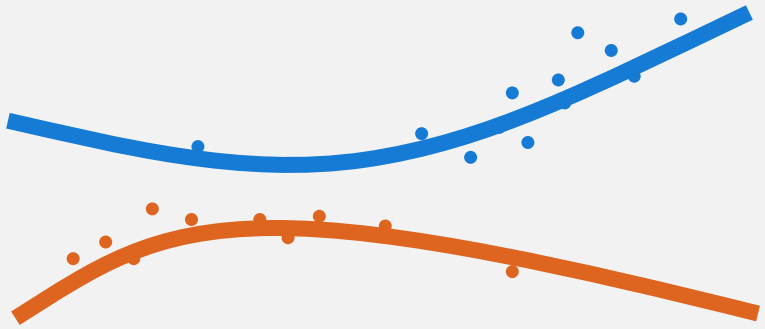


Potential outcomes, counterfactuals & conditional treatment effects

Causal Inference & Deep Learning

MIT IAP 2018

Fredrik D. Johansson

Everyone wants to make better decisions.

Predicting effects of decisions
requires **causal** reasoning

Causal inference problems are becoming

High-dimensional

What are the effects of genetics?

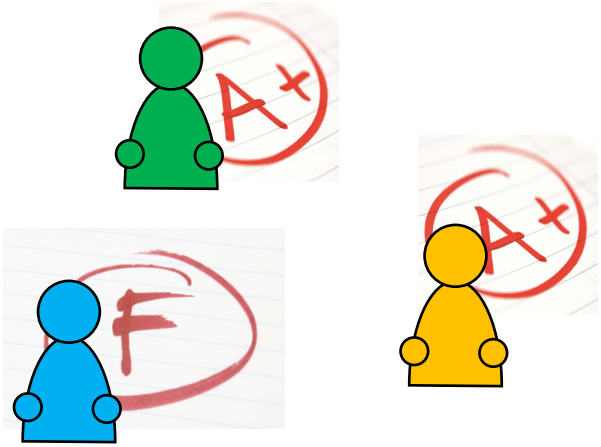
Causal inference problems are increasingly

Observational (non-experimental)

How should we treat our patients?

Causal inference problems are becoming

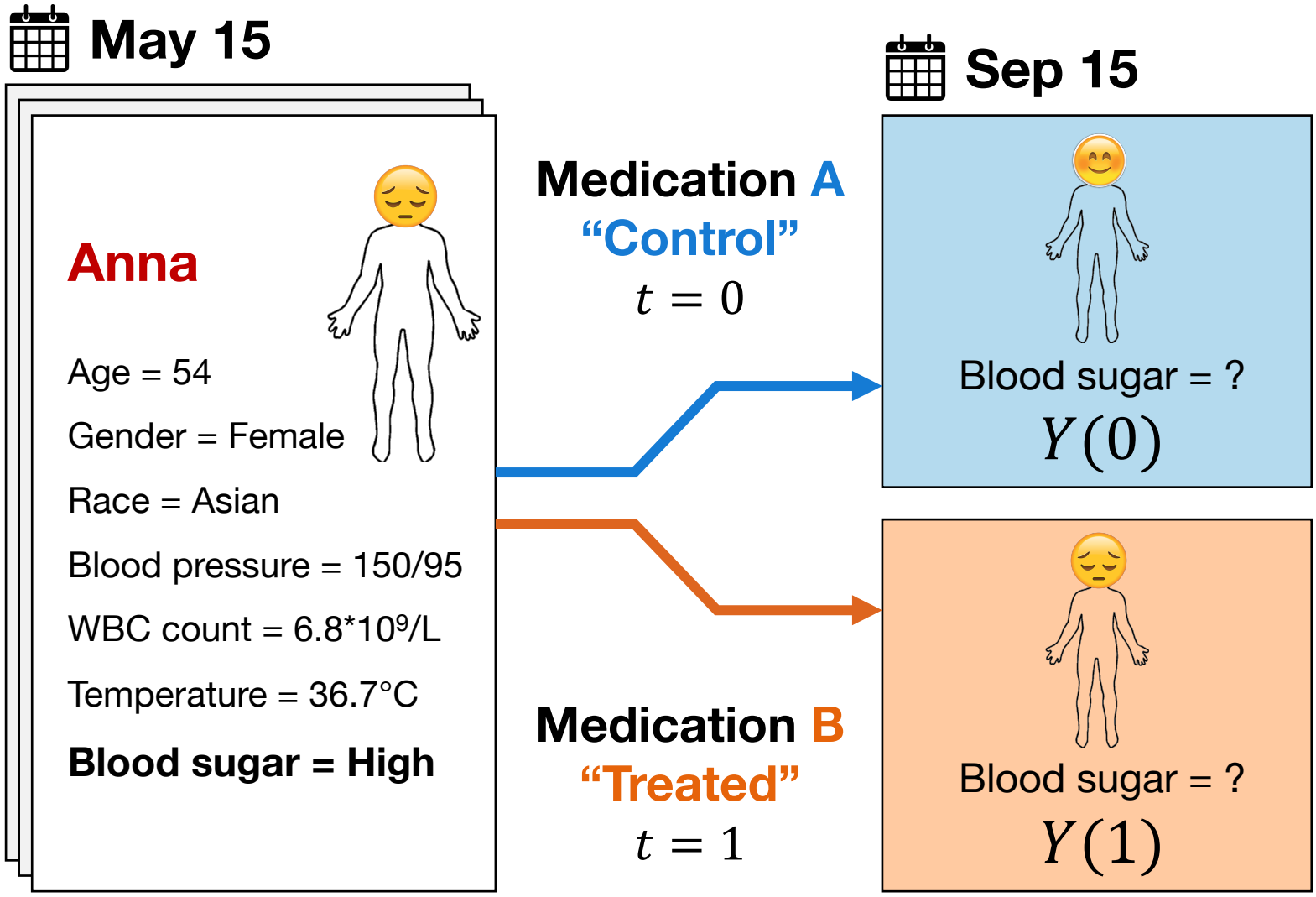
Personalized



How should we teach our students?

Why do I care about decision making?

- Clinical machine learning group (clinicalml.com)
- Many health care problems concern decision making
  - **Who** should receive which treatment?
  - **Which** lab tests should be ordered?
  - **When** should we intervene?
  - (**What** was the cause of death?)


May 15
Anna
Age = 54
Gender = Female
Race = Asian
Blood pressure = 150/95
WBC count = 6.8*10⁹/L
Temperature = 36.7°C
Blood sugar = High
Medication A
"Control"
$t = 0$
Medication B
"Treated"
$t = 1$
Sep 15
Blood sugar = ?
$Y(0)$
Blood sugar = ?
$Y(1)$

Treatment effects

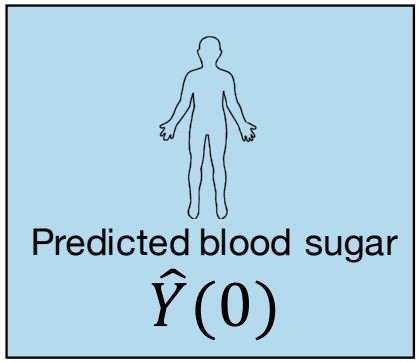
- The **effect** of treatment is the **difference** between what would have happened under each path, $\tau = Y(1) - Y(0)$

- Can be used for **population-wide** policy-making:
  Does smoking have an effect on cancer rate?

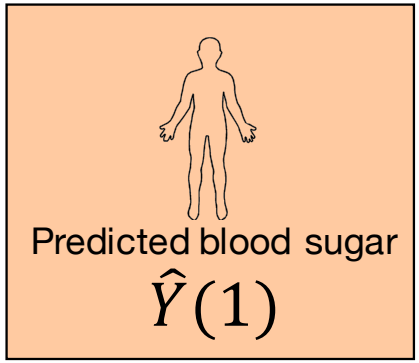
- or for **personalized** intervention:
  Which medication works best for Anna, specifically?

Machine learning approach

- **Predict** both outcomes $Y(0)$ and $Y(1)$



If $\hat{Y}(0) < \hat{Y}(1)$ give treatment $T = 0$



If $\hat{Y}(1) < \hat{Y}(0)$ give treatment $T = 1$

Supervised learning

- Fit function to historical records of patients

X	T	Y
Age	**Treatment**	**Outcome (BS)**
26	B	High
24	A	Low
…	…	…

Find $f(x, t) \approx y$

Supervised learning

- Superficially similar to many supervised learning problems

Features **Labels**

X, T

Age	Treatment
26	B
24	A
…	…

⇨

Outcome (BP)
High
Low
…

Y

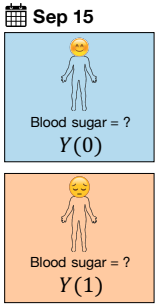
X

⇨ “Cat” Y

X

⇨ *“What is this wave?”* Y

Supervised learning



- Observe only outcome of prescribed treatment

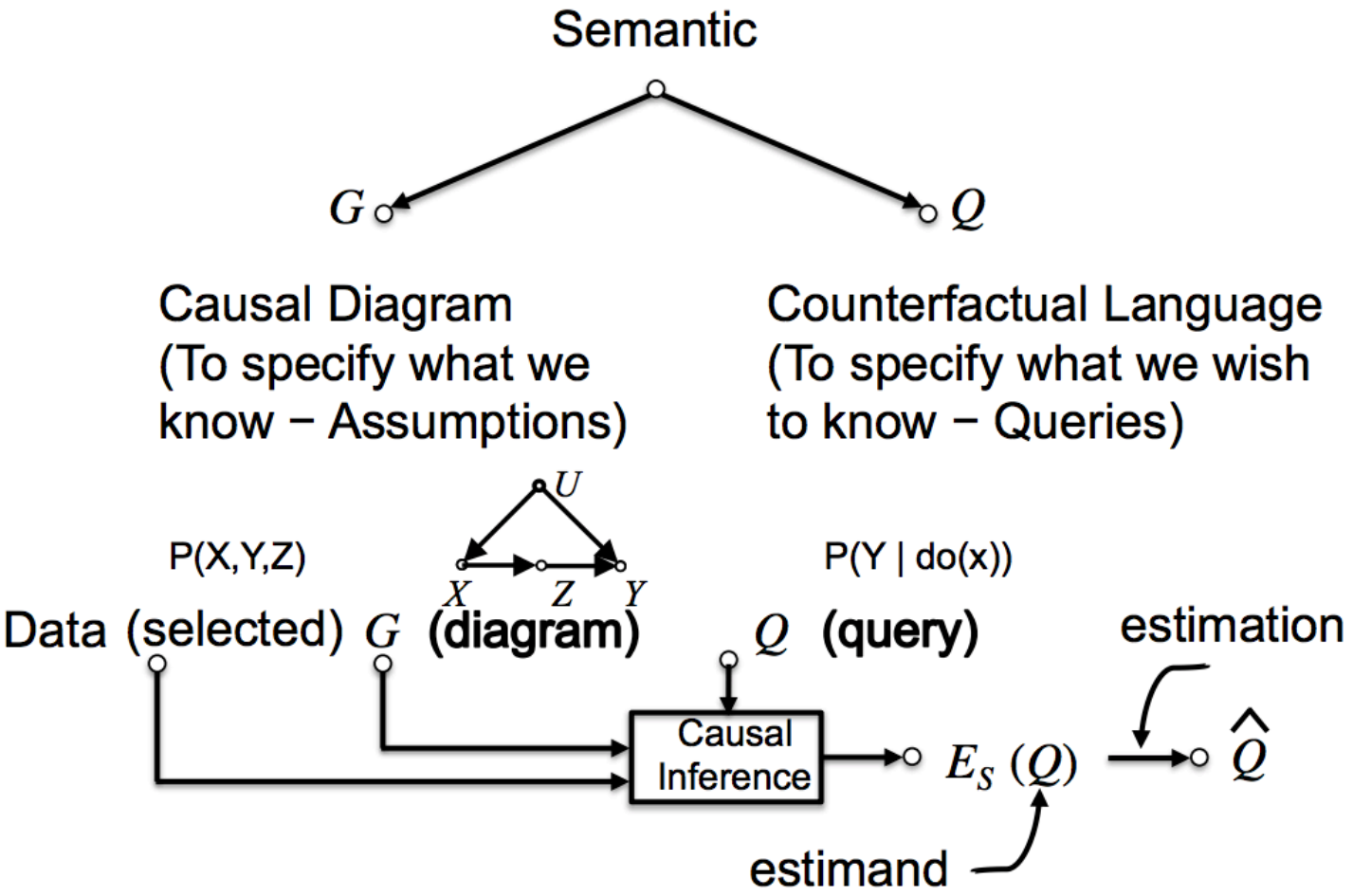
X	T	Y	Y_{cf}
Age	**Treatment**	**Outcome (BS)**	**Counterfactual**
26	B	High	**?**
24	A	Low	**?**
…	…	…	…

Find $f(x, t) \approx Y(t)$

Why is supervised learning not enough?

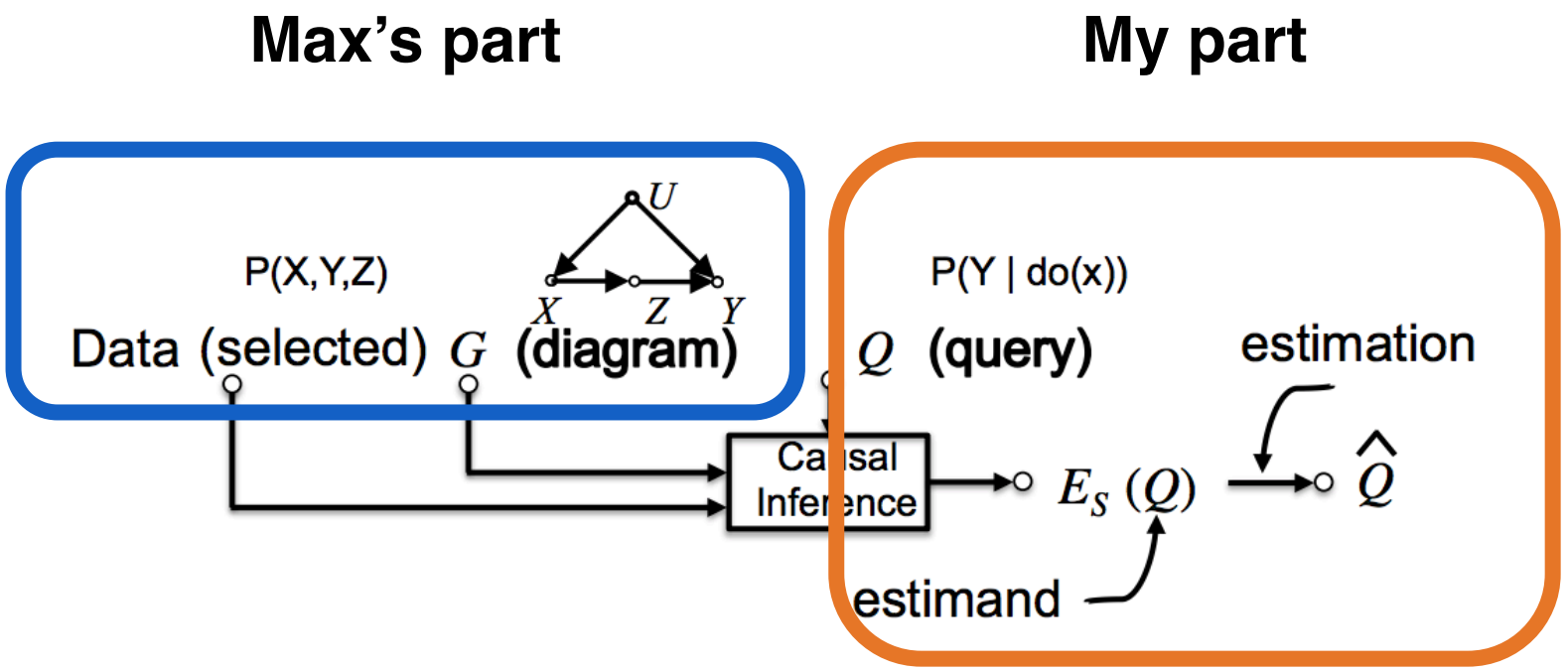
- No supervision for counterfactual outcomes!
- Counterfactual inference thought of as a **missing variables** problem or as **domain adaptation**
- **Treatment** is **unlike** other features—we do not want to e.g. remove it in variable selection

Causality and machine learning



Slide borrowed from Judea Pearl: http://causality.cs.ucla.edu/blog/wp-content/uploads/2017/12/nips-dec2017-bw.pdf

Causality and machine learning



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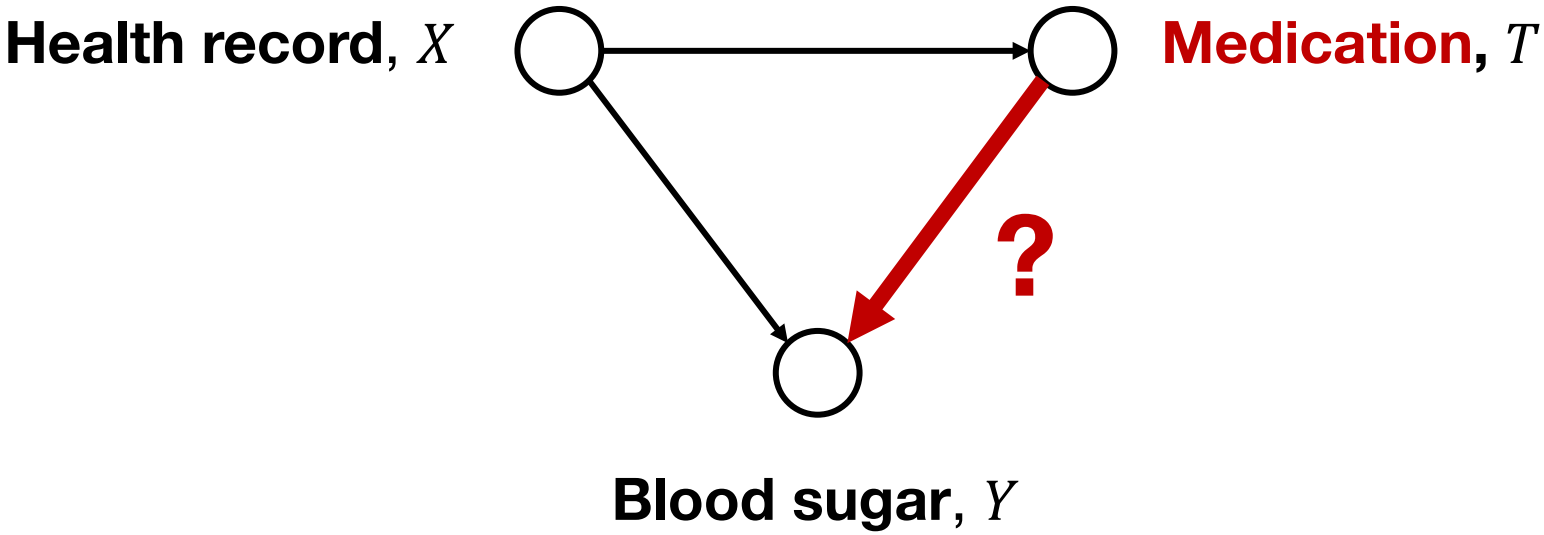
1. Potential outcomes framework

2. Supervised learning (risk minimization)

3. Adjusting for distributional shift

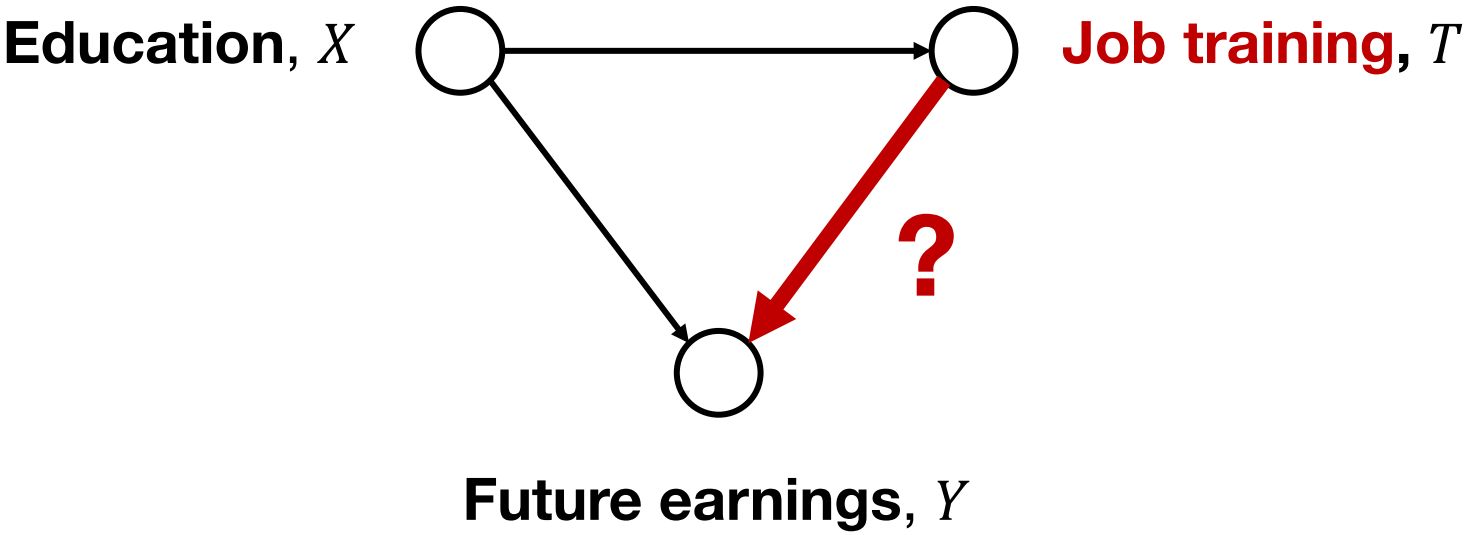
Anna's causal graph

- Does **Medication B** reduce **blood sugar**?



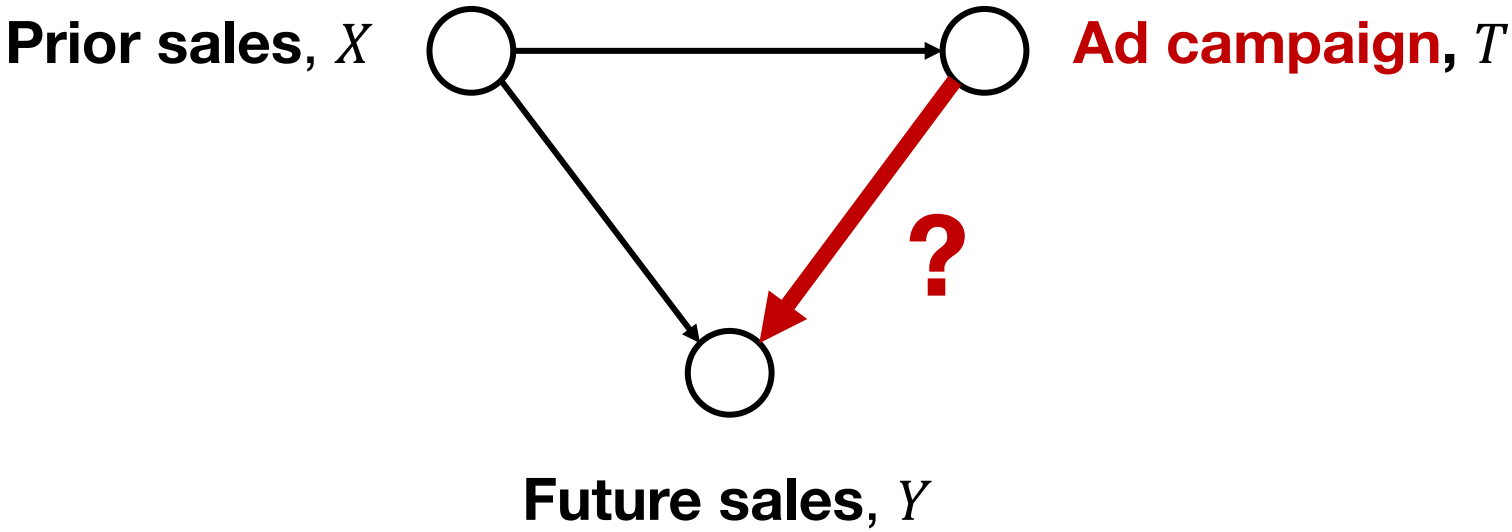
Job training

- Does **job training** increase future **earnings**?



Advertising

- Will running an **ad campaign** increase **sales**?



Potential outcomes

- The (X, T, Y) context-treatment-outcome triple is a common pattern—same graph, same queries of interest
- **Potential outcomes** (Neyman-Rubin causal model) are convenient in this setting
- Let $Y(t)$ denote the **potential** outcome under intervention t. *What **would** happen if we intervened with $T = t$?*

- Potential outcomes are complementary to causal graphs
- Interventions are often called “treatment” for historical reasons

Potential & conditional outcomes

- We use potential outcomes to differentiate between conditioning and intervening

- **Conditional** outcome: $\mathbb{E}[\, Y \mid T = 1 \,]$

  What is the expected outcome for subjects who we would currently treat with $T = 1$*?*

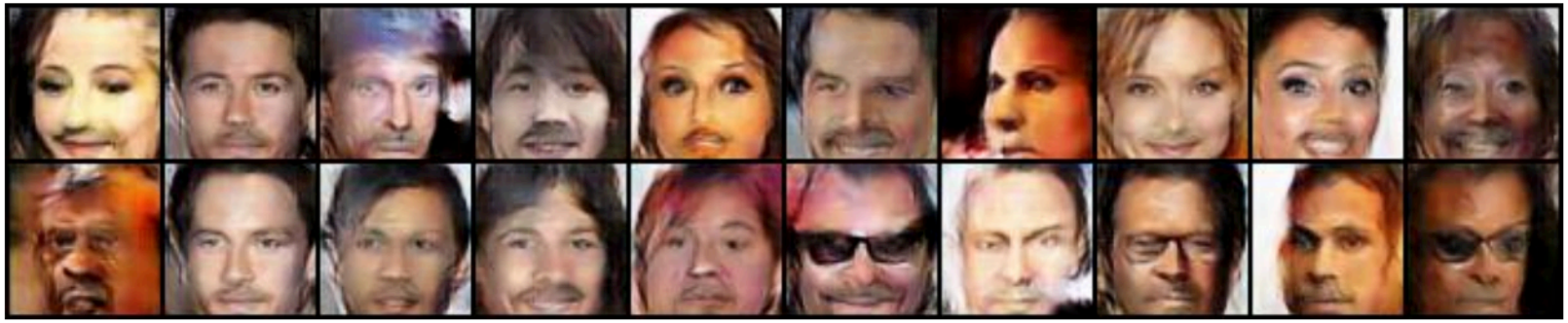
- **Potential** outcome: $\mathbb{E}[Y(1)]$

  What is the expected outcome if we were to treat **everyone***?*

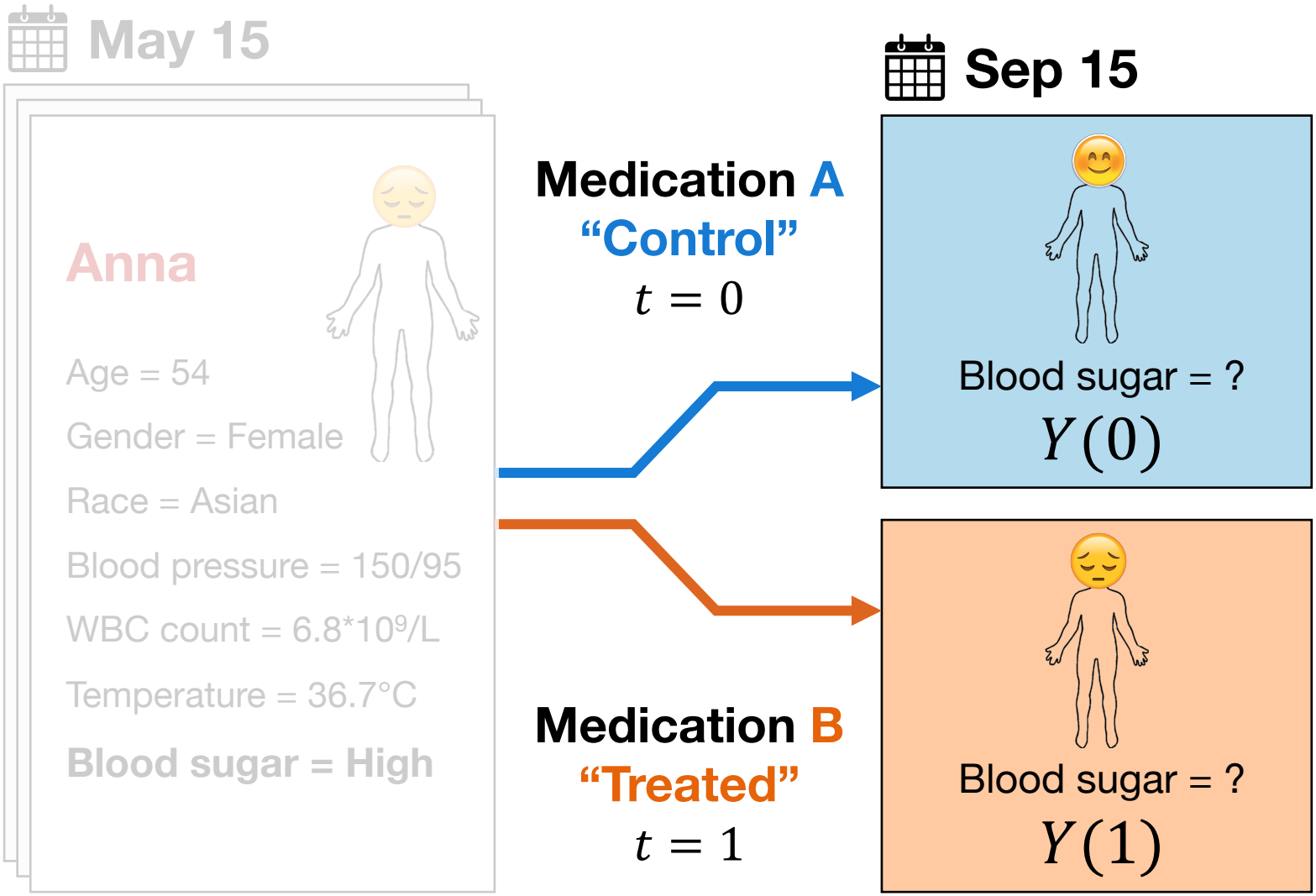
Causal GAN

- Conditioning vs intervening on mustache in synthesized photo's of faces. Conditioning: only men, Intervening, men+women

Intervening



Conditioning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$t = 1$
Sep 15
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$Y(0)$
Blood sugar = ?
$Y(1)$

Potential outcomes—Binary treatment

- Let treatment be binary: $T \in \{0, 1\}$
  and call $t = 0$ **control**, $t = 1$ **treated**

- $Y(1)$ treated outcome, $Y(0)$ control outcome

- **Factual** outcome: $Y = (1 - T)Y(0) + TY(1)$

- Joint distribution $X, T, Y \sim p(X, T, Y)$

[1]Average is taken over noise in Y

Two effects of interest

- Conditional Average Treatment Effect (**CATE**)[1]

$$\tau(x) = \mathbb{E}_p[\, Y(1) \mid X = x \,] - \mathbb{E}_p[Y(0) \mid X = x]$$

- The average effects on subjects with features $X = x$

- Can be used to **personalize** treatment:

  Should I be taking Medication B, given my current state?

[1]Average is taken over noise in Y

Two effects of interest

- (Population) Average Treatment Effect (**PATE/ATE**)

$$ATE = \mathbb{E}_p[Y(1) - Y(0)]$$

$$= \mathbb{E}_p[\tau(x)]$$

- Studied for hundreds of years

- Often the target of drug trials:

  Does Medication B work better on average?

[1]Average is taken over noise in Y

Potential outcomes & CATE

- Tabular records of patients

Age	**Treatment**	**Outcome (BS)**
26	A	High
24	B	Low
…	…	…

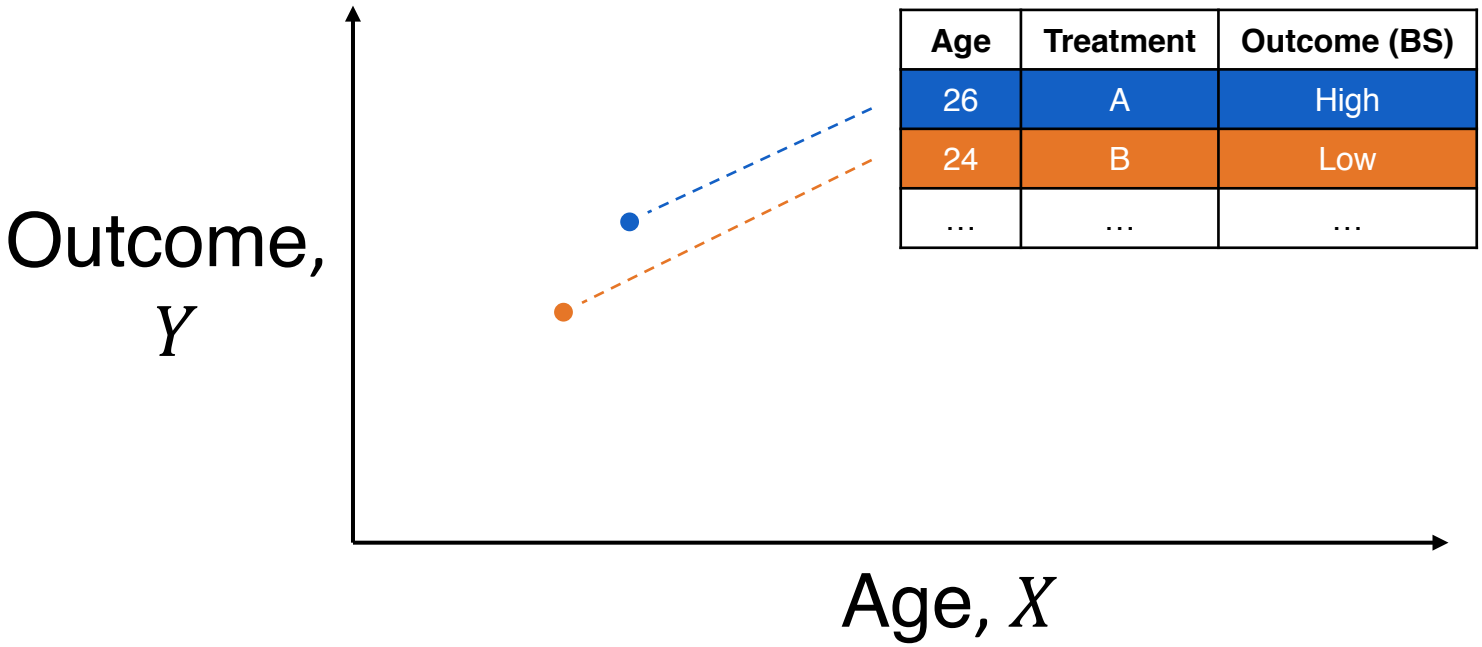
Potential outcomes & CATE

- Represent features and outcome in a plot

Age	Treatment	Outcome (BS)
26	A	High
24	B	Low
…	…	…

Potential outcomes & CATE

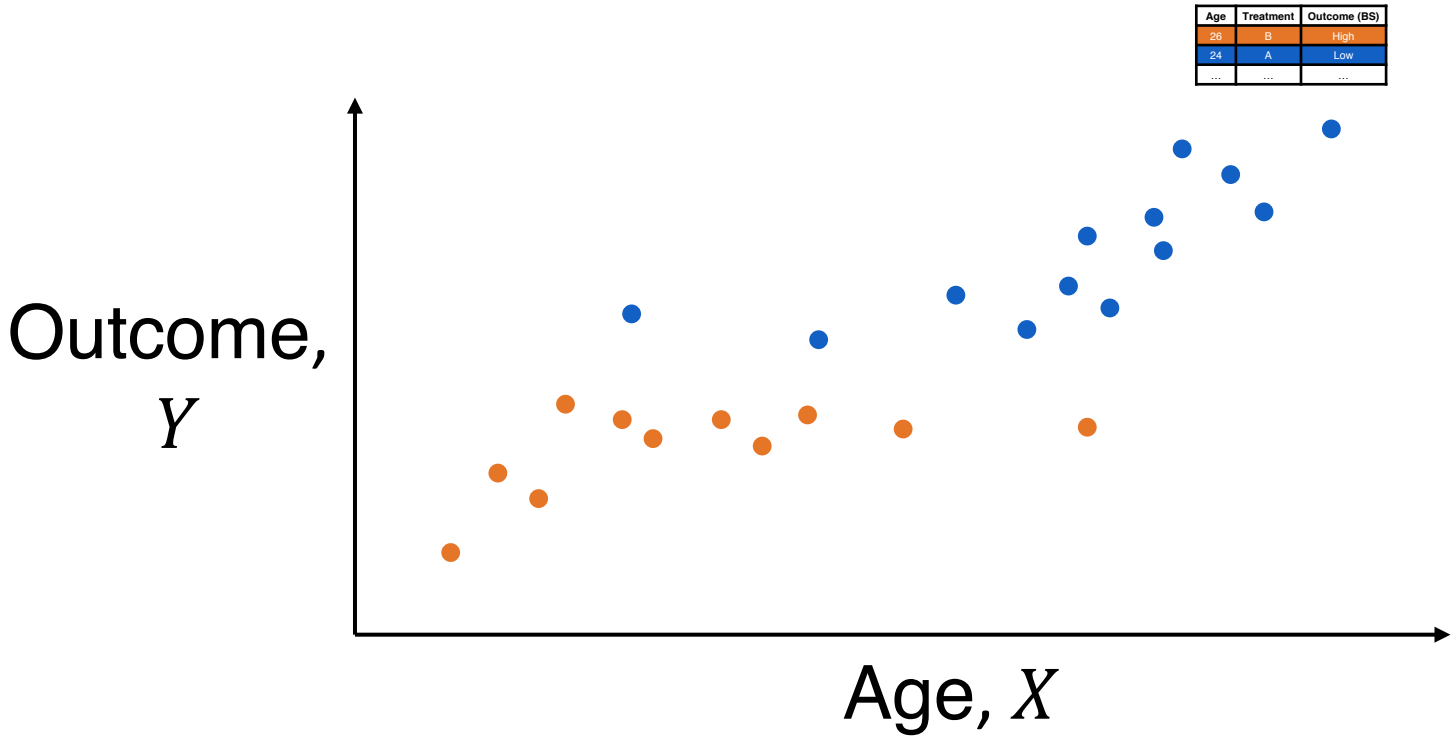
- Let color represent treatment groups



Age	Treatment	Outcome (BS)
26	A	High
24	B	Low
…	…	…

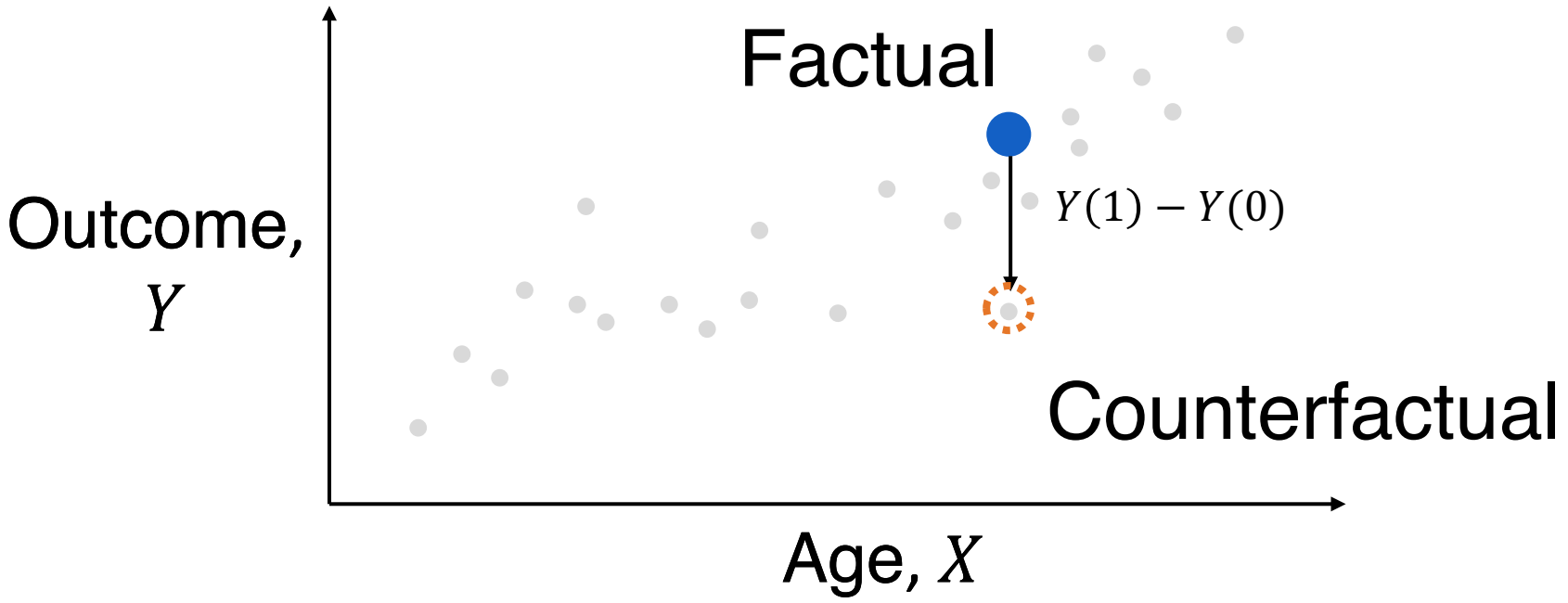
Potential outcomes & CATE

- Treatment groups need not be identically distributed (see later)



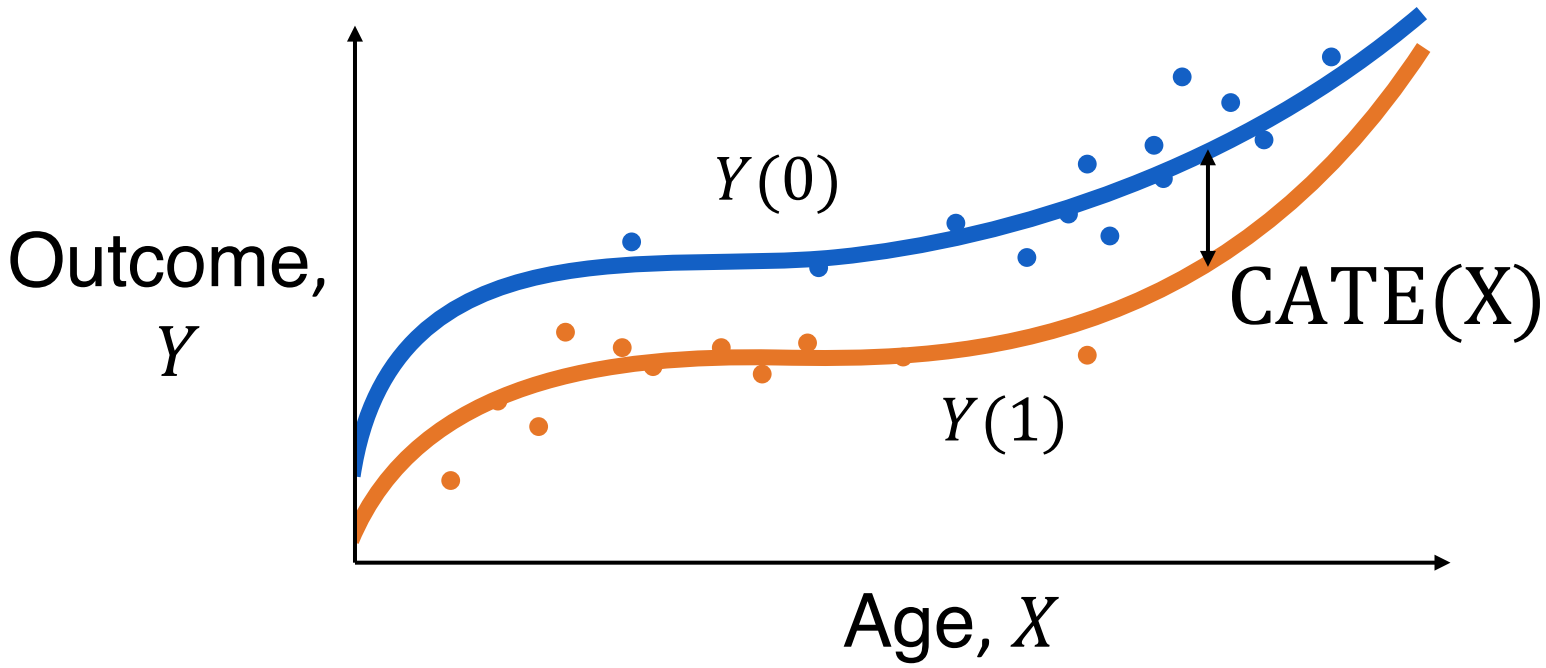
Counterfactuals

- Effect on a unit determined by (unobserved) **counterfactual**



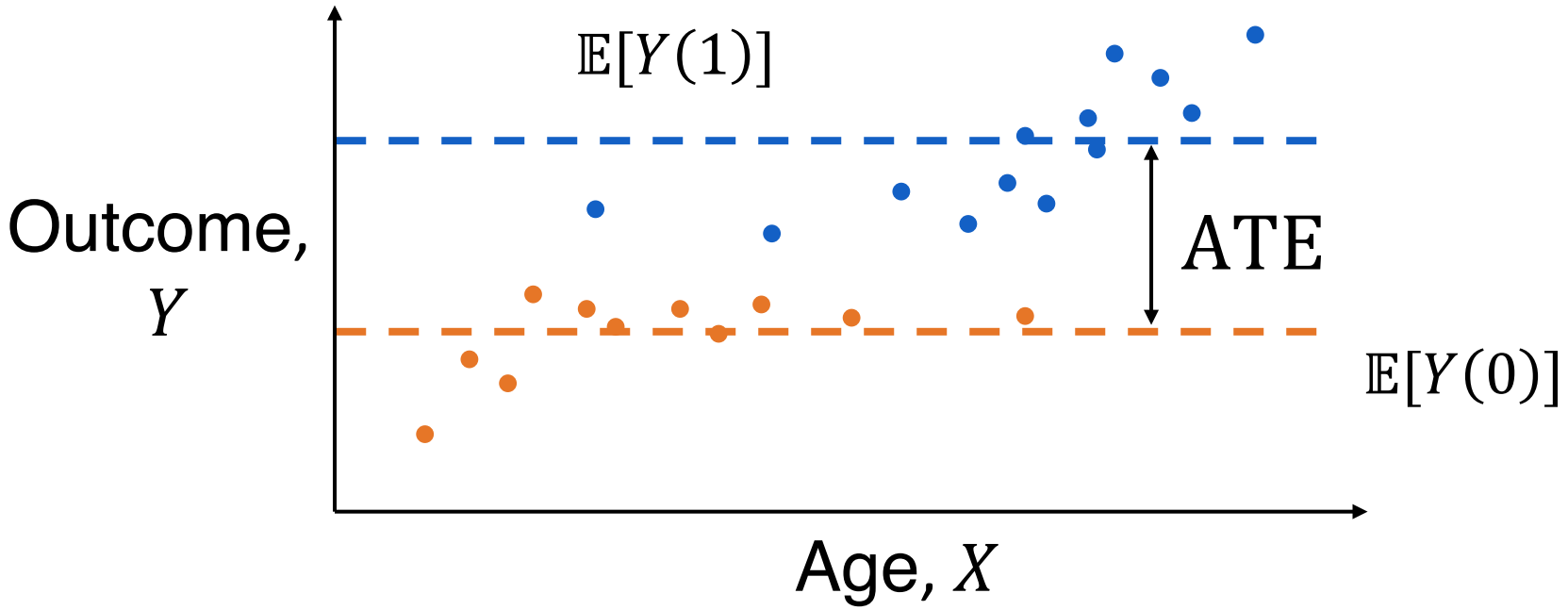
Potential outcomes & CATE

- Expected potential outcomes $Y(0), Y(1)$ are the goal



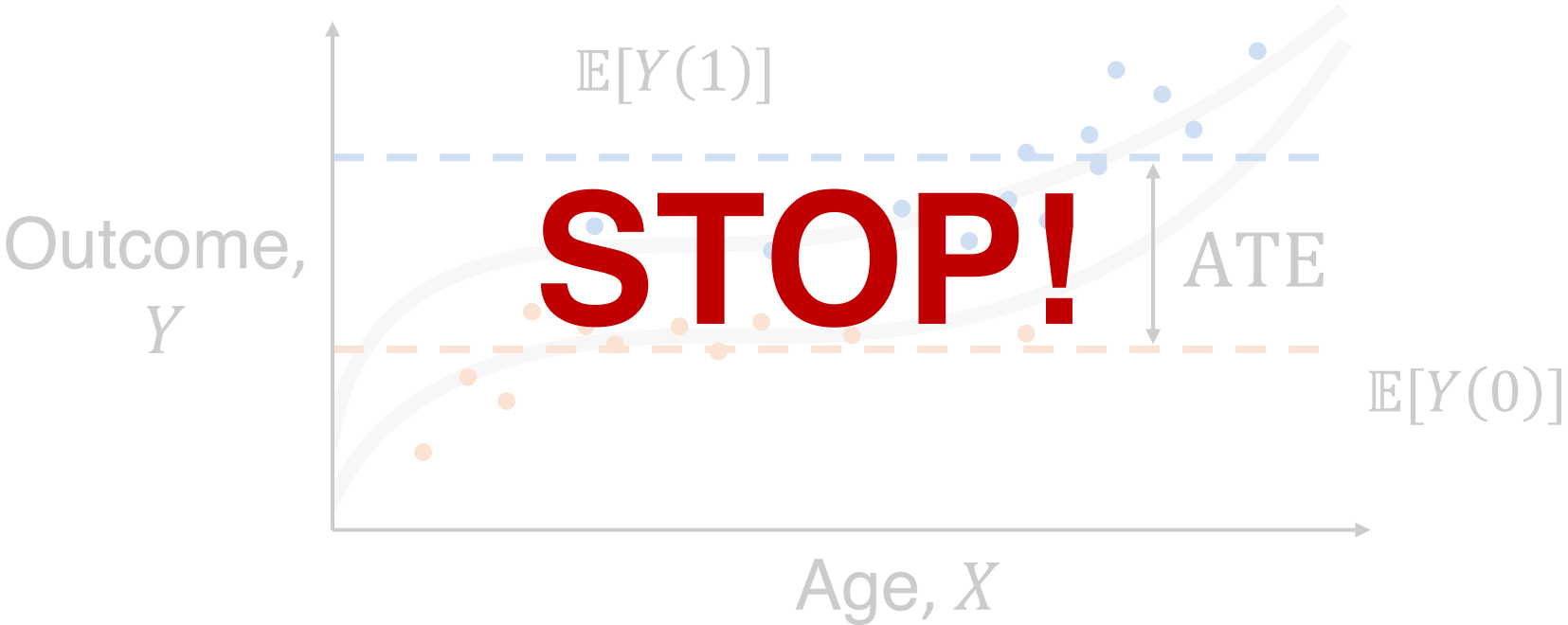
Potential outcomes & ATE

- Average treatment effect



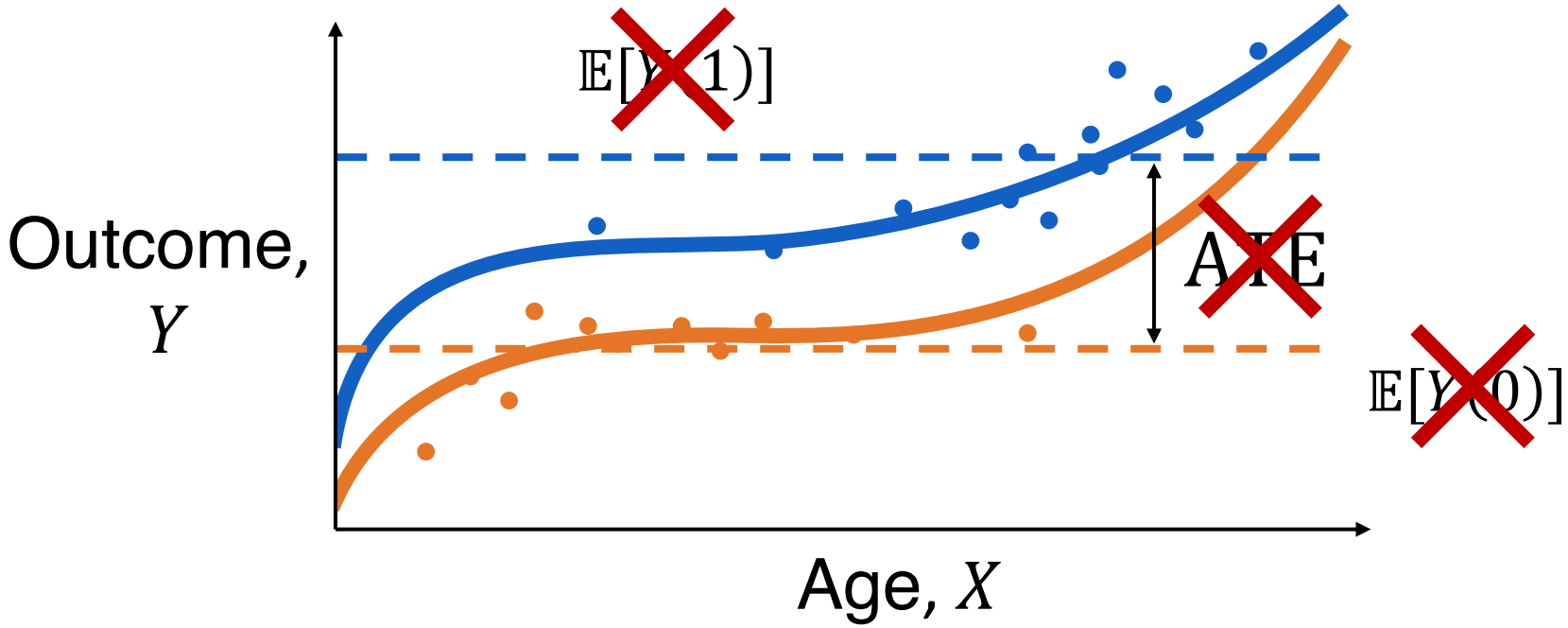
Potential outcomes & ATE

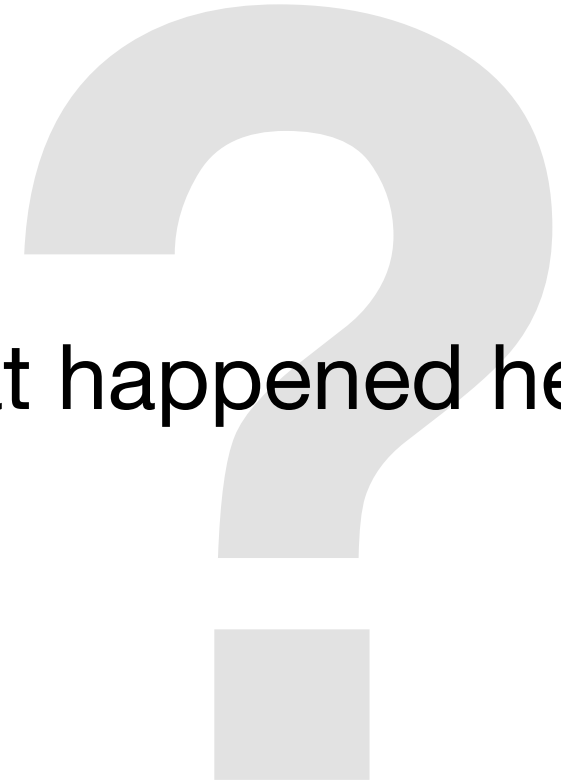
- Average treatment effect



Potential outcomes & ATE

- Average effect can't be larger than maximum conditional!

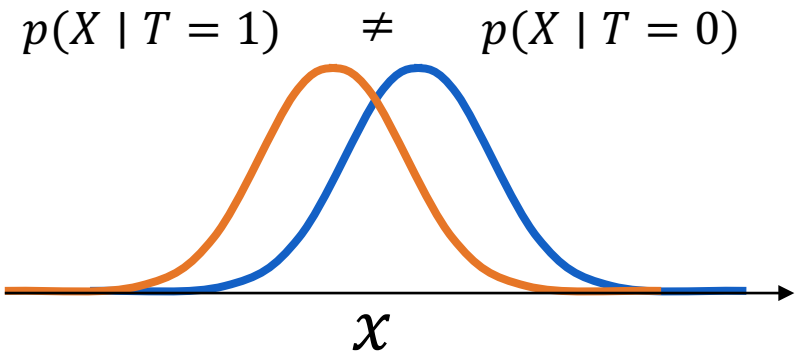


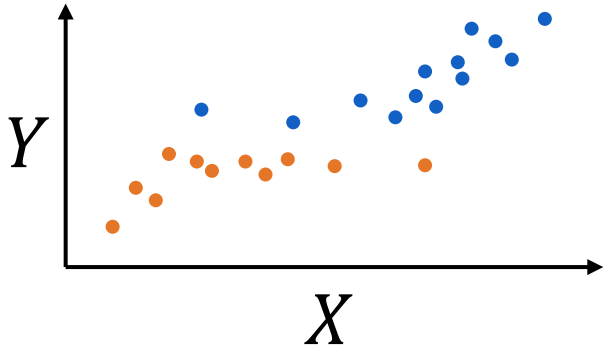


What happened here?

Treatment group imbalance

- Treatment groups are not identically distributed

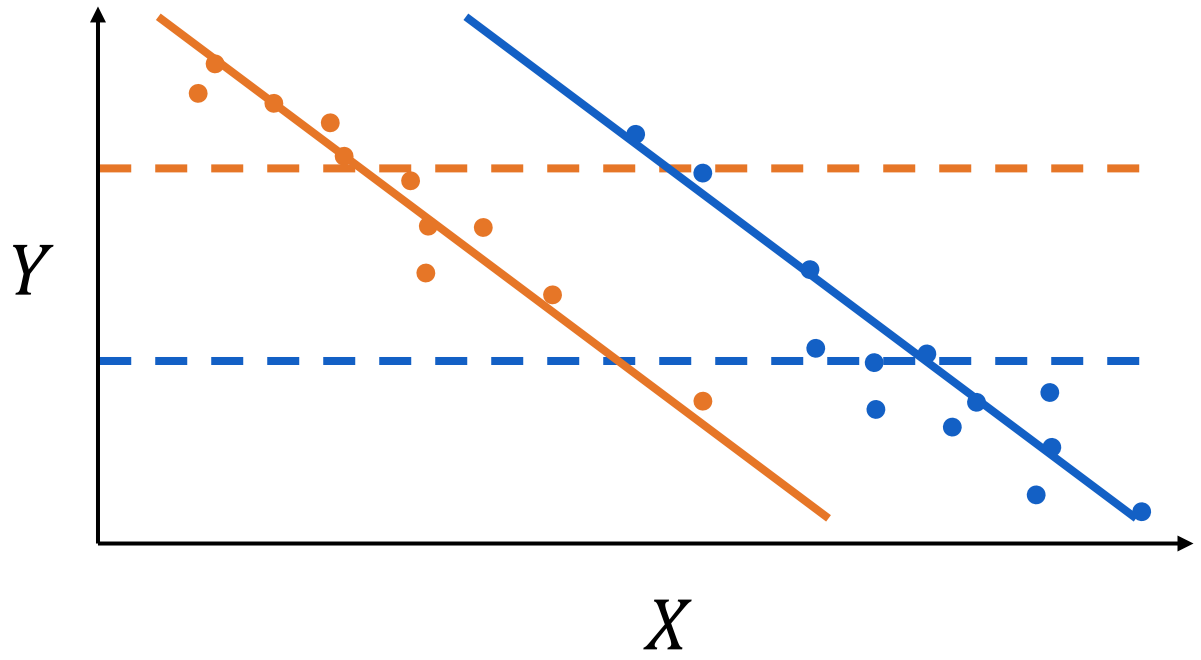




$$\underbrace{\mathbb{E}_p[\,Y \mid T = 1\,] - \mathbb{E}_p[\,Y \mid T = 0\,]}_{\text{What we computed}} \neq \underbrace{\mathbb{E}_p[Y(1) - Y(0)]}_{\text{What we want}}$$

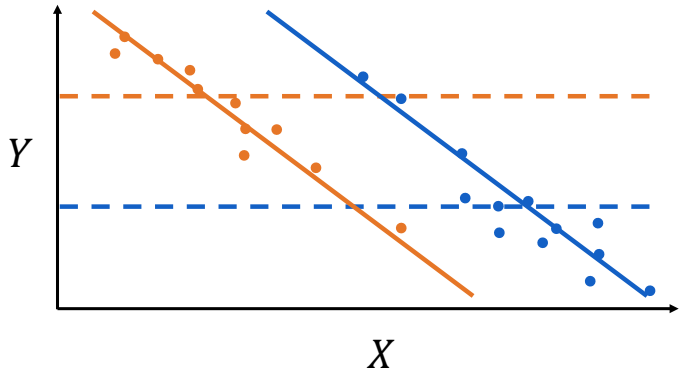
Simpsons paradox

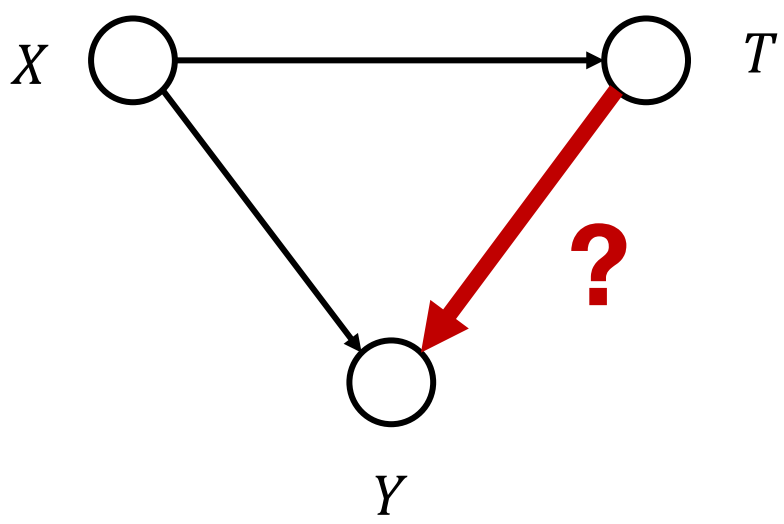
- There are examples where for **every** $x \in \mathcal{X}$, CATE is positive, but the naive ATE estimate is negative



Confounding

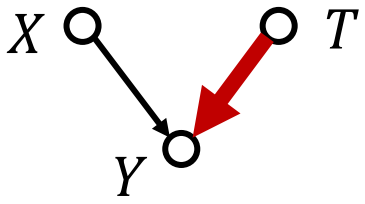
- X is a **confounder**!
- It affects both the treatment assignment T and the outcome Y
- Confounds the naïve estimate of treatment effect





Randomized controlled trials (RCT)

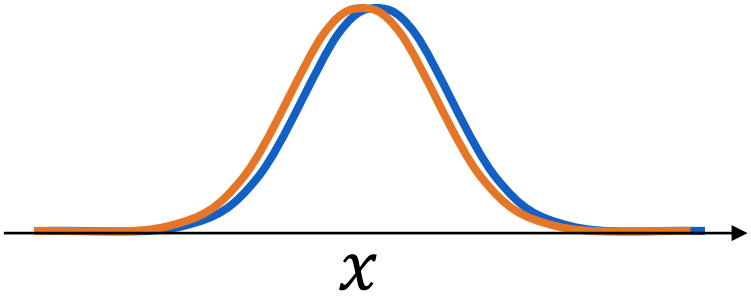
- Gold standard. Removes confounding!



- Treatment assignment is randomized: $p(T \mid X) = p(T)$

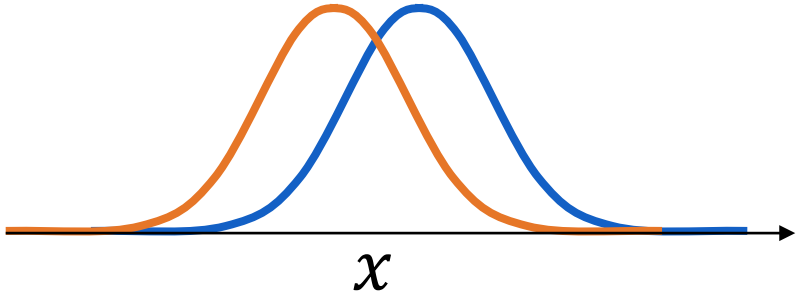
Randomized

$p(X \mid T = 1) \quad = \quad p(X \mid T = 0)$



Observational

$p(X \mid T = 1) \quad \neq \quad p(X \mid T = 0)$



Observational data

- **Randomized** controlled trials are expensive and sometimes unethical or impractical

  We can't force people to smoke

- **Observational** data is plentiful and cheap

  How are patients treated in hospitals today?

- So, how can we learn from observational data?

Assumptions in observational case

- Sufficient conditions for **identifiability**:

- **Strong ignorability**[1]: $Y_0, Y_1 \perp\!\!\!\perp T \mid X$ "No *hidden* confounders"

  All variables that affect both Y_t and T are measured

- **Overlap**: $\forall x, t\colon\ p(T = t \mid X = x) > 0$

  All treatments have non-zero probability of being observed

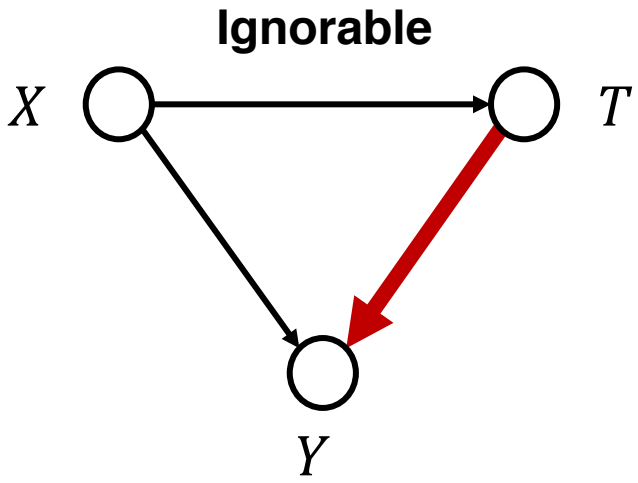
- **Stable Unit Treatment Value Assumption** (SUTVA):

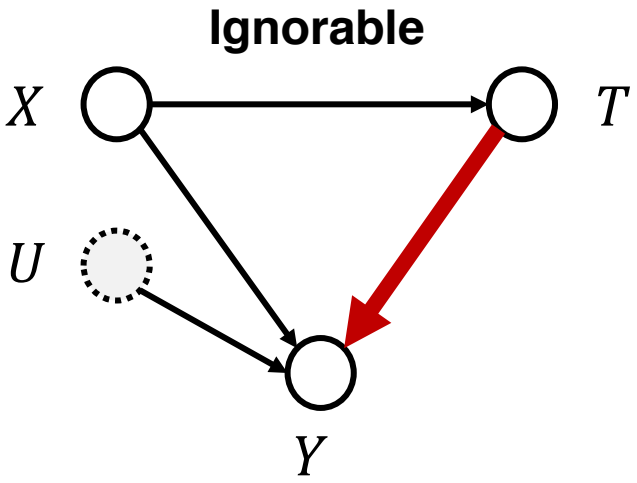
  Treatments and outcomes of different subjects are independent

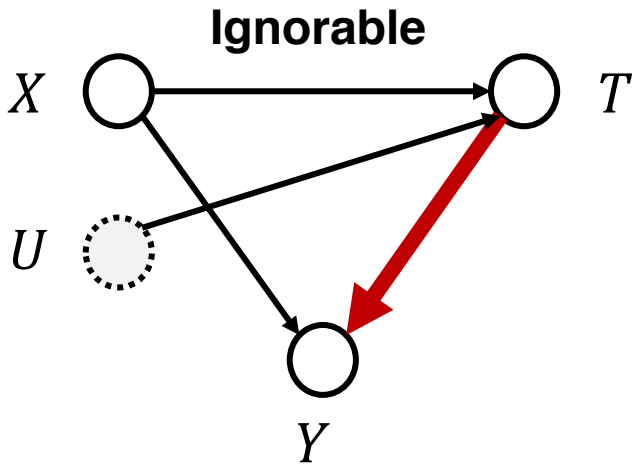
Ignorability

Measured

Unmeasured / hidden



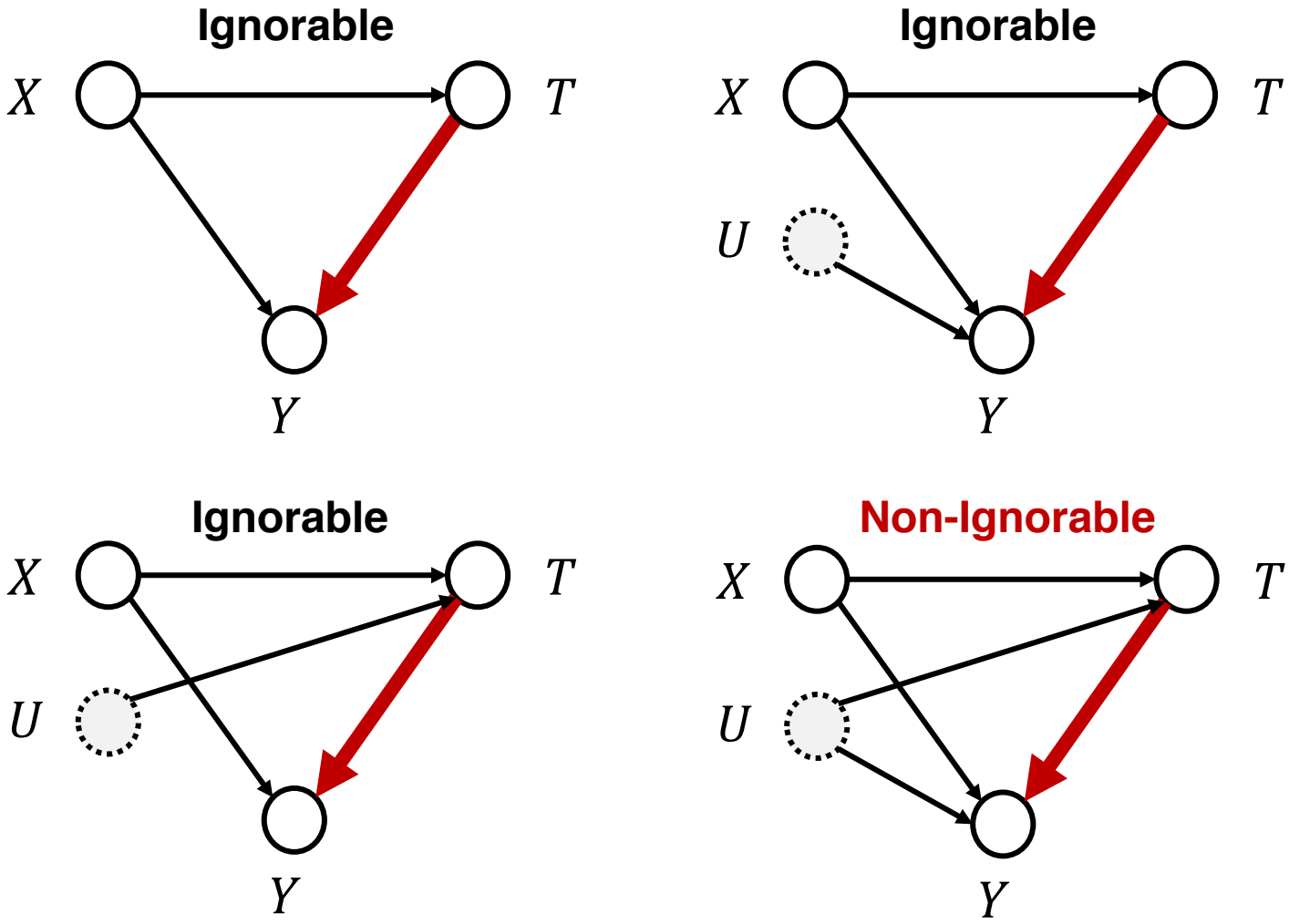




Ignorability

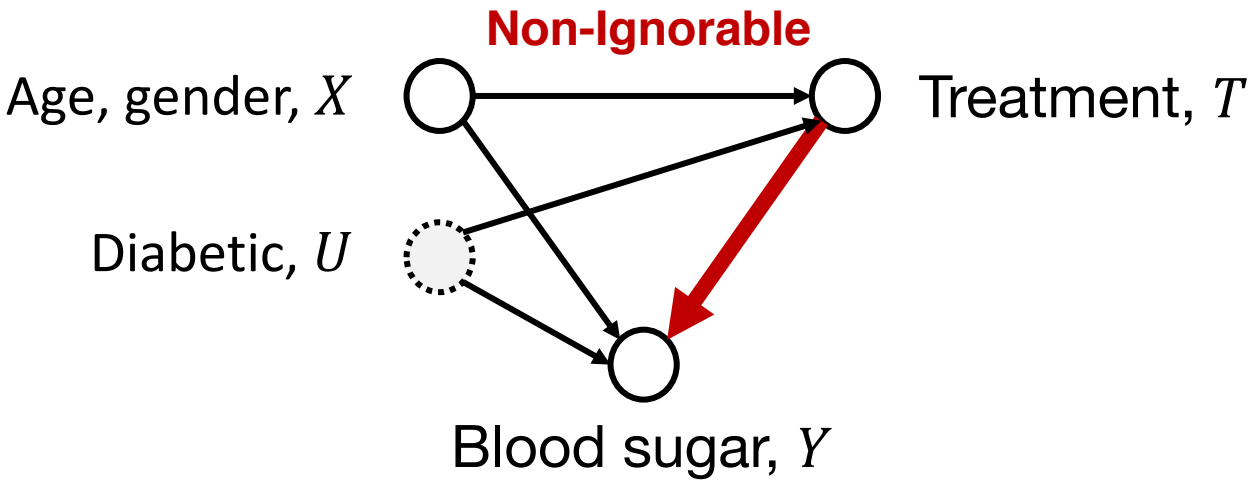
Measured

Unmeasured / hidden



Ignorability

Measured Unmeasured / hidden



Covariate adjustment

- It can be shown (on a couple of lines) that under the assumptions listed above

$$\mathbb{E}[\, Y(t) \mid x \,] = \mathbb{E}[\, Y \mid x, t \,]$$

- and as a result

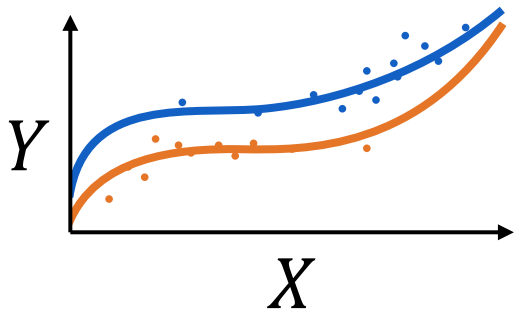
$$ATE = \mathbb{E}\Big[\mathbb{E}[\, Y \mid x, T = 1 \,] - \mathbb{E}[\, Y \mid x, T = 0 \,]\Big]$$

- We find (regression) models for $\mathbb{E}[\, Y \mid x, t \,]$ and extrapolate

Estimating both CATE and ATE

- In fact, $\mathbb{E}[\, Y \mid x, t \,]$ is sufficient to estimate both ATE and CATE under these assumptions:

$$\tau(x) = \mathbb{E}[\, Y \mid x, T = 1 \,] - \mathbb{E}[\, Y \mid x, T = 0 \,]$$



- Our job is now to estimate $\mathbb{E}[\, Y \mid x, t \,]$!

1. Potential outcomes framework

2. Supervised learning (risk minimization)

3. Adjusting for distributional shift

Supervised learning

- Machine learning in general, and deep learning in particular, is great at "function fitting" or supervised learning

- **Input:** features $X \in \mathbb{R}^d$
- **Output:** label $Y \in \mathbb{R}$

(Think of treatment as in X for now.)

- Learn from n samples $(x_1, y_1), \ldots, (x_n, y_n) \sim p(X, Y)$

Risk minimization

- Most supervised learning attempt to find models f such that

$$f(x) \approx \mathbb{E}_p[Y \mid X = x]$$

- often by the **risk minimization** principle

$$f = \operatorname*{argmin}_h R_p(h)\,, \qquad R_p(h) \coloneqq \mathbb{E}_p[(h(x) - y)^2]$$

- Unfortunately, typically only samples are available, not the full expectation

- Loss is specific to application (e.g. regression). Here, square loss

Empirical risk minimization

- A common proxy is **Empirical Risk Minimization** (ERM)

$$f = \operatorname*{argmin}_h \hat{R}_S(h), \qquad \hat{R}_S(h) \coloneqq \frac{1}{n}\sum_{i=1}^{n}(h(x_i) - y_i)^2$$

- where S is a sample from p, $S = (x_1, y_1), \ldots, (x_n, y_n)$

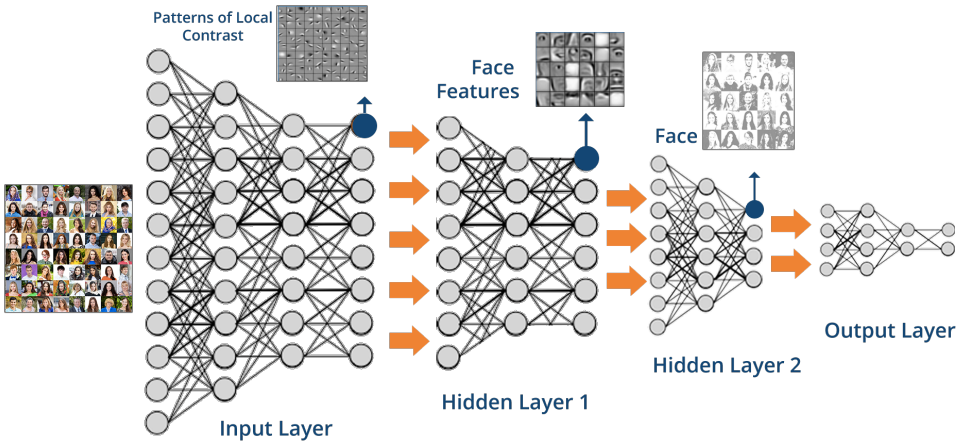
- Supported by learning theory. W.h.p. we generalize from sample

$$R_p(h) \leq \hat{R}_S(h) + \frac{\mathcal{C}}{\sqrt{n}}$$

$\mathcal{C}$ ← Model complexity

Deep learning

- Deep learning is amazing at empirical risk minimization
- Incredibly flexible models that are trained by simple algorithms



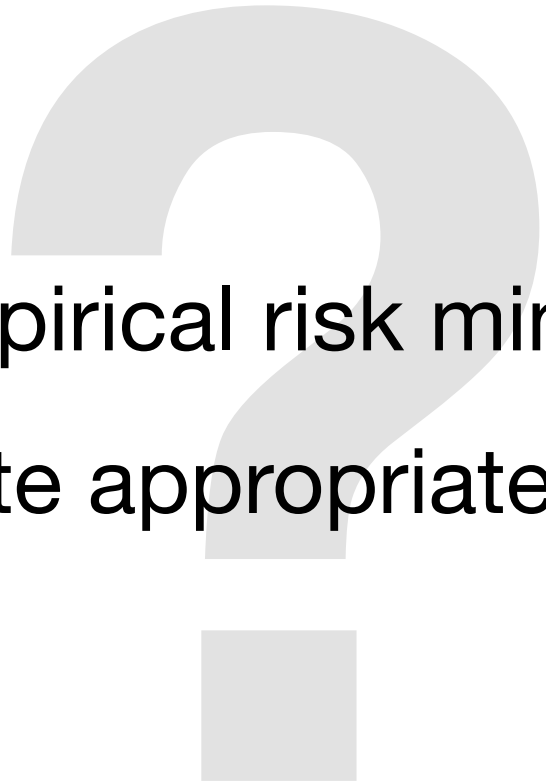
- (Opinions highly divided on how/why they generalize and don't overfit)

Estimating potential outcomes

- We consider learning hypotheses $f(x,t) \approx \mathbb{E}[\, Y \mid x, t \,]$
- Under ignorability, $f(x,t)$ estimates the potential outcome $Y(t)$
- Repeat the **risk minimization** principle for each outcome

$$f(\cdot,0) = \operatorname*{argmin}_{h_0} R_p^0(h_0)\,, \qquad R_p^0(h_0) \coloneqq \mathbb{E}_p\left[\left(h_0(x) - Y(0)\right)^2\right]$$

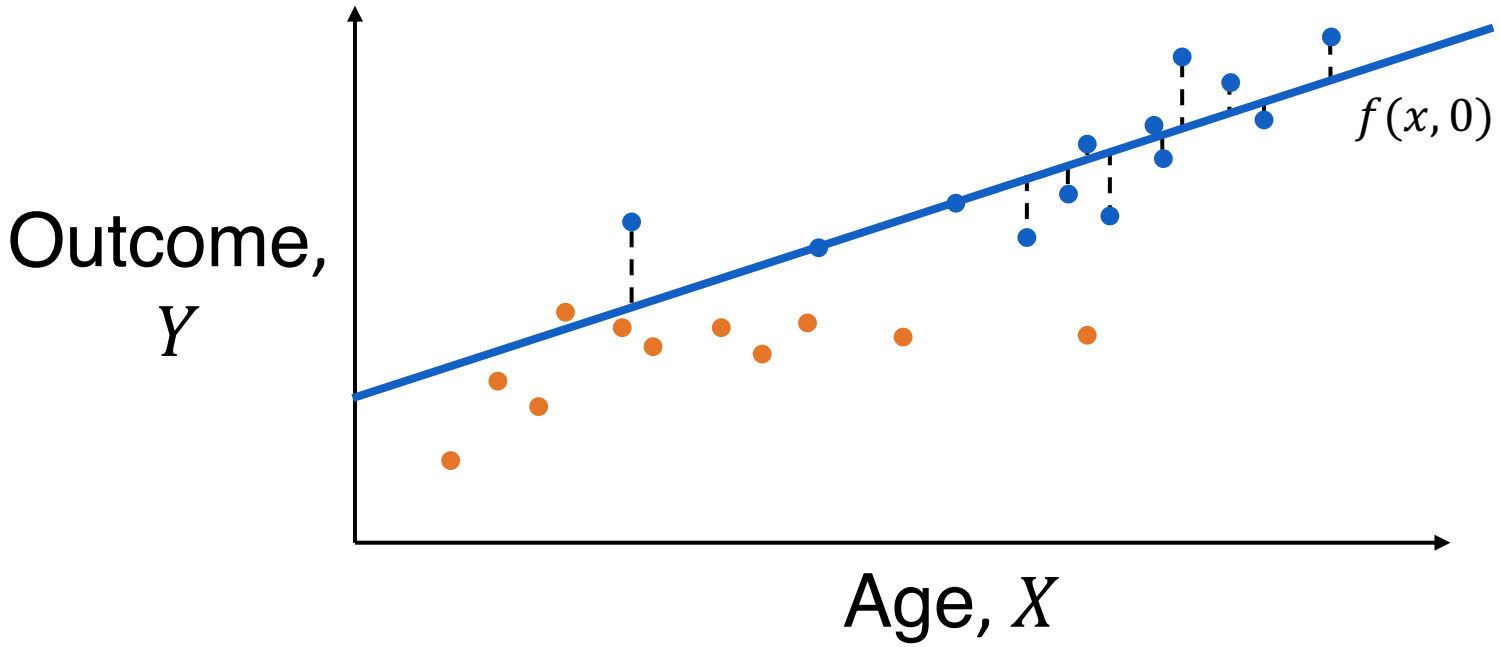
$$f(\cdot,1) = \operatorname*{argmin}_{h_1} R_p^1(h_1)\,, \qquad R_p^1(h_1) \coloneqq \mathbb{E}_p\left[\left(h_1(x) - Y(1)\right)^2\right]$$



Why is empirical risk minimization not quite appropriate here?

Estimating potential outcomes

- We don't have samples of $\mathbb{E}_p\left[\left(h_0(x) - Y(0)\right)^2\right]$ from $p(X, T)$, only from $p(X \mid T = 0)$! *We only see the control outcome for controls*



Estimating potential outcomes

- We don't have samples of $\mathbb{E}_p\left[\left(h_0(x) - Y(0)\right)^2\right]$ from $p(X, T)$, only from $p(X \mid T = 0)$! *We only see the control outcome for controls*

- No guarantee that

$$\mathbb{E}_p\left[\left(h_0(x) - Y(0)\right)^2\right] \overset{?}{\approx} \frac{1}{n}\sum_{i:t_i=0}(h_0(x_i) - y_i)^2$$

Only control group

- More on this **tomorrow**!

CATE risk minimization

- Ignoring the issue of empirical risk minimization for now, we seek an objective for **CATE**, and our estimate $\hat{\tau}_f(x)$

$$\hat{\tau}_f(x) = f(x,1) - f(x,0)$$

- We wish to minimize the risk, the **CATE MSE**,

$$R_p^{\tau}(f) = \mathbb{E}_p\left[\left(\hat{\tau}_f(x) - \tau(x)\right)^2\right]$$

- **Problem!** $\tau(x)$ is never fully observed! (And neither is $R_p^{\tau}(f)$)

Bounding CATE MSE

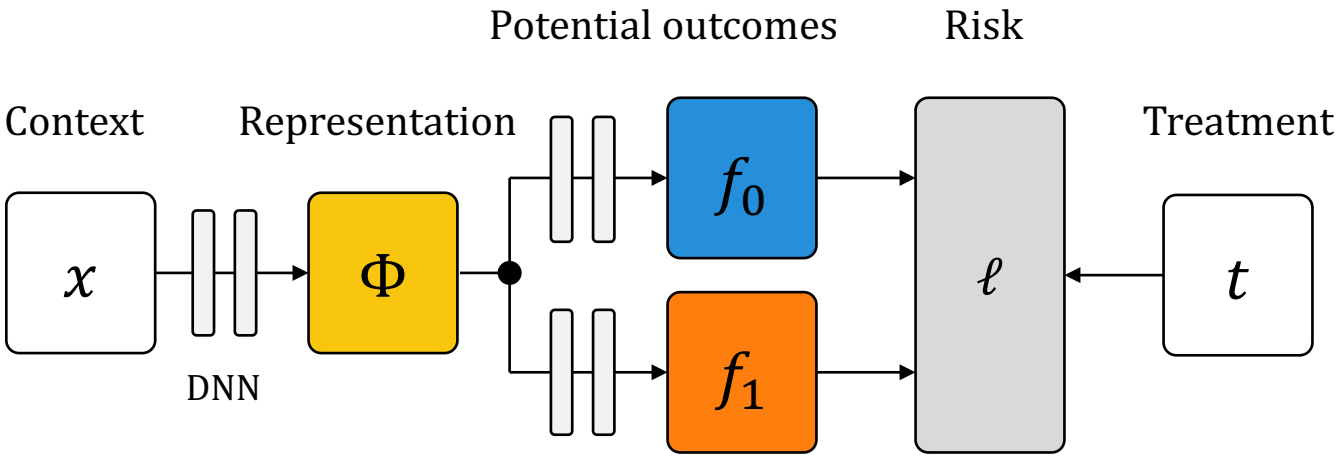
- $R_p^\tau(f)$ is not observed, but we can bound it!
- Intuitively, if $f(x,1)$ and $f(x,0)$ are good estimates, so is $\hat{\tau}_f(x)$
- In fact, it is easy to show that (w. relaxed triangle inequality)

$$R_p^\tau(f) \leq 2\left(R_p^0(f) + R_p^1(f)\right) + \sigma$$

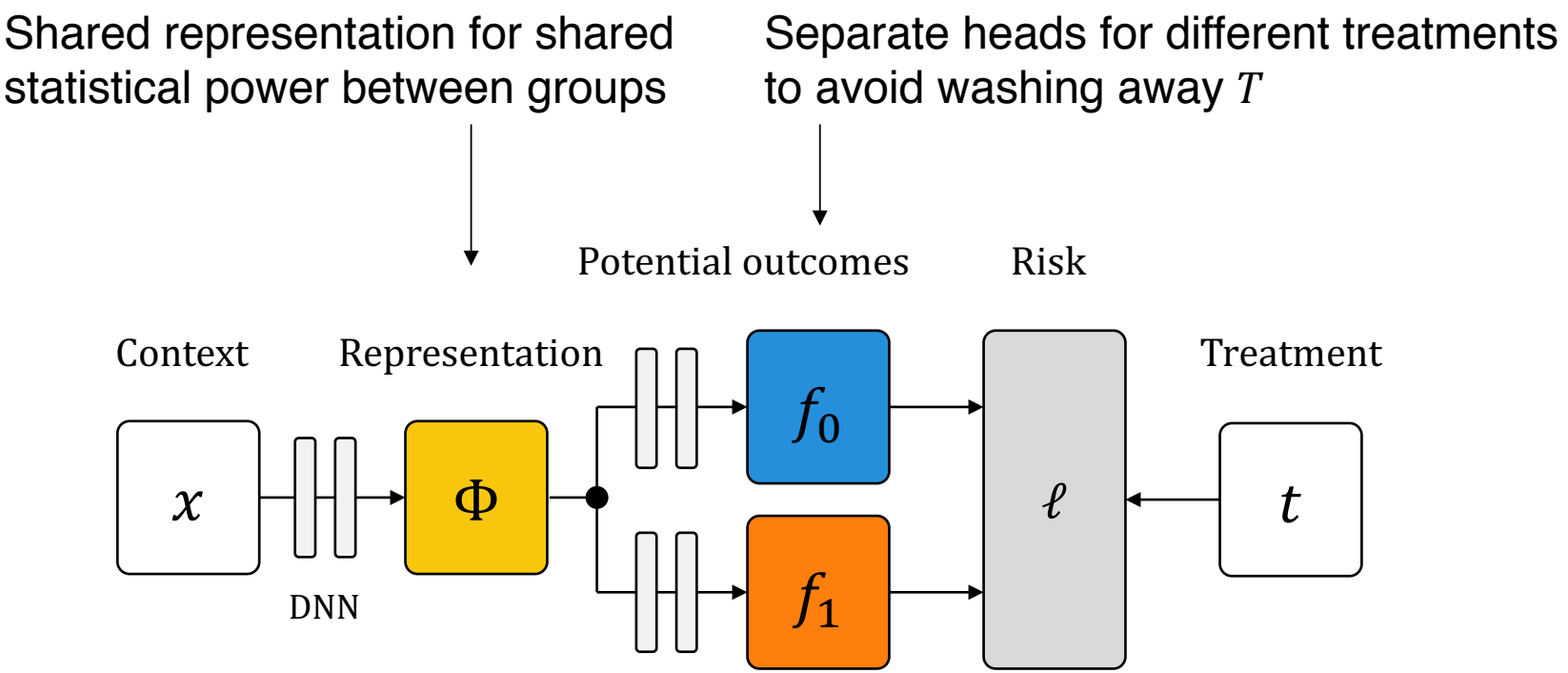
- Fitting each potential outcome well is sufficient (but not necessary)

Deep learning architecture

- Shalit, J., Sontag came up with the following architecture



Deep learning architecture



- This halved the error on a widely used causal effect benchmark!

1. Potential outcomes framework

2. Supervised learning (risk minimization)

3. Adjusting for distributional shift

Tomorrow!