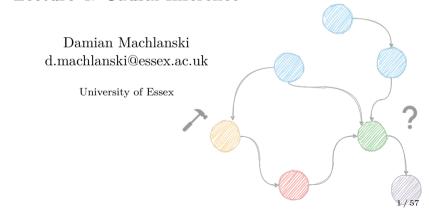
CE888: Data Science and Decision Making Lecture 4: Causal Inference



- ► Introduction
- ► Motivation
- ► Causality
- ► Methods
- ► Metrics
- ► Conclusion

THE PLAN FOR WEEK 4

► Today

INTRODUCTION

•0000

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

Do the quiz before starting the lab exercises.

Introduction

► 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

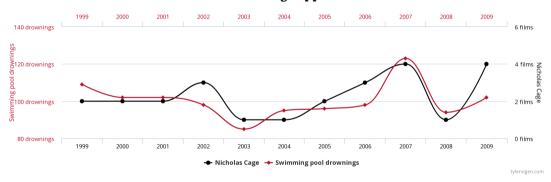
- ▶ Data science is more than just ML
- ► It's about decision making
- ► Associations vs. causal relations
- ► Correlation does not imply causation
- ▶ Also: biases and shifts within the data that skew the results
- ► Wrong conclusions -> bad decisions
- ► Complimentary to permutation tests:
 - ► PT: Is the effect statistically significant? (yes/no)
 - ► CI: How big the effect is? (number)

Spurious Correlations

INTRODUCTION

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

Films Nicolas Cage appeared in



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

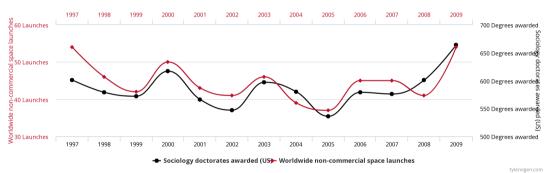
Spurious Correlations (2)

INTRODUCTION

Worldwide non-commercial space launches

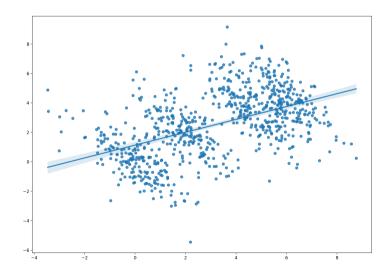
correlates with

Sociology doctorates awarded (US)

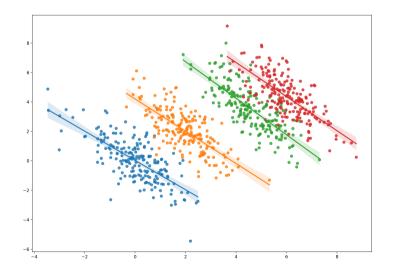


Credit: https://www.tylervigen.com/spurious-correlations

Introduction

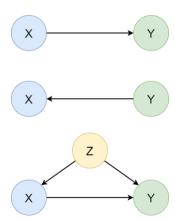


SIMPSON'S PARADOX



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 (steps 2. and 3. didn't happen)
- 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

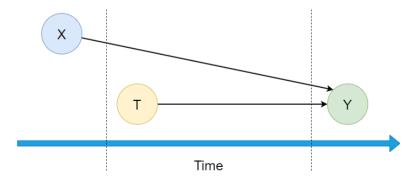
It's about finding out how a specific action affects a system of interest.

- ► 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

RANDOMISED CONTROLLED TRIALS

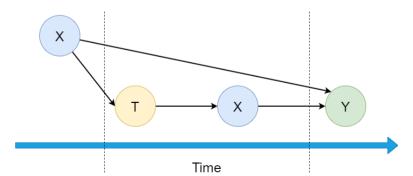
▶ Data from controlled experiments

- 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)
- \blacktriangleright (X, 1-T): predict the outcomes we haven't observed
- ightharpoonup 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

$$Effect = Y_1 - Y_0$$

#	X_1	X_2	X_3	Т	Y_0	Y_1
1/	1				20	- 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.

Causality 0.000000000

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:

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

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

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

What is the value of ATE?

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

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

TREATMENT EFFECT - CATE

INTRODUCTION

A more general way of defining effects is through conditioning:

$$CATE = \mathbb{E}\left[\mathcal{Y}_1|X=x\right] - \mathbb{E}\left[\mathcal{Y}_0|X=x\right]$$

Which stands for Conditional Average Treatment Effect.

Note the two previous effects are special cases of CATE (ATE: $x = \emptyset$, ITE: unique x).

You will likely see CATE estimators in the literature and CI packages.

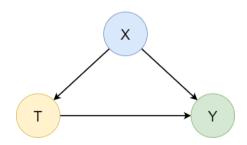
ASSUMPTIONS

- ► 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

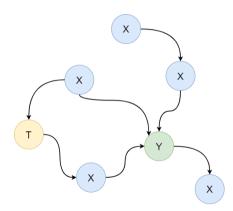


- ► This is a very simplistic view of the world
- ► Actual reality can be much more complex

Assumptions (3)

Introduction

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



Onto The Methods

Introduction

We know the theory. Now, let's do some modelling!

METHODS

Modern Approaches

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

- ► Recent surveys on modern causal inference methods ⁶ ⁷
- ► Most popular:

INTRODUCTION

- ► Inverse Propensity Weighting (IPW)
- ► Doubly-Robust
- ► Double/Debiased Machine Learning
- ► Causal Forests
- ► Meta-Learners
- ► Multiple based on neural networks (very advanced)

Too many to discuss here, but we will learn some common principles.

We will start with a simple regression, add 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

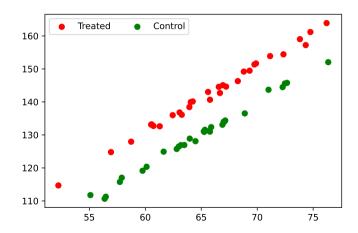
$$\widehat{ITE}(x) = \hat{\mu}(1, x) - \hat{\mu}(0, x)$$

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

S-Learner - Code

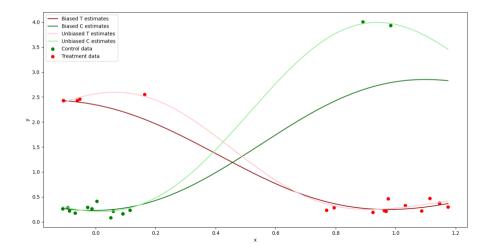
```
lr = LinearRegression()
# input: [X, T], target: Y
lr.fit(np.concatenate([x_train, t_train], axis=1), y_train)
# predict YO given [X, O] - set T=0
y0 pred = lr.predict(np.concatenate([x_test, np.zeros_like(t test)], axis=1))
# predict Y1 given [X, 1] - set T=1
y1 pred = lr.predict(np.concatenate([x test, np.ones_like(t test)], axis=1))
# effect = u1 - u0
effect_pred = y1_pred - y0_pred
```

Introduction



BIASED ESTIMATORS

Introduction



PROPENSITY SCORE

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

- ightharpoonup 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

Introduction

```
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)
# ...
```

- ▶ Treated and control distributions are often different
- ► 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)

Introduction

```
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:

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

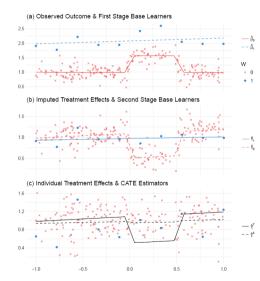
⁸http://arxiv.org/abs/1706.03461

X-Learner - Code

Introduction

```
x1 = XLearner(models=LinearRegression(), propensity_model=LogisticRegression())
x1.fit(y_train, t_train, X=x_train)
effect_pred = x1.effect(x_test)
```

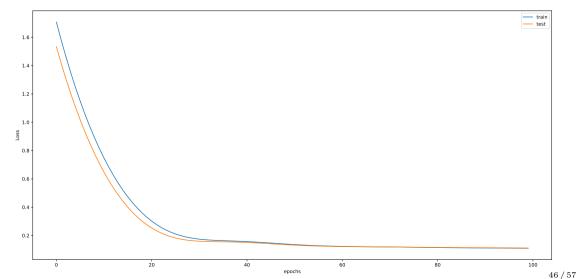
X-LEARNER - INTUITION



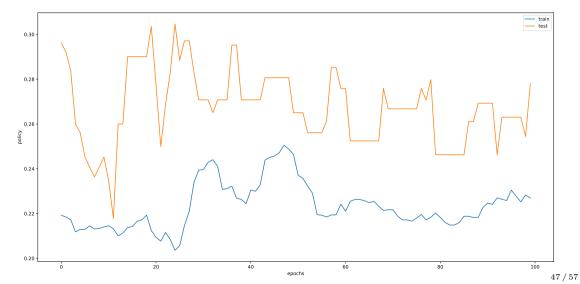
EVALUATION

- ► We have predicted some effects.
- ▶ But are they accurate?
- ► How good our model is at predicting effects?
- ► Can we use the usual metrics like MSE?

MSE



Policy Risk



ERROR ON OUTCOMES VS. EFFECTS

- ▶ Predicting accurate *outcomes* Y (MSE) is only half of the problem
- ► However, the priority is to predict accurate **effects**
- ▶ Thus, we need to measure the amount of error (ϵ) or risk (\mathcal{R}) introduced by a model with respect to predicted effects

Examples:

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

PREDICTIONS

INTRODUCTION

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

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

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

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 observaional 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

Types Of Metrics

With effect/counterfactuals

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

Without effect/counterfactuals

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

THERE IS MORE

- ► 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 assumptions
 - ► Trees, neural networks, policy learners
- ► Front-door and back-door adjustments
- ► Handling colliders, confounders, feature selection
- ▶ ..

⁹http://arxiv.org/abs/2104.04103

SUMMARY

- ► 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

CONCLUSION

ACKNOWLEDGEMENTS

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.

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WHAT'S NEXT?

INTRODUCTION

- ► Moodle quiz
 - ► A few theoretical Os
 - ► 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).