Machine Learning for Causal Inference from Observational Data

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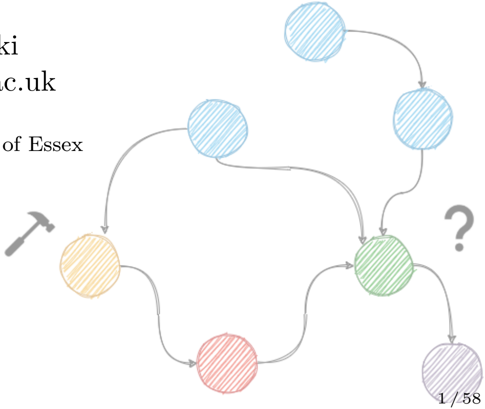


Welcome!

- Agenda
  - Slides: Introduction to Causal Inference
  - Tutorial: Guided Example with Code
  - Exercise: Do It Yourself

With some breaks in the middle as necessary.

Resources

- 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 Inference[4]

[1] `http://bayes.cs.ucla.edu/WHY/`

[2] `http://bayes.cs.ucla.edu/PRIMER/`

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

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

TOOLS

We are going to use the following:

- Python 3
- scikit-learn (ML methods)
- EconML[5] (CI estimators)
- The usual ML stack (numpy, pandas, matplotlib)
- Jupyter Notebooks

[5] https://github.com/microsoft/EconML

A Machine Learning Perspective

We will need the following:

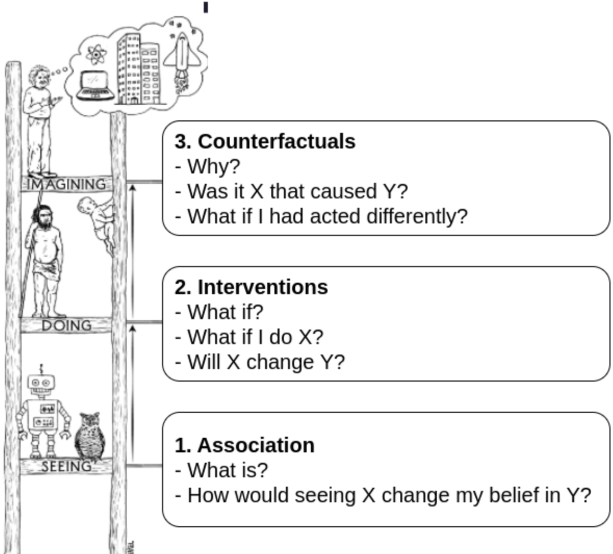
- Supervised learning - predict y given (X, y) samples
  - Regression (continuous outcome)
  - Classification (binary outcome)
- Basic data exploration
- Data pre-processing
- Training and testing
- Using metrics

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

Why Do I Need This?

- 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)

The Ladder of Causation

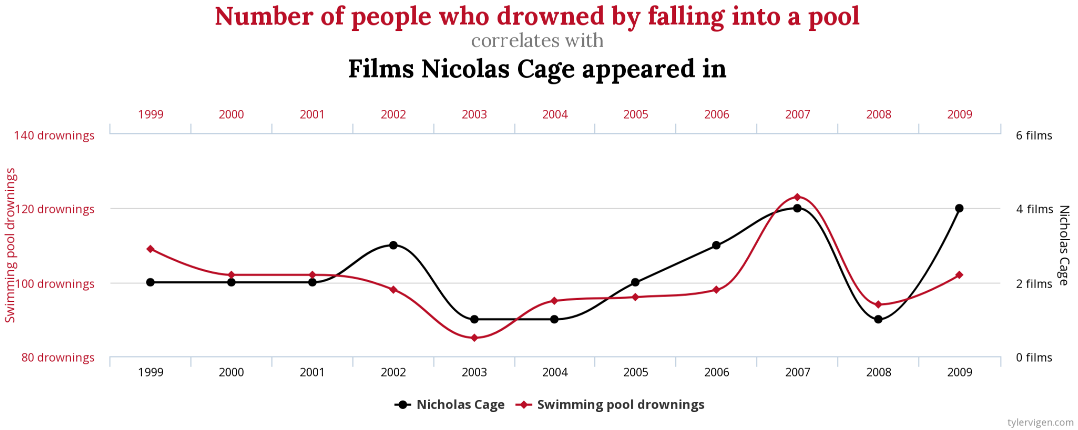


3. Counterfactuals
- Why?
- Was it X that caused Y?
- What if I had acted differently?

2. Interventions
- What if?
- What if I do X?
- Will X change Y?

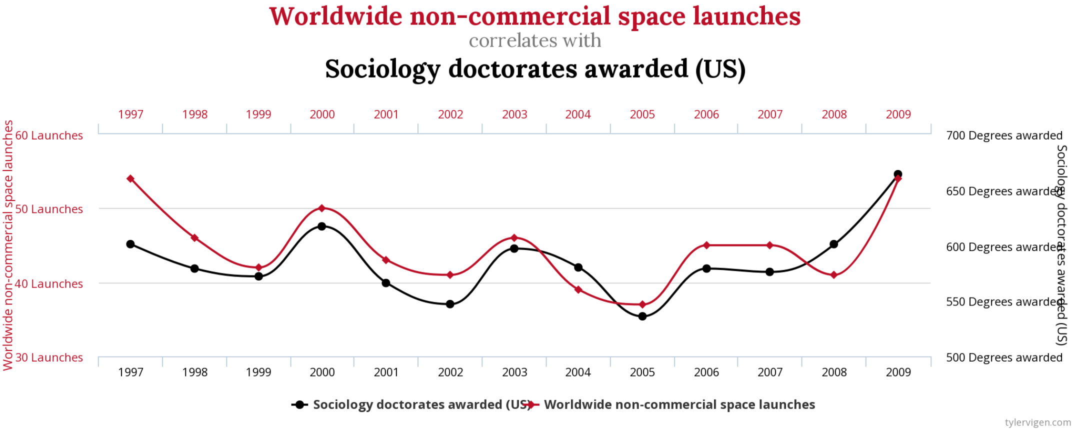
1. Association
- What is?
- How would seeing X change my belief in Y?

Spurious Correlations



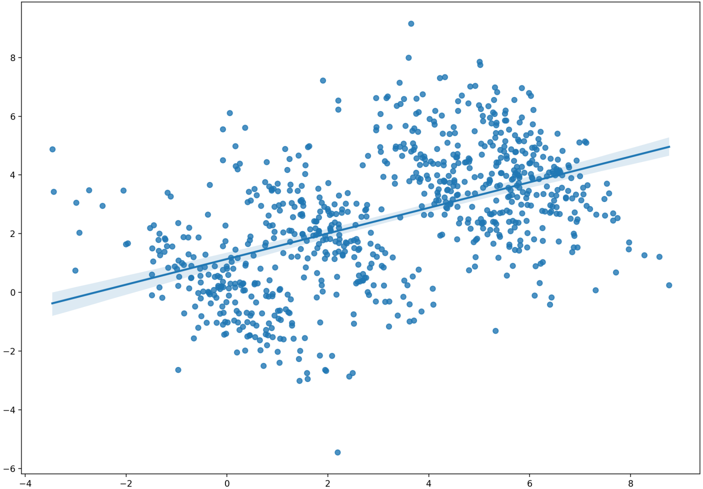
Credit: https://www.tylervigen.com/spurious-correlations

Spurious Correlations (2)

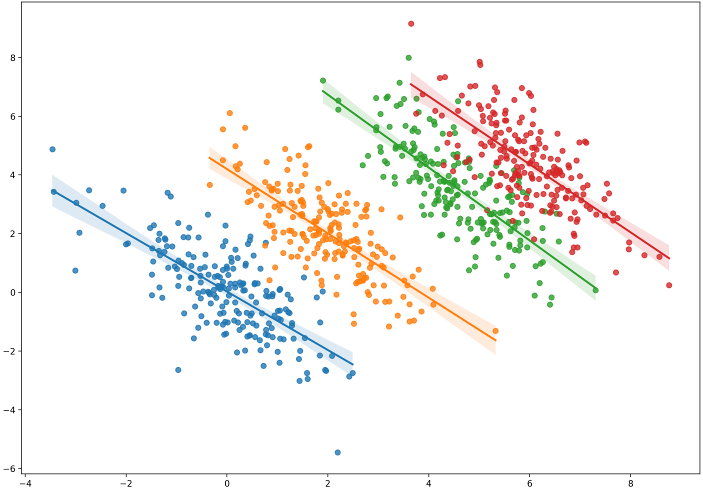


Credit: https://www.tylervigen.com/spurious-correlations

Simpson's Paradox

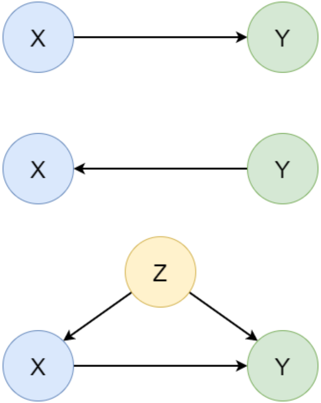


Simpson's Paradox



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

- 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

- 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

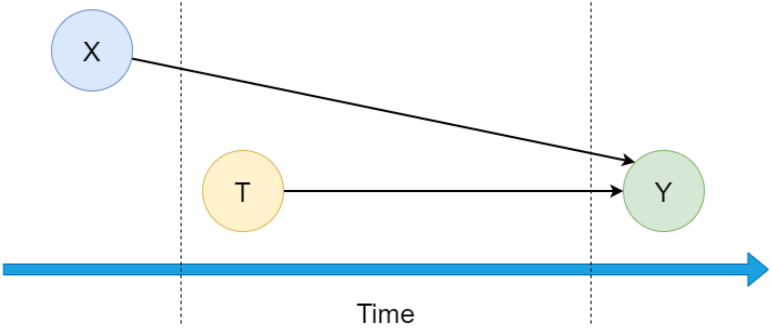
- Developing a new vaccine
- Government policy
- Recommending the best treatment for a specific patient

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

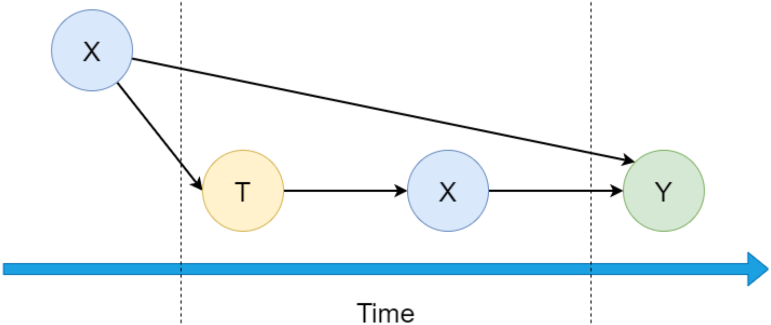
Randomised Controlled Trials

- Data from controlled experiments
- Randomised T - people assigned $T = 0$ (control) or $T = 1$ (treated)
- This mimicks observing alternative reality
- 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
- 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

- 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
- 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

More on ML vs. CI

ML

- What should be the price of this house?

CI

- How the price of this house will change if we modify it in a certain way?
- What would be the cheapest investment in the house that would increase its value the most?

Fundamentals

$$Effect = Y_1 - Y_0$$

#	X_1	X_2	X_3	T	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

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:

- $Y_0 \in \{2, 3, 1\}$
- $Y_1 \in \{3, 4, 2\}$

What is the value of ATE?

Treatment Effect - ATE Example (2)

We are given the following data:

- $Y_0 \in \{2, 3, 1\}$
- $Y_1 \in \{3, 4, 2\}$

What is the value of ATE?

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

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

Treatment Effect - CATE

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).

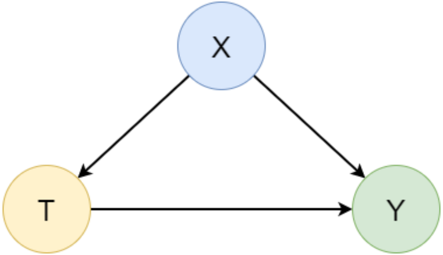
You will likely see CATE estimators in the literature and CI packages.

Assumptions

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

Assumptions (2)

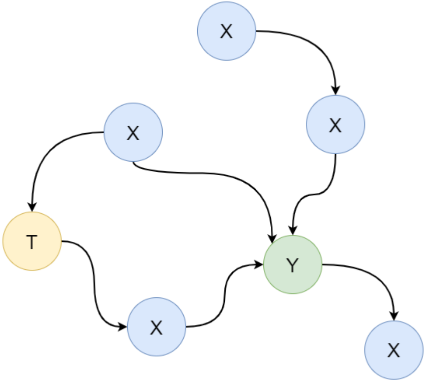
- Most CI estimators assume the *triangle* graph



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

Assumptions (3)

- Can we infer graphs from data?
- Causal discovery



Onto The Methods

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

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:
  - 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.

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

[7] https://arxiv.org/abs/2002.02770

S-Learner

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

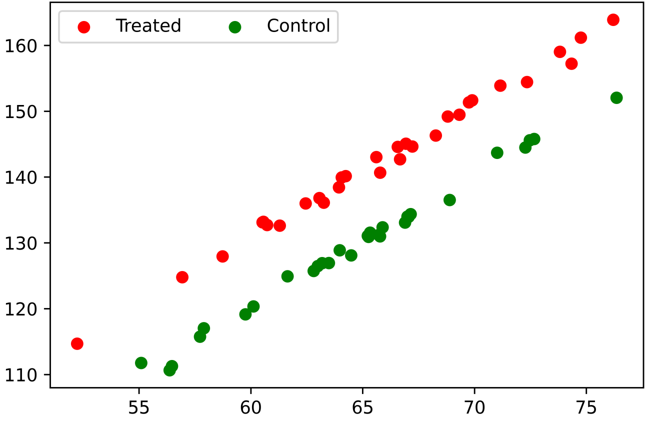
$$\widehat{ITE}(x) = \hat{\mu}(1,x) - \hat{\mu}(0,x)$$

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

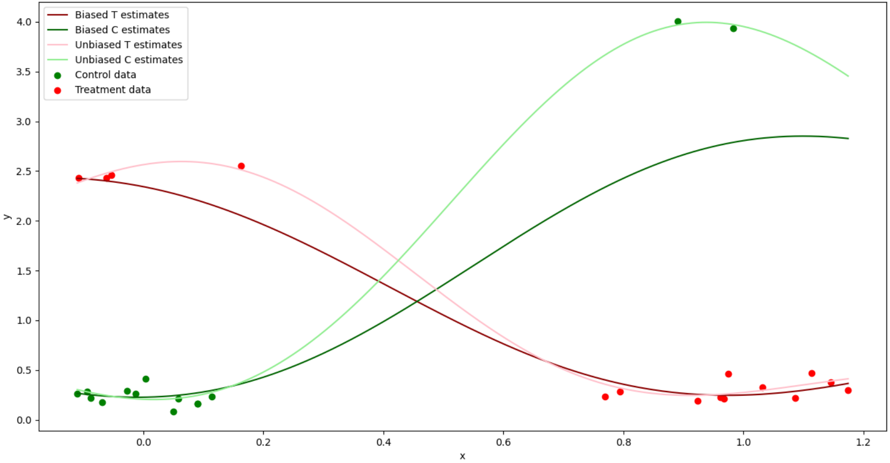
S-Learner - Code

```
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 = y1 - y0
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 $t \in \{0, 1\}$
- 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)
- Either $\hat{e}(x)$ or $\hat{\mu}(x)$ can still have bias (misspecification)
- Doubly-Robust method attempts to address that

IPW Estimator - Code

```python
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
- 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)
y1_pred = m1.predict(x_test)

effect_pred = y1_pred - y0_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 here[8]). 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:

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

[8] `http://arxiv.org/abs/1706.03461`

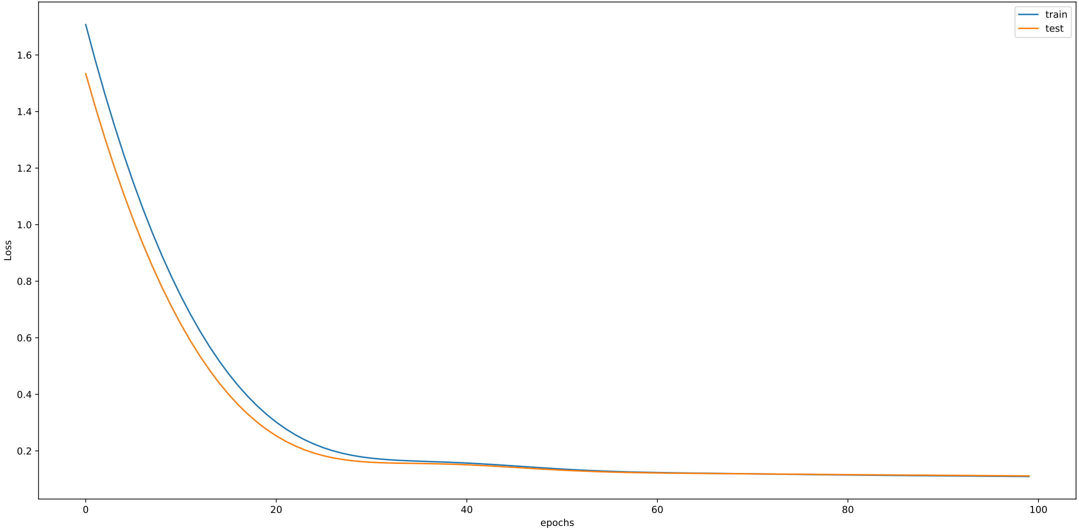
X-Learner - Code

```
xl = XLearner(models=LinearRegression(), propensity_model=LogisticRegression())

xl.fit(y_train, t_train, X=x_train)

effect_pred = xl.effect(x_test)
```

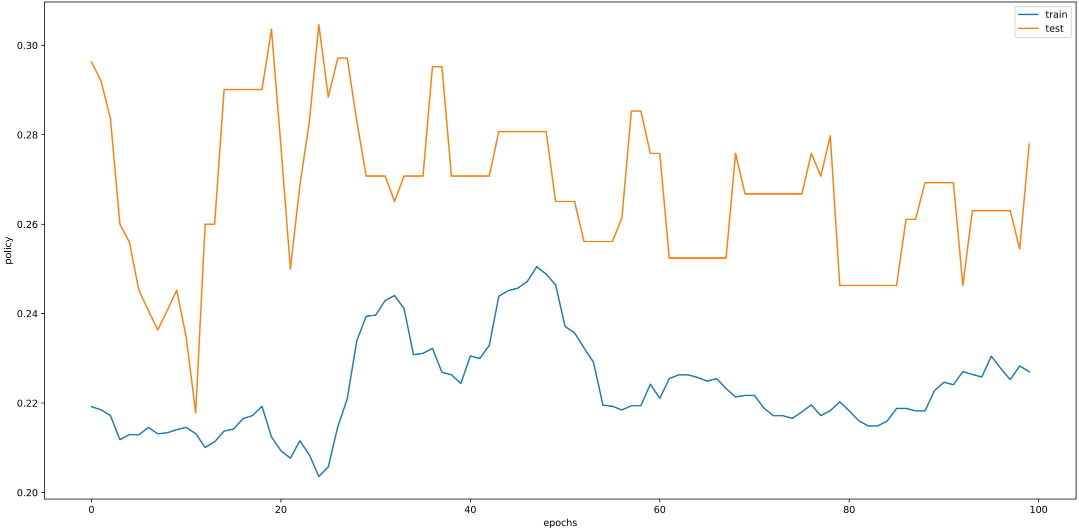
Evaluation

- 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


train
test
policy
0.20
0.22
0.24
0.26
0.28
0.30
epochs
0
20
40
60
80
100

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:

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

Model and Hyperparameter Selection

- Absolutely mandatory [9]
- Do NOT use defaults
- Search over:
  - Hyperparameters (values and types)
  - Base learners (regressors and classifiers)
  - Causal estimators
- The more the better, at the cost of increased compute

[9] https://arxiv.org/abs/2303.01412

Predictions

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).

The main purpose is to test performance of causal estimators. The focus is on methods, not data.

Some well-established causal inference datasets:

- IHDP
- Jobs
- News
- Twins
- ACIC challenges

Types Of Metrics

With effect/counterfactuals

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

Without effect/counterfactuals

- ϵ_{ATT} (ATE on the Treated)
- $\mathcal{R}_{pol}$ (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 treatments[10]
- Other methods
  - Instrumental variables
  - Relaxing the common assumptions
  - Trees, neural networks, policy learners
- Front-door and back-door adjustments
- Handling colliders, confounders, feature selection
- ...

[10] `http://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

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.

References

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What's next?

- Onto the practical parts
  - Tutorial
    - Predict ATE and measure ϵ_{ATE}
    - S-Learner, IPW and X-Learner
    - Random Forest as base regressors and classifiers
  - Exercise - IHDP
    - Predict ITE and ATE
    - Measure ϵ_{PEHE} and ϵ_{ATE}
  - Exercise - JOBS (optional)
    - Predict ATT and Policy
    - Measure ϵ_{ATT} and $\mathcal{R}_{pol}$
- Short break?