



# CAUSALLY REGULARIZED MACHINE LEARNING

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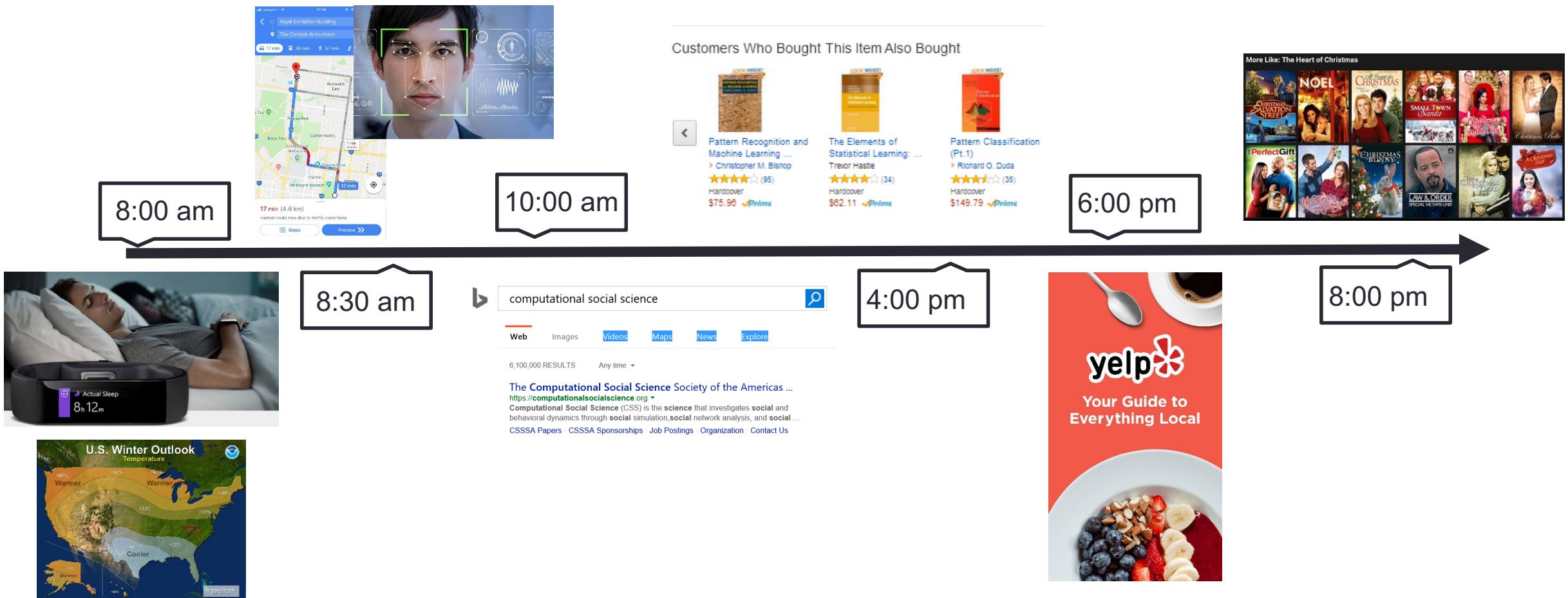
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**Bo Li**, Tsinghua University

# Predictive systems are impacting our life

- A day in our life with predictive analytics



# Even in risk-sensitive areas



Human

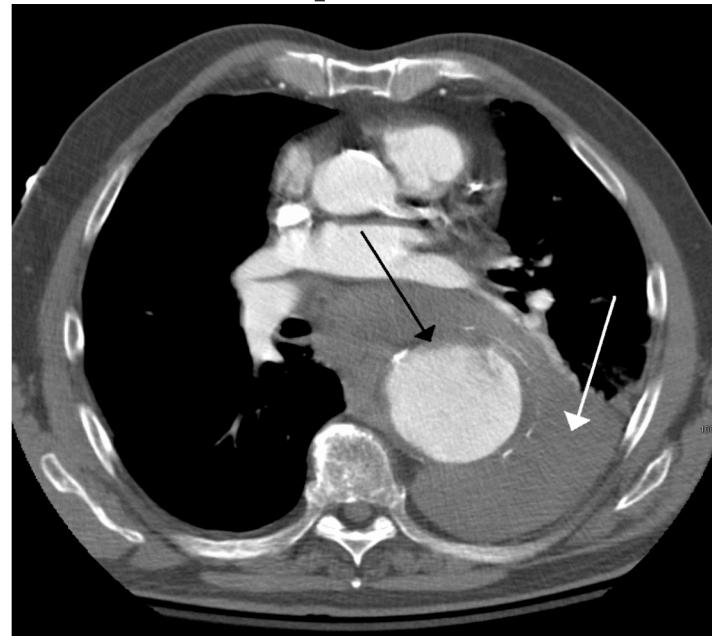


Human's risk-sensitive sense brings new challenges to today's AI

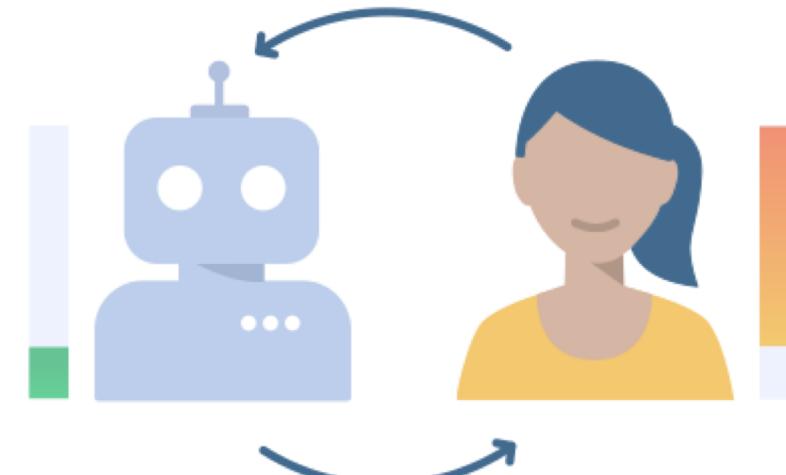
# Explainability

Most machine learning models are black-box models

**Unexplainable**



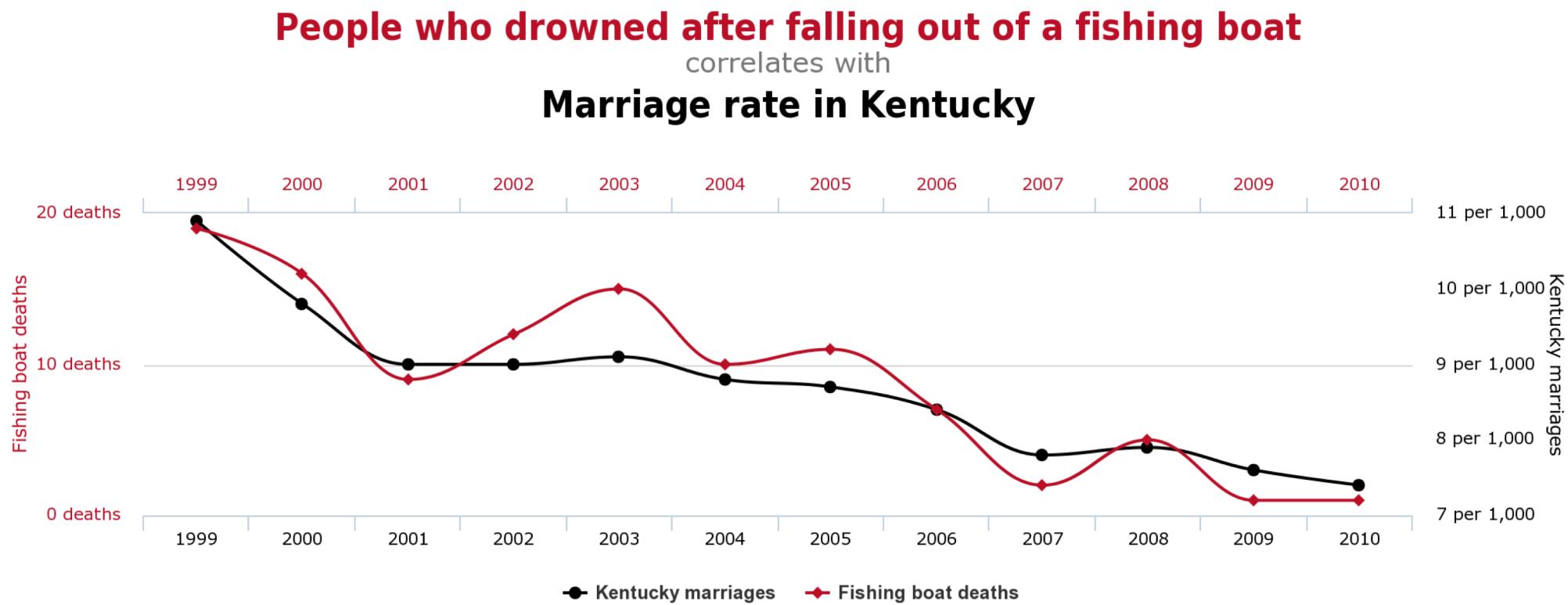
**Human in the loop**



Health Military Finance Industry

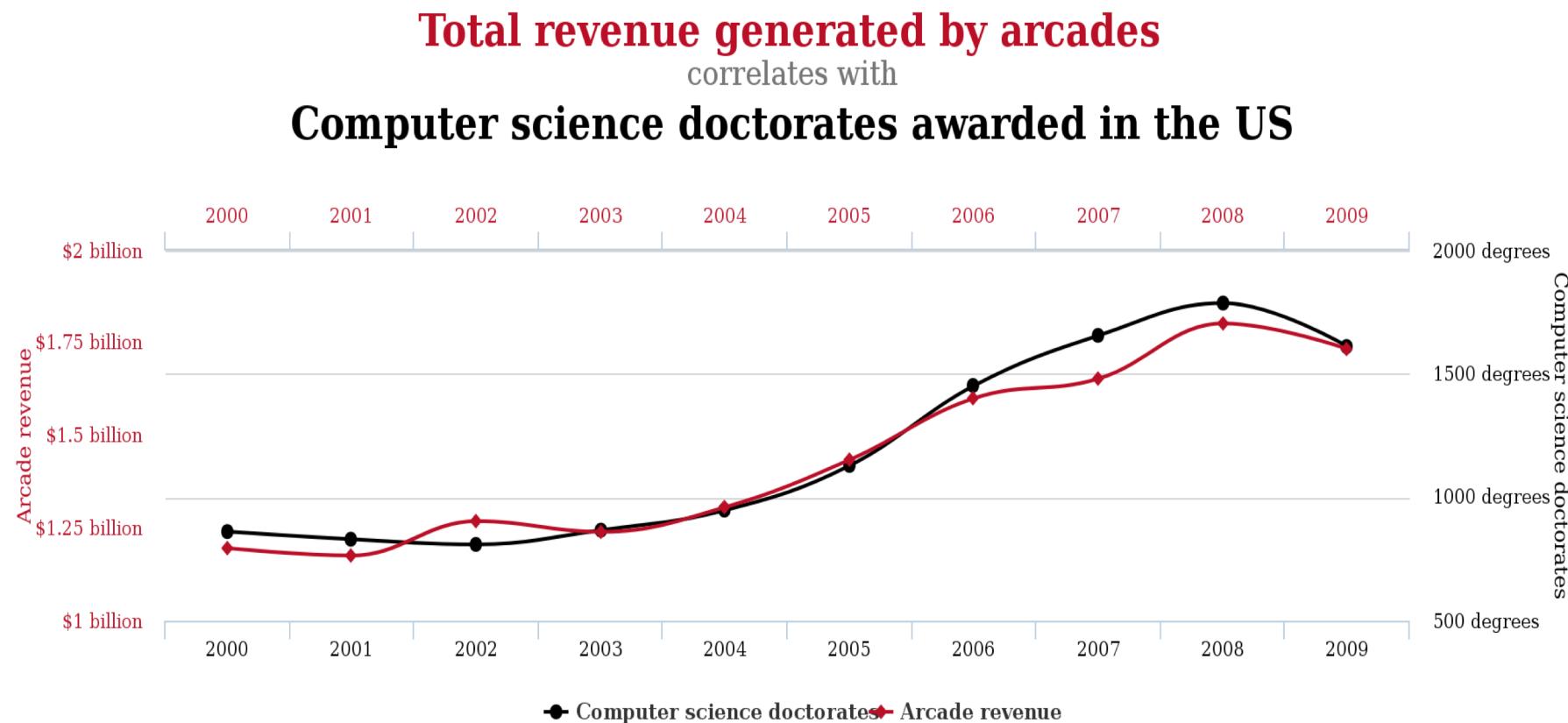
# Explainability

- Correlation is not explainable

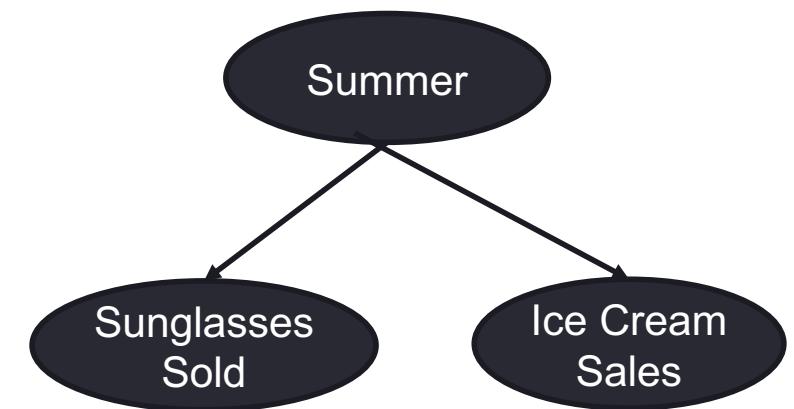
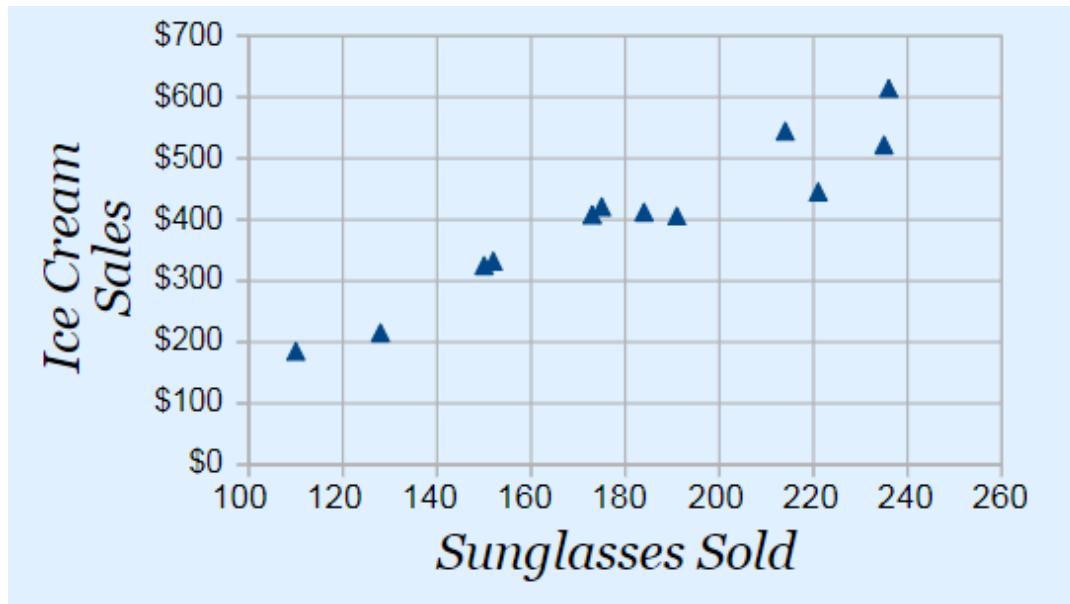


# Explainability

- Correlation is not explainable



# Explainability

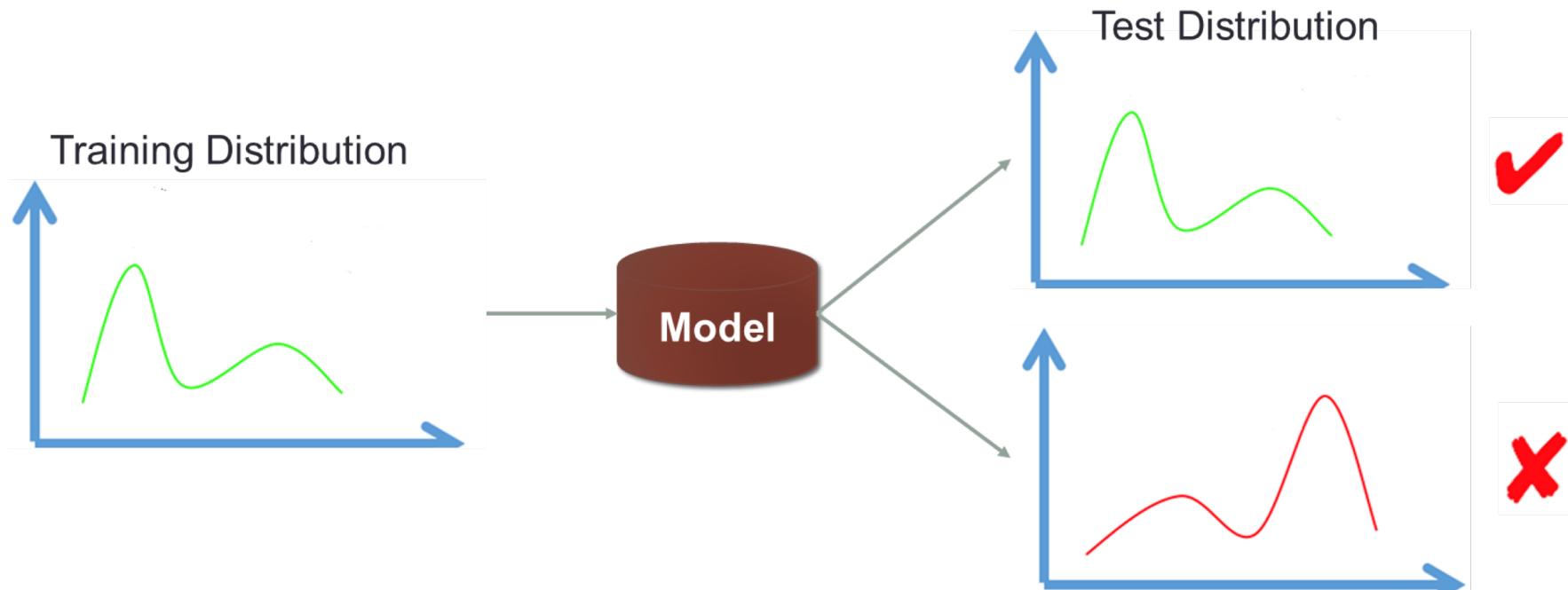


Spurious Correlation !

Correlation does not imply causation!

# Stability

Most ML methods are developed under IID hypothesis



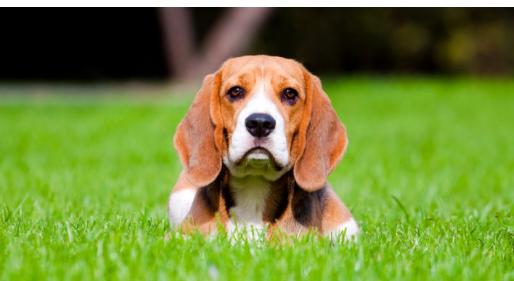
# Stability



Yes



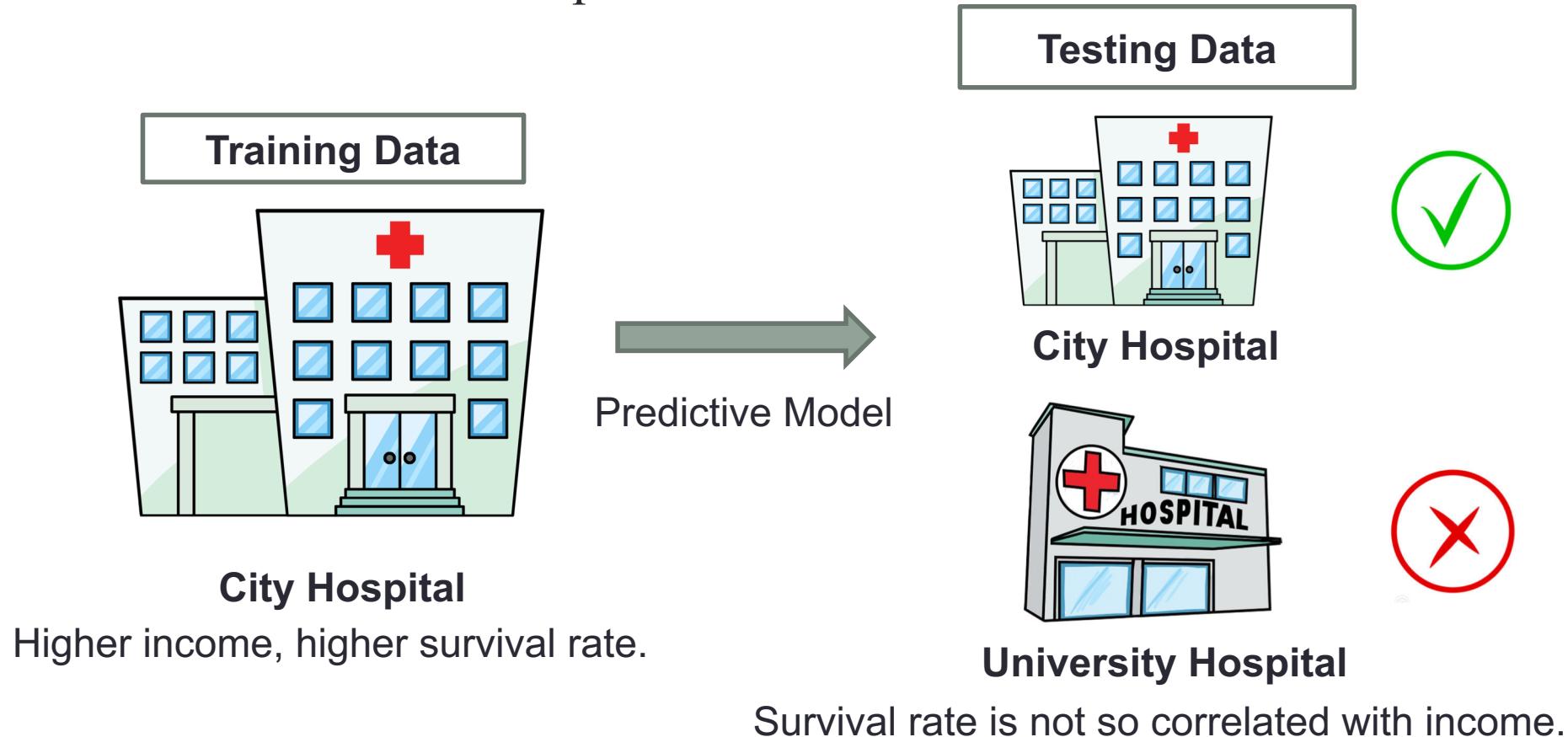
Maybe



No

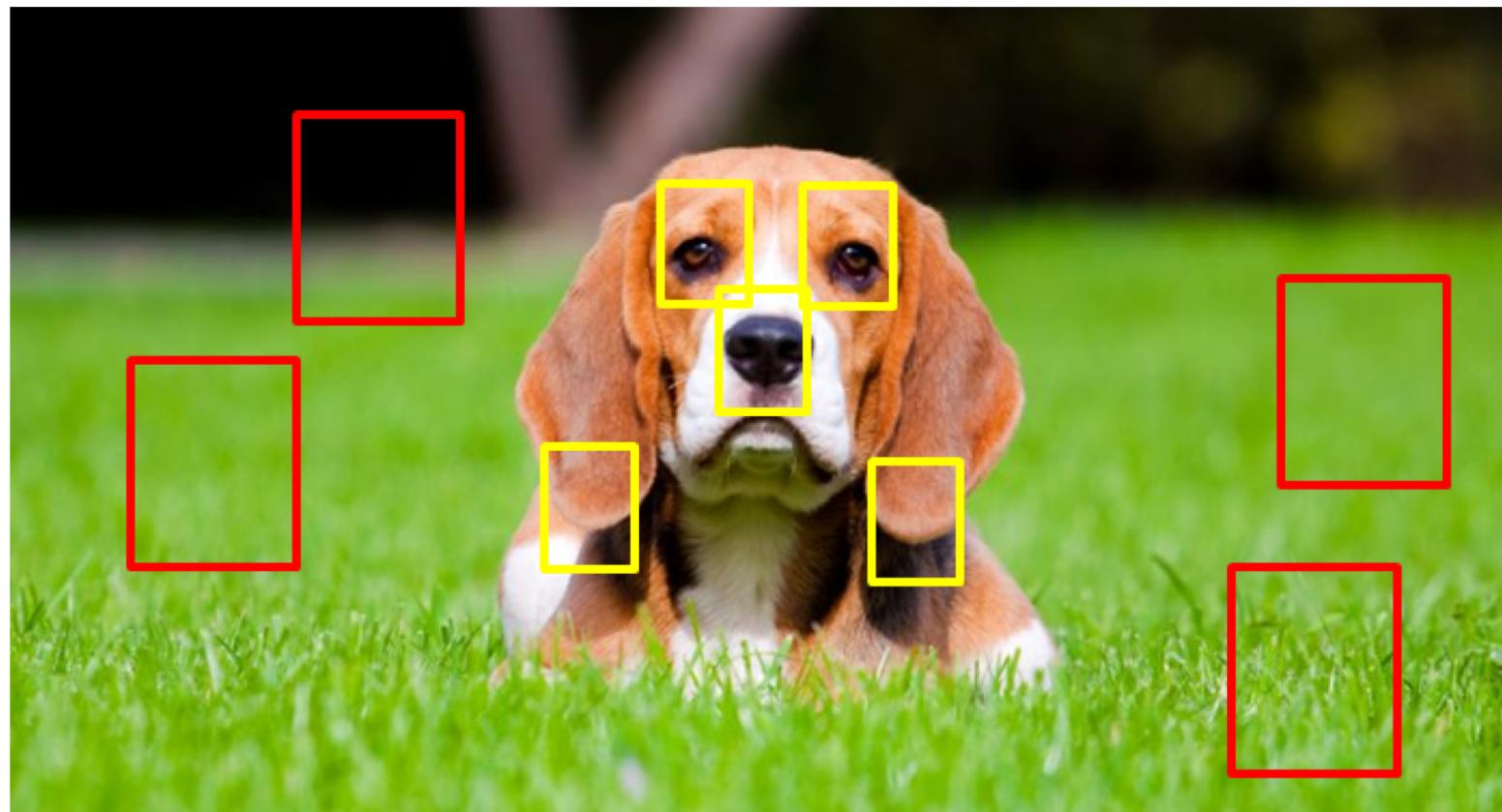
# Stability

- Cancer survival rate prediction



# Stability

Correlation v.s. Causality



# Actionability

- Does predictive models guide decision making?
- System changes algorithm from A to B at some point.
- Is the new algorithm B better?
- Say algorithm that provides promotion or discount link to a different customers



Algorithm A



Algorithm B

# Actionability

- Measure success rate (SR)

| Old Algorithm (A) | New Algorithm (B) |
|-------------------|-------------------|
| 50/1000 (5%)      | 54/1000 (5.4%)    |

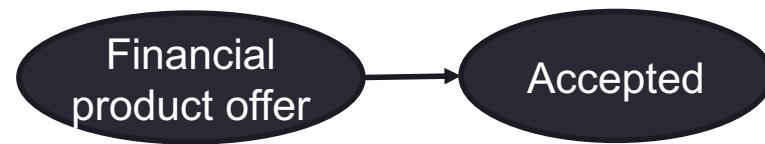


New algorithm increases overall success rate, so it is better?

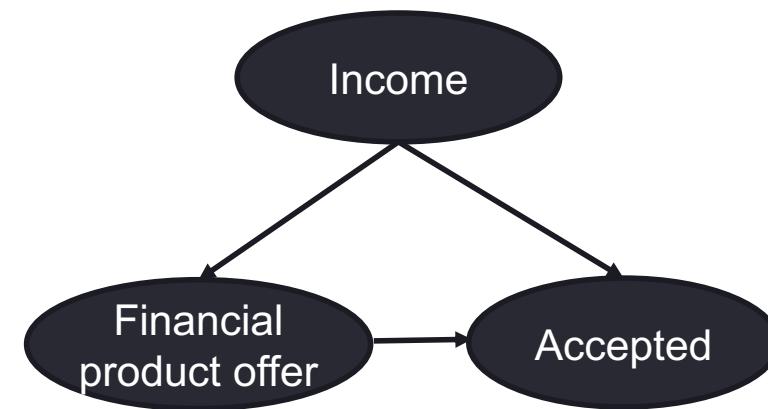
|                   | Old Algorithm (A) | New Algorithm (B) |
|-------------------|-------------------|-------------------|
| Low-income Users  | 10/400 (2.5%)     | 4/200 (2%)        |
| High-income Users | 40/600 (6.6%)     | 50/800 (6.2%)     |
| Overall           | 50/1000 (5%)      | 54/1000 (5.4%)    |

Which is better?

# Actionability



Higher success rate due to  
**algorithm**



Higher success rate due to  
**confounding bias**

Decision making is a counterfactual problem, not a predictive problem!

# Fairness

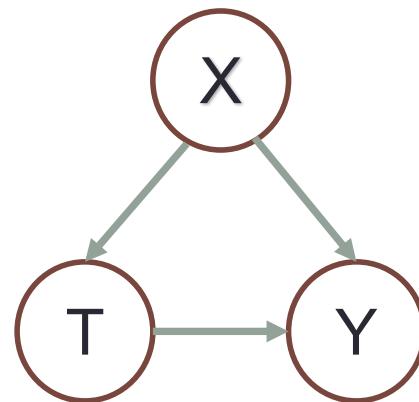


# The source of these problems: Correlation

## Correlation Framework



## Causal Framework



T: skin color  
X: income  
Y: crime rate

income—crime rate: Strong correlation  
skin color—crime rate: Strong correlation

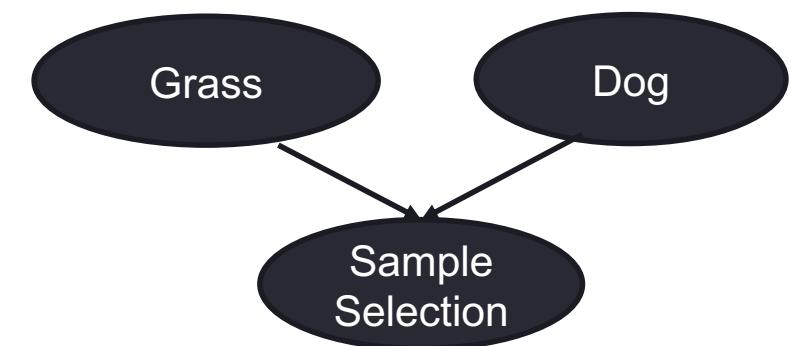
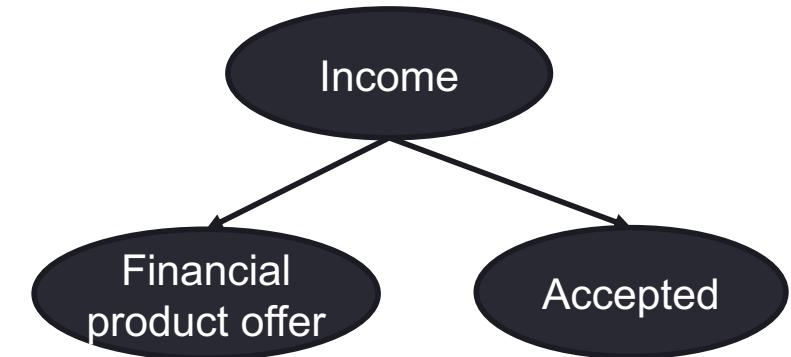
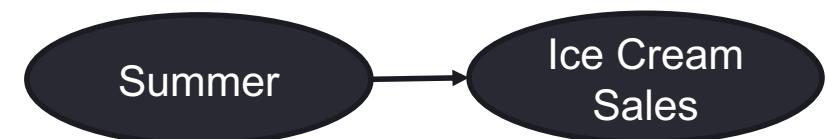
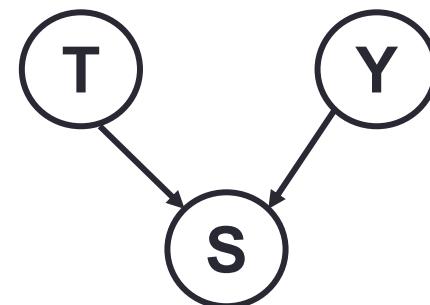
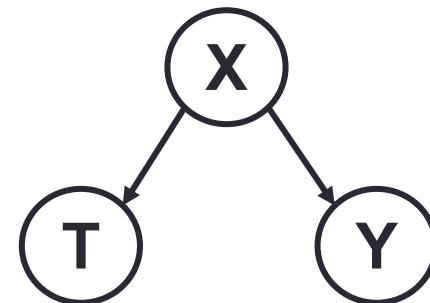


income—crime rate: Strong causation  
skin color—crime rate: Weak causation

# Correlation V.S. Causation

- Three sources of correlation:

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



# Correlation V.S. Causation

- Three sources of correlation:

- Causation
  - Causal mechanism
  - Stable and Robust

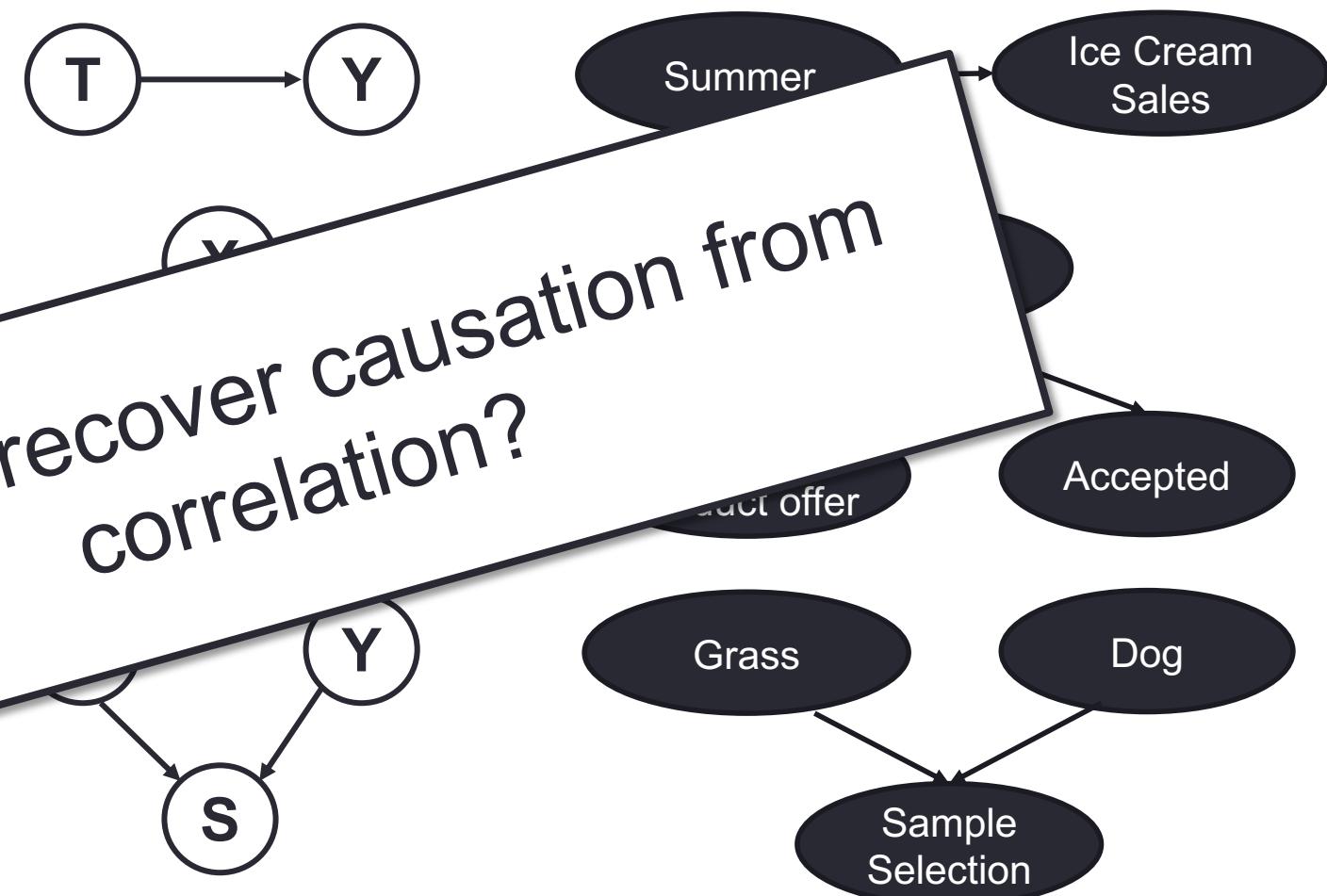
- Confounding

- Ignoring
- Spurious

- Sample Selection

- Conditional

- Spurious Correlation



# Why should we care about causality?

- Recover causation for interpretability
- Help to guide decision making
- Make stable and robust prediction in the future
- Prevent algorithmic bias

# OUTLINE

**PART I. Introduction to Causal Inference**

**PART II. Methods for Causal Inference**

**PART III. Causally Regularized Machine Learning**

**PART IV. Benchmark and Open Datasets**

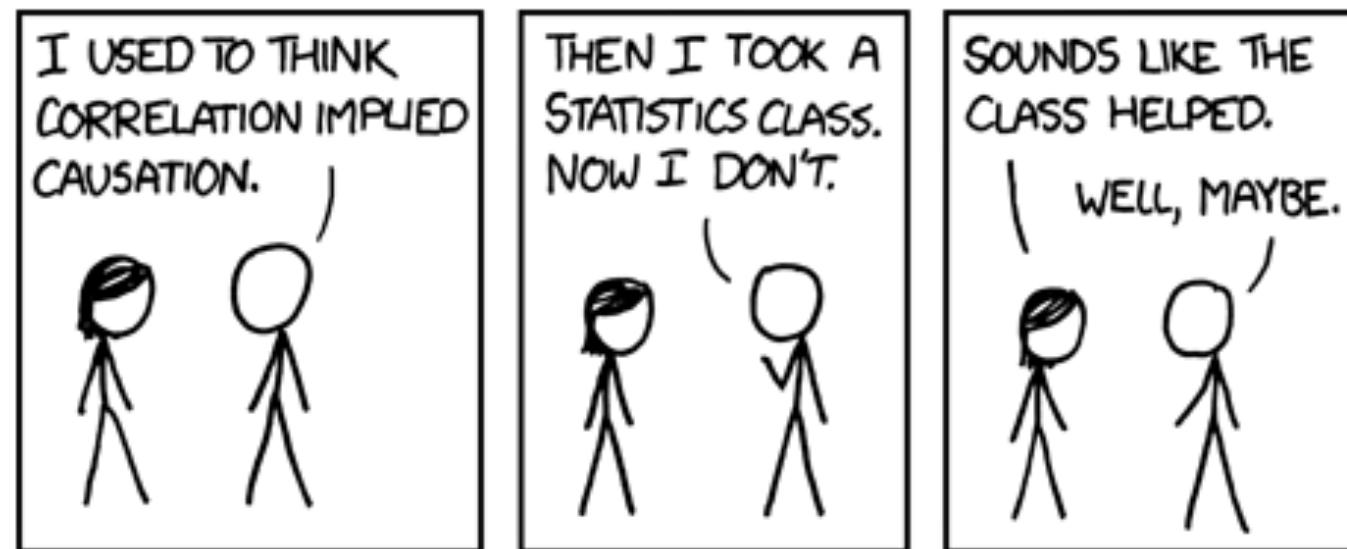
**PART V. Conclusion and Discussion**

# Cause and Effect

- Cause: The REASON why something happened
- Effect: The RESULT of what happened
- Questions of cause and effect:
  - Medicine: drug trials, effect of a drug
  - Social science: effect of a policy
  - Marketing: effect of a marketing strategy
  - ...
- **What is causality?**

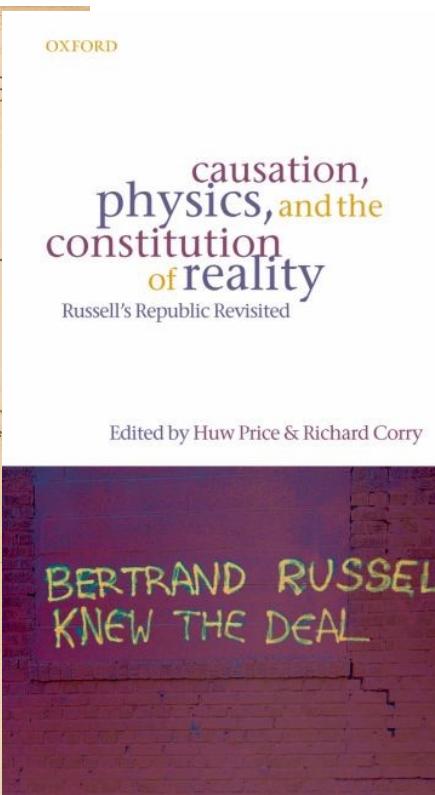
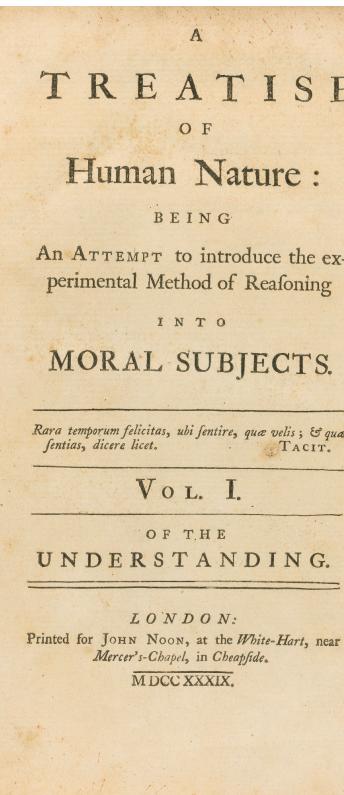
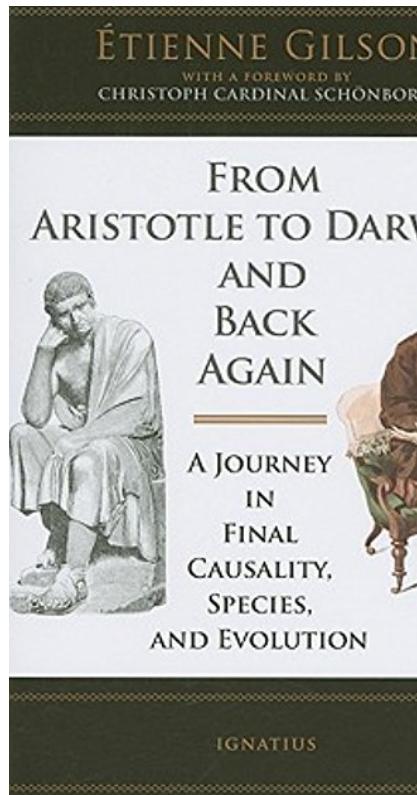


# What is causality?



# What is causality?

- A big scholarly debate, from Aristotle to Russell



# The Three Layer Causal Hierarchy

| Level  | Typical Activity            | Typical Question   | Examples   |
|--|-----------------------------|--|--|
| Observational Questions<br><br>1. Association<br>$P(y   x)$              | Seeing                      | What is?<br>How would seeing $X$ change my belief in $Y$ ?               | What does a symptom tell me about a disease?   |
|  |                             |  | What does a survey tell us about the election results?   |
| Action Questions<br><br>2. Intervention<br>$P(y   do(x), z)$             | Doing,<br>Intervening       | What if?<br>What if I do $X$ ?   | What if I take aspirin, will my headache be cured?   |
|  |                             |  | What if we ban cigarettes?   |
| Counterfactuals Questions<br><br>3. Counterfactuals<br>$P(y_x   x', y')$ | Imagining,<br>Retrospection | Why?<br>Was it $X$ that caused $Y$ ?<br>What if I had acted differently? | Was it the aspirin that stopped my headache?   |
|  |                             |  | Would Kennedy be alive had Oswald not shot him?<br>What I had not been smoking the past 2 years? |

# A practical definition

Definition: T causes Y if and only if  
changing T leads to a change in Y,  
keep everything else constant.

Causal effect is defined as the magnitude by which Y is changed by a unit change in T.

Called the “interventionist” interpretation of causality.

\**Interventionist* definition [<http://plato.stanford.edu/entries/causation-mani/>]

# Causal Effect Estimation

- Treatment Variable:  $T = 1$  or  $T = 0$
- Potential Outcome:  $Y(T = 1)$  and  $Y(T = 0)$
- Average Causal Effect of Treatment (ATE):

$$ATE = E[Y(T = 1) - Y(T = 0)]$$

- Counterfactual Problem:

$$Y(T = 1) \quad \text{or} \quad Y(T = 0)$$



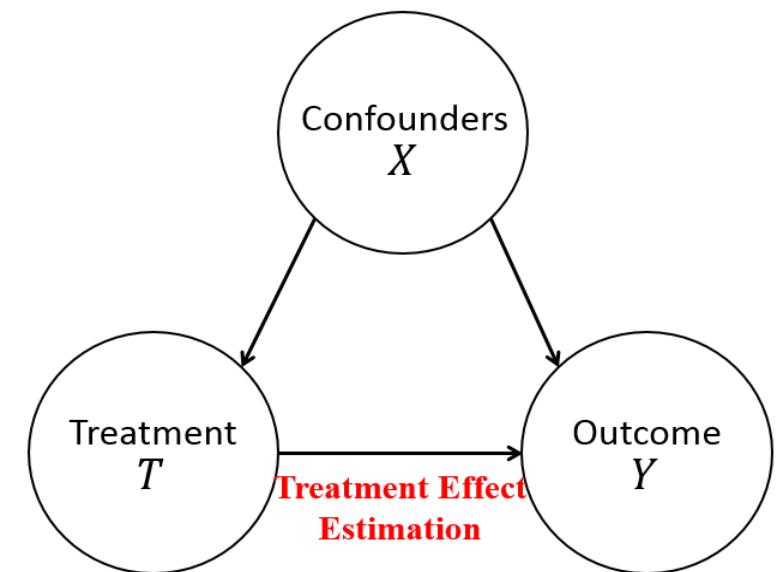
# Counterfactual Problem

| Person | T | $Y_{T=1}$ | $Y_{T=0}$ |
|--------|---|-----------|-----------|
| P1     | 1 | 0.4       | ?         |
| P2     | 0 | ?         | 0.6       |
| P3     | 1 | 0.3       | ?         |
| P4     | 0 | ?         | 0.1       |
| P5     | 1 | 0.5       | ?         |
| P6     | 0 | ?         | 0.5       |
| P7     | 0 | ?         | 0.1       |

- Two key points for causal effect estimation
  - Changing T
  - Keeping everything else constant
- For each person, observe only one: either  $Y_{t=1}$  or  $Y_{t=0}$
- For different group ( $T=1$  and  $T=0$ ), something else are not constant

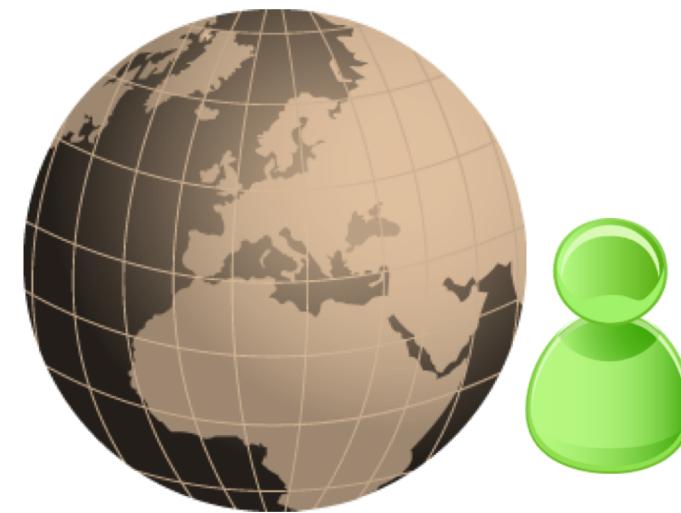
# Potential Outcome Framework

- Confounders X: everything else
- Why keep everything else constant:
  - Confounders X influences both T and Y
  - Y's change could be induced by change of T or since X changed both T and Y?
- In different group, keep confounders the same!



# Ideal Solution: Counterfactual World

- Reason about a world that does not exist
- Everything is the same on real and counterfactual worlds, but the treatment


$$Y(T = 1)$$

$$Y(T = 0)$$

# Randomized Experiments are the “Gold Standard”



- Drawbacks of randomized experiments:
  - Cost
  - Unethical

# Randomized Experiments are the “Gold Standard”

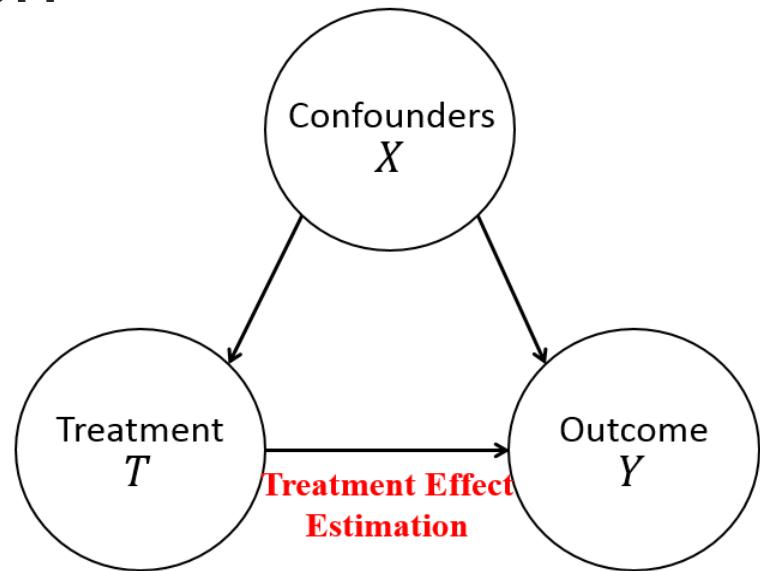
- Drawbacks
  - Cost
  - Unethical



What can we do when an experiment is  
not possible?  
Observational Studies!

# Recap: Causal Effect and Potential Outcome

- Two key points for causal effect estimation
  - Changing T
  - Keeping everything else (X) constant
- Counterfactual Problem
$$Y(T = 1) \quad \text{or} \quad Y(T = 0)$$
- Ideal Solution: Counterfactual World
- “Gold Standard”: Randomized Experiments
- We will discuss other solutions in Section 2.



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# Causal Inference with Observational Data

- **Average Treatment Effect (ATE)** represents the mean (average) difference between the potential outcome of units under **treated ( $T=1$ )** and **control ( $T=0$ )** status.

$$ATE = E[Y(T = 1) - Y(T = 0)]$$

- **Treated ( $T=1$ ):** taking a particular medication
- **Control ( $T=0$ ):** not taking any medications
- **ATE:** the causal effect of the particular medication



# Causal Inference with Observational Data



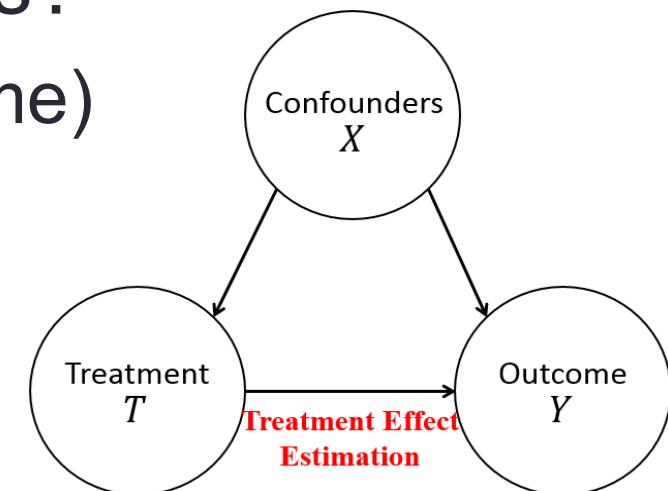
- Counterfactual Problem:

$$Y(T = 1) \quad \text{or} \quad Y(T = 0)$$

- Can we estimate ATE by directly comparing the average outcome between treated and control groups?

- Yes with randomized experiments ( $X$  are the same)
  - No with observational data ( $X$  might be different)

- Two key points:
    - Changing T ( $T=1$  and  $T=0$ )
    - Keeping everything else (Confounder X) constant



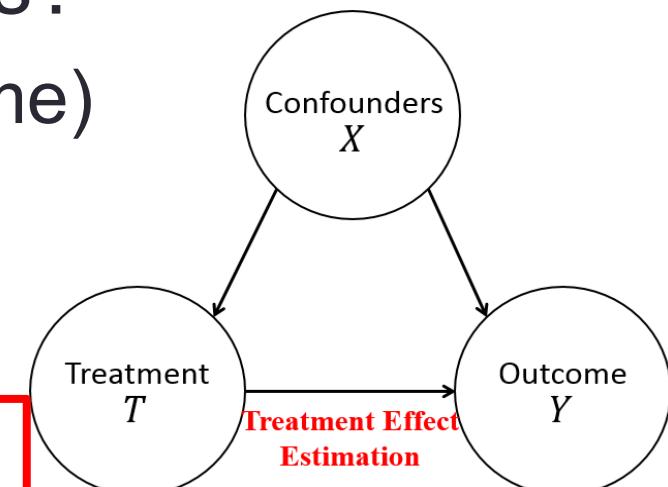
# Causal Inference with Observational Data

- Counterfactual Problem:

$$Y(T = 1) \quad \text{or} \quad Y(T = 0)$$

- Can we estimate ATE by directly comparing the average outcome between treated and control groups?
  - Yes with randomized experiments ( $X$  are the same)
  - No with observational data ( $X$  might be different)
- Two key points:

**Balancing Confounders' Distribution**



# Methods for Causal Inference

- **Matching**
- **Propensity Score Based Methods**
  - Propensity Score Matching
  - Inverse of Propensity Weighting (IPW)
  - Doubly Robust
  - Data-Driven Variable Decomposition (D<sup>2</sup>VD)
- **Directly Confounder Balancing**
  - Entropy Balancing
  - Approximate Residual Balancing
  - Differentiated Confounder Balancing (DCB)

# Assumptions of Causal Inference

- **A1: Stable Unit Treatment Value (SUTV):** The effect of treatment on a unit is independent of the treatment assignment of other units

$$P(Y_i|T_i, T_j, X_i) = P(Y_i|T_i, X_i)$$

- **A2: Unconfoundedness:** The distribution of treatment is independent of potential outcome when given the observed variables

$$T \perp (Y(0), Y(1)) | X$$

No unmeasured confounders

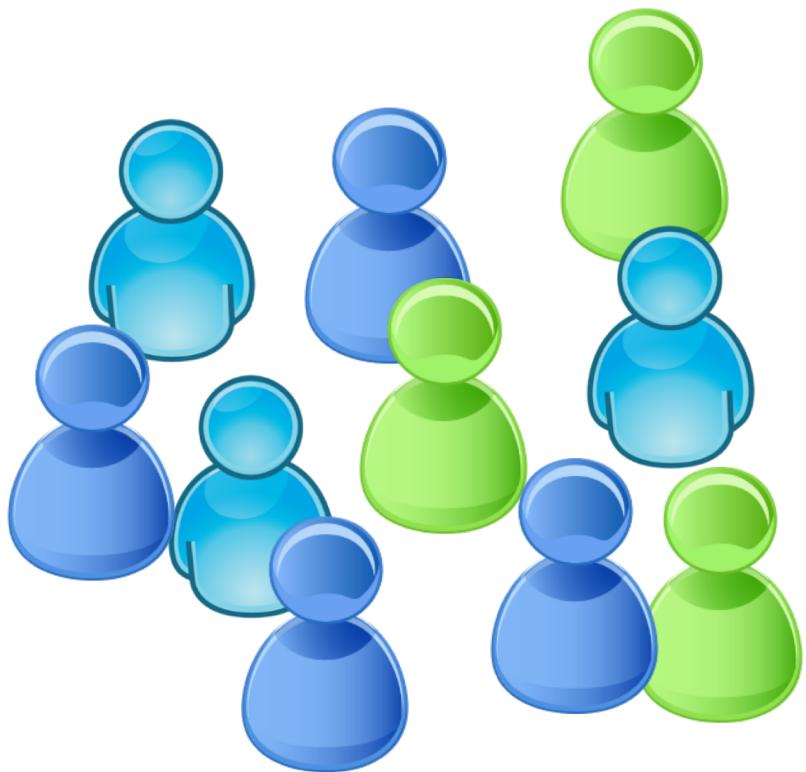
- **A3: Overlap:** Each unit has nonzero probability to receive either treatment status when given the observed variables

$$0 < P(T = 1|X = x) < 1$$

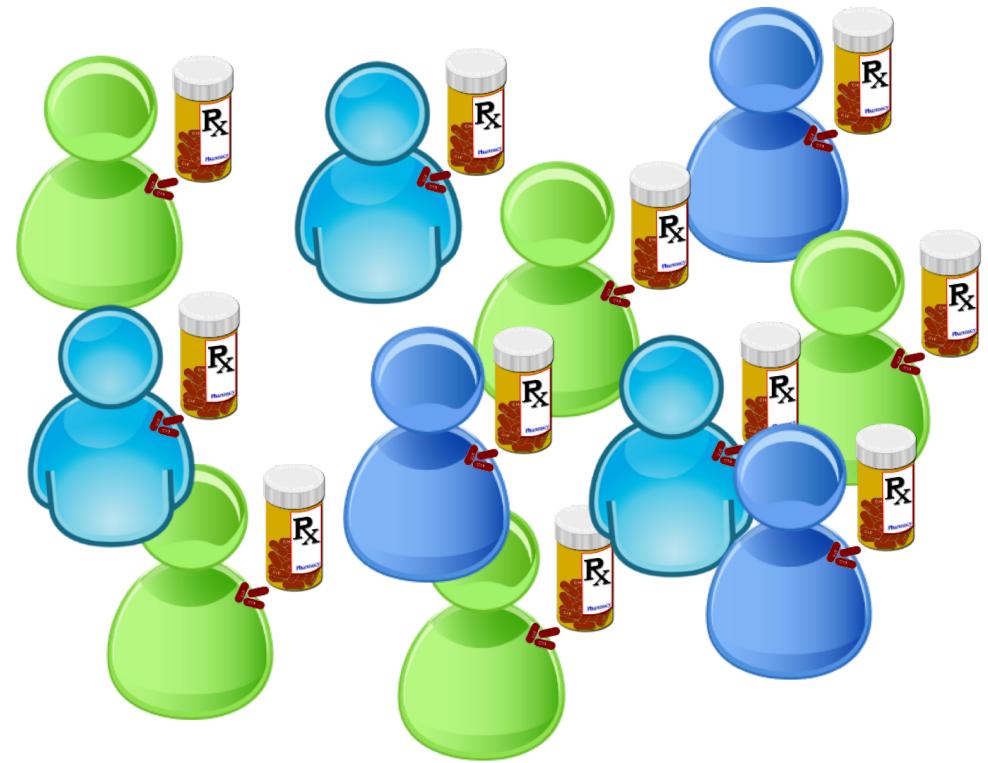
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# Matching

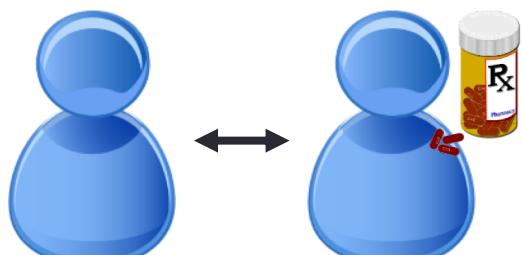
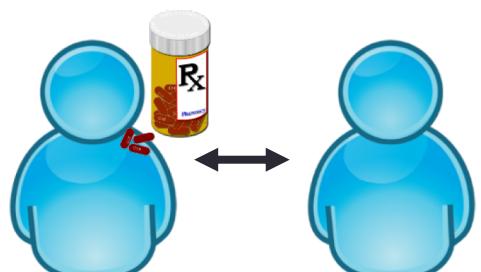
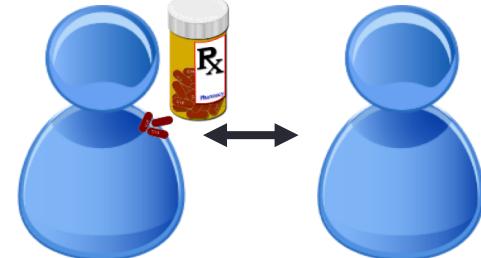
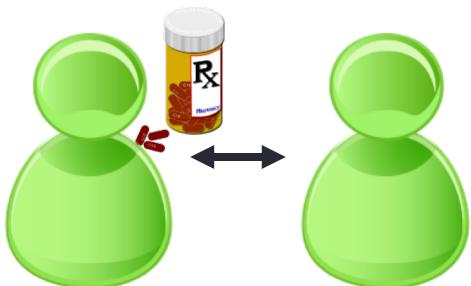
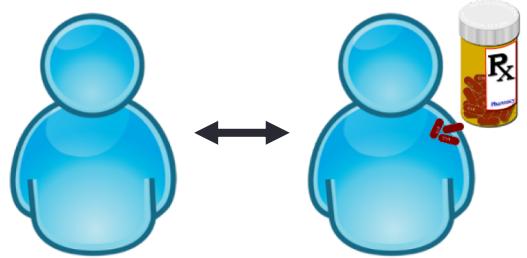
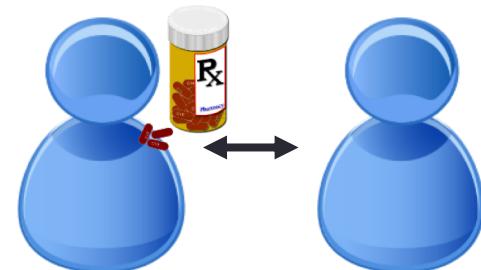
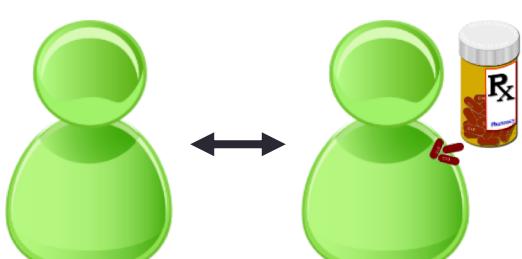
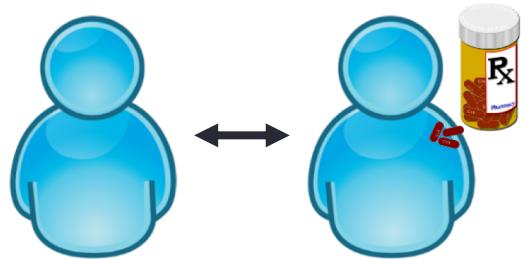


$T = 0$



$T = 1$

# Matching

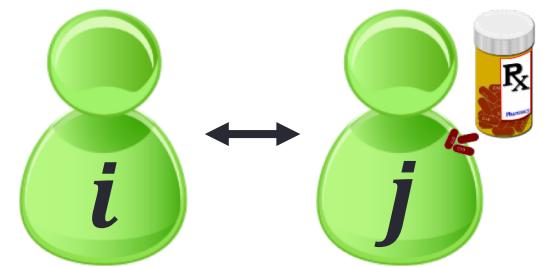


# Matching

- Identify pairs of treated ( $T=1$ ) and control ( $T=0$ ) units whose confounders  $X$  are similar or even identical to each other

$$\text{Distance}(X_i, X_j) \leq \epsilon$$

- Paired units provide the everything else (Confounders) approximate constant
- Average the difference in outcomes with in pairs to calculate the average causal effect
- Smaller  $\epsilon$ : less bias, but higher variance



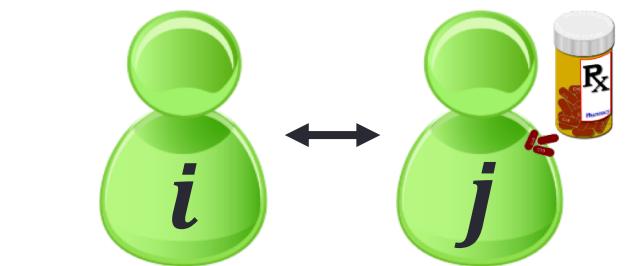
# Matching

- Exactly Matching:

$$\text{Distance}(X_i, X_j) = \begin{cases} 0, & X_i = X_j \\ \infty, & X_i \neq X_j \end{cases}$$

- Use this in low-dimensional settings

- But in high-dimensional settings, there will be few exact matches



$$\text{Distance}(X_i, X_j) \leq \epsilon$$

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# Propensity Score Based Methods

- Propensity score  $e(X)$  is the probability of a unit to be treated

$$e(X) = P(T = 1 | X)$$

- Then, Rubin shows that the propensity score is sufficient to control or summarized the information of confounders

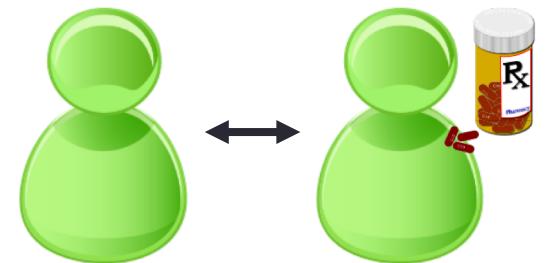
$$T \perp\!\!\!\perp X | e(X) \quad \Rightarrow \quad T \perp\!\!\!\perp (Y(1), Y(0)) | e(X)$$

- Propensity score are rarely observed, need to be estimated

# Propensity Score Matching

- Estimating propensity score:  $\hat{e}(X) = P(T = 1|X)$ 
  - **Supervised learning:** predicting a known label T based on observed covariates X.
  - Conventionally, use logistic regression
- Matching pairs by distance between propensity score:
 
$$Distance(X_i, X_j) \leq \epsilon$$

$$Distance(X_i, X_j) = |\hat{e}(X_i) - \hat{e}(X_j)|$$
- High dimensional challenge: transferred from matching to PS estimation



# Methods for Causal Inference

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# Inverse of Propensity Weighting (IPW)

- Why weighting with inverse of propensity score is helpful?
  - Propensity score induces the distribution bias on confounders X

$$e(X) = P(T = 1|X)$$

| Unit | $e(X)$ | $1 - e(X)$ | #units | #units<br>(T=1) | #units<br>(T=0) |
|------|--------|------------|--------|-----------------|-----------------|
| A    | 0.7    | 0.3        | 10     | 7               | 3               |
| B    | 0.6    | 0.4        | 50     | 30              | 20              |
| C    | 0.2    | 0.8        | 40     | 8               | 32              |

| Unit | #units<br>(T=1) | #units<br>(T=0) |
|------|-----------------|-----------------|
| A    | 10              | 10              |
| B    | 50              | 50              |
| C    | 40              | 40              |

Confounders  
are the same!

Distribution Bias

Reweighting by inverse of propensity score:

$$w_i = \frac{T_i}{e_i} + \frac{1 - T_i}{1 - e_i}$$

# Inverse of Propensity Weighting (IPW)

- Estimating ATE by IPW [1]:

$$w_i = \frac{T_i}{e_i} + \frac{1 - T_i}{1 - e_i}$$

$$ATE_{IPW} = \frac{1}{n} \sum_{i=1}^n \frac{T_i Y_i}{\hat{e}(X_i)} - \frac{1}{n} \sum_{i=1}^n \frac{(1 - T_i) Y_i}{1 - \hat{e}(X_i)}$$

- Interpretation: IPW creates a pseudo-population where the confounders are the same between treated and control groups.
- Why does this work? Consider  $\frac{1}{n} \sum_{i=1}^n \frac{T_i Y_i}{\hat{e}(X_i)}$

# Inverse of Propensity Weighting (IPW)

- If:  $\hat{e}(X) = e(X)$ , the *true propensity score*

$$E \left\{ \frac{TY}{e(X)} \right\} = E \left\{ \frac{TY_1}{e(X)} \right\} = E \left[ E \left\{ \frac{TY_1}{e(X)} | Y_1, X \right\} \right] \quad (1) \quad \textcolor{green}{Y = T * Y_1 + (1 - T) * Y_0}$$

$$= E \left\{ \frac{Y_1}{e(X)} E(T|Y_1, X) \right\} = E \left\{ \frac{Y_1}{e(X)} \textcolor{blue}{E(T|X)} \right\} \quad (2) \quad \textcolor{red}{T \perp (Y_1, Y_0) | X}$$

$$= E \left\{ \frac{Y_1}{e(X)} e(X) \right\} = E(Y_1) \quad (3) \quad \textcolor{blue}{e(X) = E(T|X)}$$

- Similarly:  $E \left\{ \frac{(1 - T)Y}{1 - e(X)} \right\} = E(Y_0)$   $ATE = E[Y(1) - Y(0)]$

# Inverse of Propensity Weighting (IPW)

- **If:**  $\hat{e}(X) = e(X)$ , the *true propensity score*, the IPW estimator is *unbiased*

$$ATE_{IPW} = \frac{1}{n} \sum_{i=1}^n \frac{T_i Y_i}{\hat{e}(X_i)} - \frac{1}{n} \sum_{i=1}^n \frac{(1 - T_i) Y_i}{1 - \hat{e}(X_i)} = E(Y_1 - Y_0)$$

- Widely used in many applications
- **But** requires the propensity score model is correct
- High variance when  $e$  is close to 0 or 1

# Methods for Causal Inference

- **Matching**
- **Propensity Score Based Methods**
  - Propensity Score Matching
  - Inverse of Propensity Weighting (IPW)
  - **Doubly Robust**
  - Data-Driven Variable Decomposition (D<sup>2</sup>VD)
- **Directly Confounder Balancing**
  - Entropy Balancing
  - Approximate Residual Balancing
  - Differentiated Confounder Balancing

# Doubly Robust

- Recap:  $ATE = E[Y(T = 1) - Y(T = 0)]$

- Simple outcome regression:

$$m_1 = E(Y|T = 1, X) \quad \text{and} \quad m_0 = E(Y|T = 0, X)$$

- Unbiased if the regression models are correct

- IPW estimator:

- Unbiased if the propensity score model is correct

- Doubly Robust [2]: combine both approaches

# Doubly Robust

$$m_0 = E(Y|T=0, X)$$

$$m_1 = E(Y|T=1, X)$$

- Estimating ATE with Doubly Robust estimator:

$$\begin{aligned} ATE_{DR} &= \frac{1}{n} \sum_{i=1}^n \left[ \frac{T_i Y_i}{\hat{e}(X_i)} - \frac{\{T_i - \hat{e}(X_i)\}}{\hat{e}(X_i)} \hat{m}_1(X_i) \right] \\ &\quad - \frac{1}{n} \sum_{i=1}^n \left[ \frac{(1 - T_i) Y_i}{1 - \hat{e}(X_i)} + \frac{\{T_i - \hat{e}(X_i)\}}{1 - \hat{e}(X_i)} \hat{m}_0(X_i) \right] \end{aligned}$$

- *Unbiased* if either **propensity score** or **regression** model is correct
- This property is referred to as *double robustness*

# Doubly Robust

- Theoretical Proof:

$$\begin{aligned}
 & E \left[ \frac{TY}{\hat{e}(X_i)} - \frac{\{T - \hat{e}(X_i)\}}{\hat{e}(X_i)} \hat{m}_1(X_i) \right] \\
 = & E \left[ \frac{TY_1}{\hat{e}(X_i)} - \frac{\{T - \hat{e}(X_i)\}}{\hat{e}(X_i)} \hat{m}_1(X_i) \right] \\
 = & E \left[ Y_1 + \frac{\{T - \hat{e}(X_i)\}}{\hat{e}(X_i)} \{Y_1 - \hat{m}_1(X_i)\} \right] \\
 = & E(Y_1) + \boxed{E \left[ \frac{\{T - \hat{e}(X_i)\}}{\hat{e}(X_i)} \{Y_1 - \hat{m}_1(X_i)\} \right]}
 \end{aligned}$$

# Doubly Robust

$$m_0 = E(Y|T=0, X)$$

$$m_1 = E(Y|T=1, X)$$

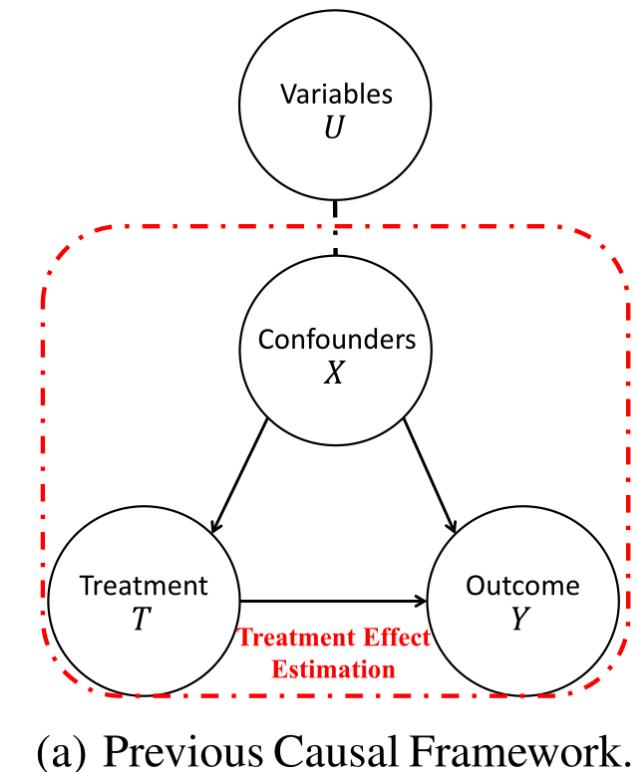
- Estimating ATE with Doubly Robust estimator:

$$\begin{aligned} ATE_{DR} &= \frac{1}{n} \sum_{i=1}^n \left[ \frac{T_i Y_i}{\hat{e}(X_i)} - \frac{\{T_i - \hat{e}(X_i)\}}{\hat{e}(X_i)} \hat{m}_1(X_i) \right] \\ &\quad - \frac{1}{n} \sum_{i=1}^n \left[ \frac{(1 - T_i) Y_i}{1 - \hat{e}(X_i)} + \frac{\{T_i - \hat{e}(X_i)\}}{1 - \hat{e}(X_i)} \hat{m}_0(X_i) \right] \end{aligned}$$

- *Unbiased if propensity score or regression model is correct*
- This property is referred to as *double robustness*
- But may be very biased if both models are incorrect

# Propensity Score based Methods

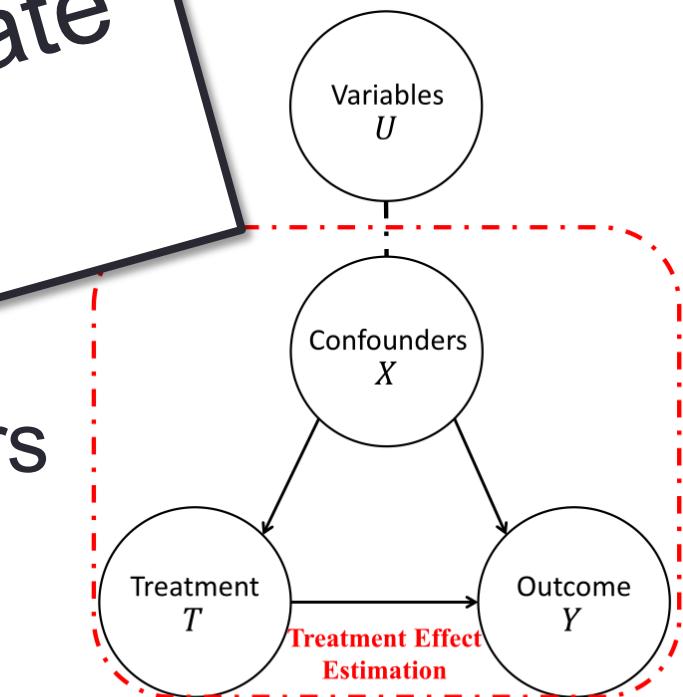
- Recap:
  - Propensity Score Matching
  - Inverse of Propensity Weighting
  - Doubly Robust
- Need to estimate propensity score
  - Treat all observed variables as confounders
  - In Big Data Era, High dimensional data
  - But, not all variables are confounders



# Propensity Score based Methods

- Recap:
  - Propensity Score Matching
  - Inverse of Propensity Weighting
  - Doubly Robust
- Need to
  - Treat all other variables as confounders
  - In Big Data setting, high dimensional data
  - But, not all variables are confounders

How to automatically separate  
the confounders?

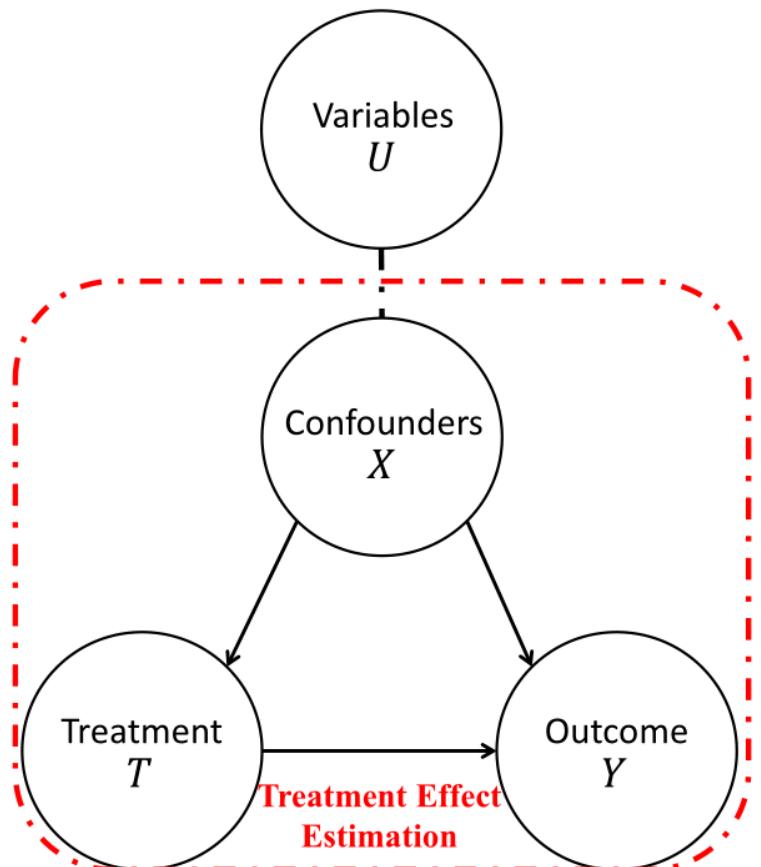


(a) Previous Causal Framework.

# Methods for Causal Inference

- Matching
- Propensity Score Based Methods
  - Propensity Score Matching
  - Inverse of Propensity Weighting (IPW)
  - Doubly Robust
  - Data-Driven Variable Decomposition (D<sup>2</sup>VD)
- Directly Confounder Balancing
  - Entropy Balancing
  - Approximate Residual Balancing
  - Differentiated Confounder Balancing (DCB)

# Inverse of Propensity Weighting (IPW)



(a) Previous Causal Framework.

- Treat all observed variables  $\mathbf{U}$  as confounders  $\mathbf{X}$

- Propensity Score Estimation:

$$e(\mathbf{U}) = p(T = 1|\mathbf{U}) = p(T = 1|\mathbf{X}) = e(\mathbf{X})$$

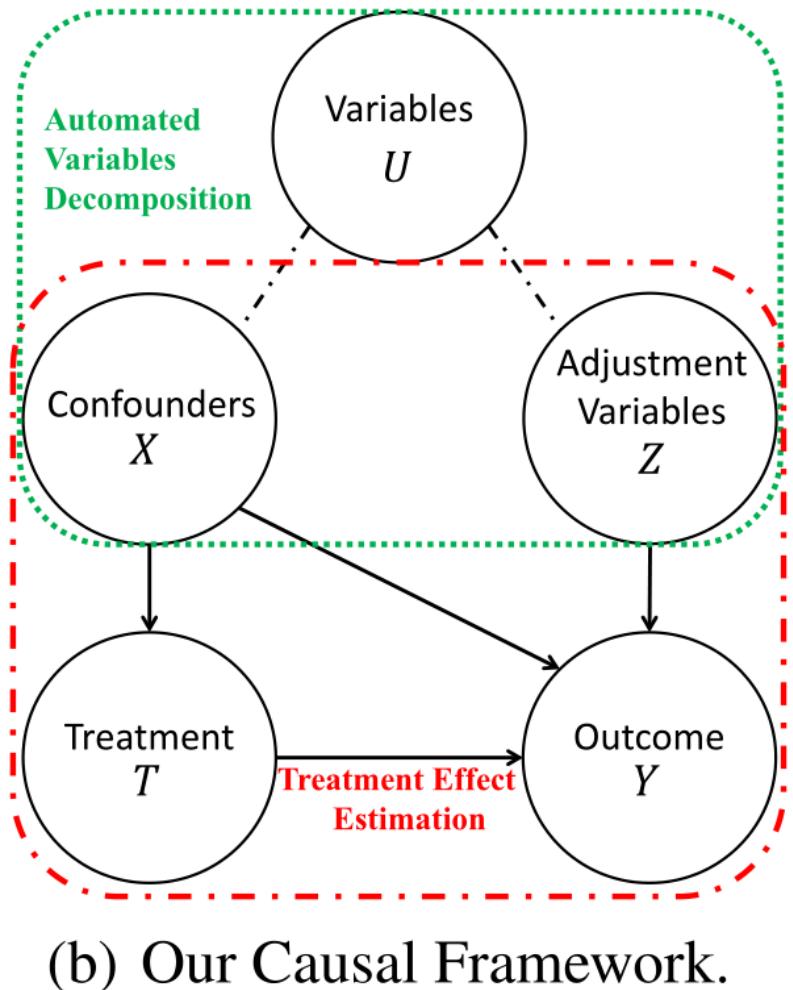
- Adjusted Outcome:

$$Y^* = Y^{obs} \cdot \frac{T - e(\mathbf{U})}{e(\mathbf{U}) \cdot (1 - e(\mathbf{U}))} = Y^{obs} \cdot \frac{T - e(\mathbf{X})}{e(\mathbf{X}) \cdot (1 - e(\mathbf{X}))}$$

- IPW ATE Estimator:

$$\widehat{ATE}_{IPW} = \widehat{E}(Y^*)$$

# Data-Driven Variable Decomposition (D<sup>2</sup>VD)



- **Separateness Assumption:**
  - All observed variables  $U$  can be decomposed into three sets: **Confounders  $X$** , **Adjustment Variables  $Z$** , and **Irrelevant variables  $I$**  (Omitted).
- **Propensity Score Estimation:**

$$e(\mathbf{X}) = p(T = 1 | \mathbf{X})$$
- **Adjusted Outcome:**

$$Y^+ = (Y^{obs} - \phi(\mathbf{Z})) \cdot \frac{T - e(\mathbf{X})}{e(\mathbf{X}) \cdot (1 - e(\mathbf{X}))}$$
- **Our D<sup>2</sup>VD ATE Estimator:**

$$\widehat{ATE}_{D^2VD} = \widehat{E}(Y^+)$$

# Data-Driven Variable Decomposition (D<sup>2</sup>VD)

- **Confounders Separation & ATE Estimation.**
- With our D<sup>2</sup>VD estimator:

$$\widehat{ATE}_{D^2VD} = \widehat{E}(Y^+) = E \left( (Y^{obs} - \phi(\mathbf{Z})) \cdot \frac{T - e(\mathbf{X})}{e(\mathbf{X}) \cdot (1 - e(\mathbf{X}))} \right)$$

- By minimizing following objective function:

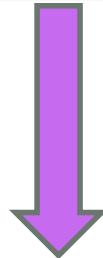
$$\text{minimize } \|Y^+ - h(\mathbf{U})\|^2.$$

- We can estimate the ATE as:

$$\widehat{ATE}_{D^2VD} = \widehat{E}(h(\mathbf{U}))$$

# Data-Driven Variable Decomposition (D<sup>2</sup>VD)

$$\text{minimize} \quad \|Y^+ - h(\mathbf{U})\|^2 \quad \text{Where} \quad Y^+ = \left( Y^{obs} - \phi(\mathbf{Z}) \right) \cdot \frac{T - e(\mathbf{X})}{e(\mathbf{X}) \cdot (1 - e(\mathbf{X}))}$$



$$e(\mathbf{X}) = \frac{1}{1 + \exp(-\mathbf{X}\beta)} \quad \phi(\mathbf{Z}) = \mathbf{Z}\alpha,$$

**Replace  $\mathbf{X}, \mathbf{Z}$  with  $\mathbf{U}$**        $h(\mathbf{U}) = \mathbf{U}\gamma,$

$$\begin{aligned} & \text{minimize} \quad \|(Y^{obs} - \mathbf{U}\alpha) \odot W(\beta) - \mathbf{U}\gamma\|_2^2, \quad \text{Where} \quad W(\beta) := \frac{T - e(\mathbf{U})}{e(\mathbf{U}) \cdot (1 - e(\mathbf{U}))} \\ & s.t. \quad \sum_{i=1}^m \log(1 + \exp((1 - 2T_i) \cdot U_i\beta)) < \tau, \\ & \quad \|\alpha\|_1 \leq \lambda, \quad \|\beta\|_1 \leq \delta, \quad \|\gamma\|_1 \leq \eta, \quad \|\alpha \odot \beta\|_2^2 = 0. \end{aligned}$$

$\alpha, \beta, \gamma$

- Adjustment variables:  $\mathbf{Z} = \{\mathbf{U}_i : \hat{\alpha}_i \neq 0\}$
- Confounders:  $\mathbf{X} = \{\mathbf{U}_i : \hat{\beta}_i \neq 0\}$
- Treatment Effect:  $\widehat{ATE}_{D^2VD} = E(\mathbf{U}\hat{\gamma})$

# Data-Driven Variable Decomposition (D<sup>2</sup>VD)

## Bias Analysis:

Our D<sup>2</sup>VD algorithm is unbiased to estimate causal effect

**THEOREM 1.** *Under assumptions 1-4, we have*

$$E(Y^+|X, Z) = E(Y(1) - Y(0)|X, Z).$$

## Variance Analysis:

The asymptotic variance of Our D<sup>2</sup>VD algorithm is smaller

**THEOREM 2.** *The asymptotic variance of our adjusted estimator  $\widehat{ATE}_{adj}$  is no greater than IPW estimator  $\widehat{ATE}_{IPW}$ :*

$$\sigma_{adj}^2 \leq \sigma_{IPW}^2.$$

# Data-Driven Variable Decomposition ( $D^2VD$ )

- OUR: *Data-Driven Variable Decomposition ( $D^2VD$ )*
- Baselines
  - *Directly Estimator (dir)*: ignores confounding bias
  - *IPW Estimator (IPW)*: treats all variables as confounders
  - *Doubly Robust Estimator (DR)*: IPW+regression
  - *Non-Separation Estimator ( $D^2VD-$ )*: no variables separation

# Data-Driven Variable Decomposition (D<sup>2</sup>VD)

- Dataset generation:
  - Sample size  $m=\{1000,5000\}$
  - Dimension of observed variables  $n=\{50,100,200\}$
  - Observed variables:  $\mathbf{U} = (\mathbf{X}, \mathbf{Z}, \mathbf{I})$   
 $\mathbf{x}_1, \dots, \mathbf{x}_{n_x}, \mathbf{z}_1, \dots, \mathbf{z}_{n_z}, \mathbf{i}_1, \dots, \mathbf{i}_{n_i} \stackrel{iid}{\sim} \mathcal{N}(0, 1),$
- Treatment: logistic and misspecified  
 $T_{logit} \sim Bernoulli(1/(1 + \exp(-\sum_{i=1}^{n_x} x_i)))$  and  
 $T_{missp} = 1 \text{ if } \sum_{i=1}^{n_x} x_i > 0.5, T_{missp} = 0 \text{ otherwise.}$
- Outcome:

$$Y = \sum_{j=\frac{n_x}{2}}^{n_x} \mathbf{x}_j \cdot \omega_j + \sum_{k=1}^{n_z} \mathbf{z}_k \cdot \rho_k + T + \mathcal{N}(0, 2),$$

# Data-Driven Variable Decomposition (D<sup>2</sup>VD)

- Dataset generation:

The true treatment effect in synthetic data is 1.

- Observed variables:  $\mathbf{U} = (\mathbf{X}, \mathbf{Z}, \mathbf{I})$   
 $\mathbf{x}_1, \dots, \mathbf{x}_{n_x}, \mathbf{z}_1, \dots, \mathbf{z}_{n_z}, \mathbf{i}_1, \dots, \mathbf{i}_{n_i} \stackrel{iid}{\sim} \mathcal{N}(0, 1),$
- Treatment: logistic and misspecified  
 $T_{logit} \sim Bernoulli(1/(1 + \exp(-\sum_{i=1}^{n_x} x_i)))$  and  
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- Outcome:

$$Y = \sum_{j=\frac{n_x}{2}}^{n_x} \mathbf{x}_j \cdot \omega_j + \sum_{k=1}^{n_z} \mathbf{z}_k \cdot \rho_k + T + \mathcal{N}(0, 2),$$

# Data-Driven Variable Decomposition (D<sup>2</sup>VD)

- Experimental Results on Synthetic Data:  $Bias = |\widehat{ATE} - ATE|$

| $T/m$                         | $n$                           | $n = 50$     |              |              |              | $n = 100$    |              |              |              | $n = 200$    |              |              |              |
|-------------------------------|-------------------------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
|                               |                               | Estimator    | Bias         | SD           | MAE          | RMSE         | Bias         | SD           | MAE          | RMSE         | Bias         | SD           | MAE          |
| $T = T_{logit}$<br>$m = 1000$ | $\widehat{ATE}_{dir}$         | 0.418        | 0.409        | 0.479        | 0.582        | 0.302        | 0.490        | 0.472        | 0.571        | 0.405        | 0.628        | 0.574        | 0.720        |
|                               | $\widehat{ATE}_{IPW + lasso}$ | 0.078        | 0.310        | 0.252        | 0.317        | 0.097        | 0.356        | 0.295        | 0.366        | 0.073        | 0.328        | 0.267        | 0.320        |
|                               | $\widehat{ATE}_{DR + lasso}$  | 0.060        | 0.181        | 0.152        | 0.189        | 0.067        | 0.190        | 0.155        | 0.199        | 0.081        | 0.181        | 0.169        | 0.190        |
|                               | $\widehat{ATE}_{D^2VD(-)}$    | 0.053        | 0.138        | 0.124        | 0.146        | 0.064        | 0.130        | 0.117        | 0.144        | <b>0.018</b> | 0.170        | 0.128        | 0.162        |
|                               | $\widehat{ATE}_{D^2VD}$       | <b>0.045</b> | <b>0.108</b> | <b>0.091</b> | <b>0.116</b> | <b>0.019</b> | <b>0.114</b> | <b>0.093</b> | <b>0.115</b> | 0.067        | <b>0.144</b> | <b>0.130</b> | <b>0.152</b> |
| $T = T_{logit}$<br>$m = 5000$ | $\widehat{ATE}_{dir}$         | 0.418        | 0.170        | 0.418        | 0.451        | 0.659        | 0.181        | 0.659        | 0.681        | 0.523        | 0.412        | 0.555        | 0.653        |
|                               | $\widehat{ATE}_{IPW + lasso}$ | 0.036        | 0.201        | 0.163        | 0.202        | 0.034        | 0.222        | 0.194        | 0.213        | <b>0.032</b> | 0.341        | 0.274        | 0.325        |
|                               | $\widehat{ATE}_{DR + lasso}$  | 0.051        | 0.079        | 0.071        | 0.094        | 0.106        | 0.075        | 0.114        | 0.127        | 0.055        | 0.084        | 0.086        | 0.096        |
|                               | $\widehat{ATE}_{D^2VD(-)}$    | 0.112        | 0.080        | 0.118        | 0.137        | 0.114        | 0.102        | 0.121        | 0.150        | 0.164        | 0.076        | 0.164        | 0.179        |
|                               | $\widehat{ATE}_{D^2VD}$       | <b>0.033</b> | <b>0.072</b> | <b>0.061</b> | <b>0.078</b> | <b>0.023</b> | <b>0.073</b> | <b>0.061</b> | <b>0.073</b> | 0.042        | <b>0.068</b> | <b>0.062</b> | <b>0.076</b> |
| $T = T_{missp}$<br>$m = 1000$ | $\widehat{ATE}_{dir}$         | 0.664        | 0.387        | 0.670        | 0.766        | 0.273        | 0.445        | 0.436        | 0.518        | 0.380        | 0.766        | 0.691        | 0.848        |
|                               | $\widehat{ATE}_{IPW + lasso}$ | 0.266        | 0.279        | 0.319        | 0.384        | 0.298        | 0.295        | 0.328        | 0.417        | 0.191        | 0.482        | 0.403        | 0.514        |
|                               | $\widehat{ATE}_{DR + lasso}$  | 0.138        | 0.187        | 0.174        | 0.231        | 0.253        | 0.197        | 0.269        | 0.320        | <b>0.050</b> | 0.218        | 0.170        | 0.222        |
|                               | $\widehat{ATE}_{D^2VD(-)}$    | 0.269        | 0.162        | 0.270        | 0.313        | 0.129        | 0.162        | 0.170        | 0.206        | 0.175        | 0.207        | 0.236        | 0.269        |
|                               | $\widehat{ATE}_{D^2VD}$       | <b>0.066</b> | <b>0.113</b> | <b>0.102</b> | <b>0.129</b> | <b>0.019</b> | <b>0.119</b> | <b>0.101</b> | <b>0.120</b> | 0.059        | <b>0.177</b> | <b>0.149</b> | <b>0.184</b> |
| $T = T_{missp}$<br>$m = 5000$ | $\widehat{ATE}_{dir}$         | 0.446        | 0.180        | 0.446        | 0.480        | 0.587        | 0.323        | 0.587        | 0.662        | 0.778        | 0.246        | 0.778        | 0.812        |
|                               | $\widehat{ATE}_{IPW + lasso}$ | 0.148        | 0.133        | 0.161        | 0.198        | 0.172        | 0.167        | 0.199        | 0.239        | 0.142        | 0.224        | 0.206        | 0.263        |
|                               | $\widehat{ATE}_{DR + lasso}$  | 0.119        | 0.073        | 0.123        | 0.139        | 0.100        | 0.067        | 0.107        | 0.120        | 0.127        | 0.079        | 0.127        | 0.148        |
|                               | $\widehat{ATE}_{D^2VD(-)}$    | 0.112        | 0.070        | 0.119        | 0.132        | 0.058        | <b>0.067</b> | 0.069        | 0.086        | 0.068        | 0.055        | 0.073        | 0.086        |
|                               | $\widehat{ATE}_{D^2VD}$       | <b>0.033</b> | <b>0.055</b> | <b>0.052</b> | <b>0.063</b> | <b>0.039</b> | 0.068        | <b>0.066</b> | <b>0.075</b> | <b>0.032</b> | <b>0.047</b> | <b>0.049</b> | <b>0.055</b> |

# Data

- 1. The direct estimator is failed under all settings.
- 2. IPW and DR estimators are good when  $T=T_{\text{logit}}$ , but poor when  $T=T_{\text{missp}}$ .
- 3. D<sup>2</sup>VD(-) has no variables separation, get similar results with DR estimator.
- 4. D<sup>2</sup>VD can improve accuracy and reduce variance for ATE estimation.

| $T/m$                                | n  | n = 50       |              |              |              | n = 100      |              |              |              | n = 200      |              |              |              |
|--------------------------------------|--|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
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| $T = T_{\text{missp}}$<br>$m = 5000$ | $\widehat{\text{ATE}}_{\text{dir}}$                | 0.446        | 0.180        | 0.446        | 0.480        | 0.587        | 0.323        | 0.587        | 0.662        | 0.778        | 0.246        | 0.778        | 0.812        |
|                                      | $\widehat{\text{ATE}}_{\text{IPW} + \text{lasso}}$ | 0.148        | 0.133        | 0.161        | 0.198        | 0.172        | 0.167        | 0.199        | 0.239        | 0.142        | 0.224        | 0.206        | 0.263        |
|                                      | $\widehat{\text{ATE}}_{\text{DR} + \text{lasso}}$  | 0.119        | 0.073        | 0.123        | 0.139        | 0.100        | 0.067        | 0.107        | 0.120        | 0.127        | 0.079        | 0.127        | 0.148        |
|                                      | $\widehat{\text{ATE}}_{\text{D}^2\text{VD}(-)}$    | 0.112        | 0.070        | 0.119        | 0.132        | 0.058        | <b>0.067</b> | 0.069        | 0.086        | 0.068        | 0.055        | 0.073        | 0.086        |
|                                      | $\widehat{\text{ATE}}_{\text{D}^2\text{VD}}$       | <b>0.033</b> | <b>0.055</b> | <b>0.052</b> | <b>0.063</b> | <b>0.039</b> | 0.068        | <b>0.066</b> | <b>0.075</b> | <b>0.032</b> | <b>0.047</b> | <b>0.049</b> | <b>0.055</b> |

# Data-Driven Variable Decomposition (D<sup>2</sup>VD)

- Experimental Results on Synthetic Data:

Table 3: Separation results of confounders  $\mathbf{X}$  and adjustment variables  $\mathbf{Z}$ . The closer to  $\mathbf{1}$  for TPR and TNR is better.

|            |              | $T = T_{\text{logit}}$ |       |           |       |           |       |
|------------|--------------|------------------------|-------|-----------|-------|-----------|-------|
|            |              | $n = 50$               |       | $n = 100$ |       | $n = 200$ |       |
| $m$        |              | TPR                    | TNR   | TPR       | TNR   | TPR       | TNR   |
| $m = 1000$ | $\mathbf{X}$ | 1.000                  | 0.917 | 0.977     | 0.948 | 0.966     | 0.906 |
|            | $\mathbf{Z}$ | 1.000                  | 0.973 | 1.000     | 0.983 | 1.000     | 0.984 |
| $m = 5000$ | $\mathbf{X}$ | 1.000                  | 0.923 | 1.000     | 0.887 | 0.994     | 0.989 |
|            | $\mathbf{Z}$ | 1.000                  | 0.975 | 1.000     | 0.987 | 1.000     | 0.994 |

| $T = T_{\text{missp}}$ |              |       |       |       |       |       |       |
|------------------------|--------------|-------|-------|-------|-------|-------|-------|
| $m$                    |              | TPR   | TNR   | TPR   | TNR   | TPR   | TNR   |
| $m = 1000$             | $\mathbf{X}$ | 1.000 | 0.844 | 0.997 | 0.866 | 0.867 | 0.977 |
|                        | $\mathbf{Z}$ | 1.000 | 0.982 | 1.000 | 0.987 | 1.000 | 0.983 |
| $m = 5000$             | $\mathbf{X}$ | 1.000 | 0.843 | 1.000 | 0.837 | 0.998 | 0.965 |
|                        | $\mathbf{Z}$ | 1.000 | 0.986 | 1.000 | 0.990 | 1.000 | 0.994 |

TPR: true positive rate  
TNR: true negative rate

Our D<sup>2</sup>VD algorithm can precisely separate the confounders and adjustment variables.

# Experiments on Real World Data



- **Dataset Description:**
  - Online advertising campaign (**LONGCHAMP**)
  - Users Feedback: 14,891 LIKE; 93,108 DISLIKE
  - 56 Features for each user
    - Age, gender, #friends, device, user setting on WeChat

- **Experimental Setting:**
    - Outcome  $Y$ : users feedback
    - Treatment  $T$ : one feature
    - Observed Variables  $U$ : other features
- $\leftarrow$   $Y = 1$ , if LIKE  
 $Y = 0$ , if DISLIKE

# Experiments Results

- ATE Estimation.

| No. | Features                           | $\widehat{ATE}_{D^2VD}$ (SD) | $\widehat{ATE}_{IPW}$ (SD) | $\widehat{ATE}_{DR}$ (SD) | $ATE_{matching}$ |
|-----|------------------------------------|------------------------------|----------------------------|---------------------------|------------------|
| 1   | No. friends (> 166)                | 0.295 (0.018)                | 0.240 (0.026)              | 0.297(0.021)              | 0.276            |
| 2   | Age (> 33)                         | -0.284 (0.014)               | -0.235 (0.029)             | -0.302(0.068)             | -0.263           |
| 3   | Share Album to Strangers           | 0.229 (0.030)                | 0.236 (0.030)              | -0.034(0.021)             | n/a              |
| 4   | With Online Payment                | 0.226 (0.019)                | 0.260 (0.029)              | 0.244(0.028)              | n/a              |
| 5   | With High-Definition Head Portrait | 0.218 (0.028)                | 0.203 (0.032)              | 0.237(0.046)              | n/a              |
| 6   | With WeChat Album                  | 0.191 (0.014)                | 0.237 (0.021)              | 0.097(0.050)              | n/a              |
| 7   | With Delicacy Plugin               | 0.124 (0.038)                | -0.253 (0.037)             | 0.067(0.051)              | 0.099            |
| 8   | Device (iOS)                       | 0.100 (0.024)                | 0.206 (0.012)              | 0.060(0.021)              | 0.085            |
| 9   | Add friends by Drift Bottle        | -0.098 (0.012)               | 0.016 (0.019)              | -0.115(0.015)             | -0.032           |
| 10  | Gender (Male)                      | -0.073 (0.017)               | -0.240 (0.029)             | 0.065(0.055)              | -0.097           |

1. Our D<sup>2</sup>VD estimator evaluate the ATE more accuracy.
2. Our D<sup>2</sup>VD estimator can reduce the variance of estimated ATE.
3. Younger Ladies are with higher probability to like the LONGCHAMP ads.

# Experiments Results

- Variables Decomposition.

Table 4: Confounders and adjusted variables when we set feature “Add friends by Shake” as treatment.

| Confounders                         | Adjustment Variables |
|-------------------------------------|----------------------|
| Add friends by Drift Bottle         | No. friends          |
| Add friends by People Nearby        | Age                  |
| Add friends by QQ Contacts          | With WeChat Album    |
| Without Friends Confirmation Plugin | Device               |

1. The confounders are many other ways for adding friends on WeChat.
2. The adjustment variables have significant effect on outcome.
3. Our D<sup>2</sup>VD algorithm can precisely separate the confounders and adjustment variables.

# Summary: Propensity Score based Methods

- Propensity Score Matching (PSM):
  - Units matching by their propensity score
- Inverse of Propensity Weighting (IPW):
  - Units reweighted by inverse of propensity score
- Doubly Robust (DR):
  - Combing IPW and regression
- **Data-Driven Variable Decomposition (D<sup>2</sup>VD):**
  - Automatically separate the confounders and adjustment variables
  - Confounder: estimate propensity score for IPW
  - Adjustment variables: regression on outcome for reducing variance
  - Improving accuracy and reducing variance on treatment effect estimation
- **But, these methods need propensity score model is correct**

$$e(X) = P(T = 1|X)$$

Treat all observed variables as confounder, ignoring non-confounders

# Methods for Causal Inference

- **Matching**
- **Propensity Score Based Methods**
  - Propensity Score Matching
  - Inverse of Propensity Weighting (IPW)
  - Doubly Robust
  - Data-Driven Variable Decomposition (D<sup>2</sup>VD)
- **Directly Confounder Balancing**
  - Entropy Balancing
  - Approximate Residual Balancing
  - Differentiated Confounder Balancing (DCB)

# Causal Inference with Observational Data

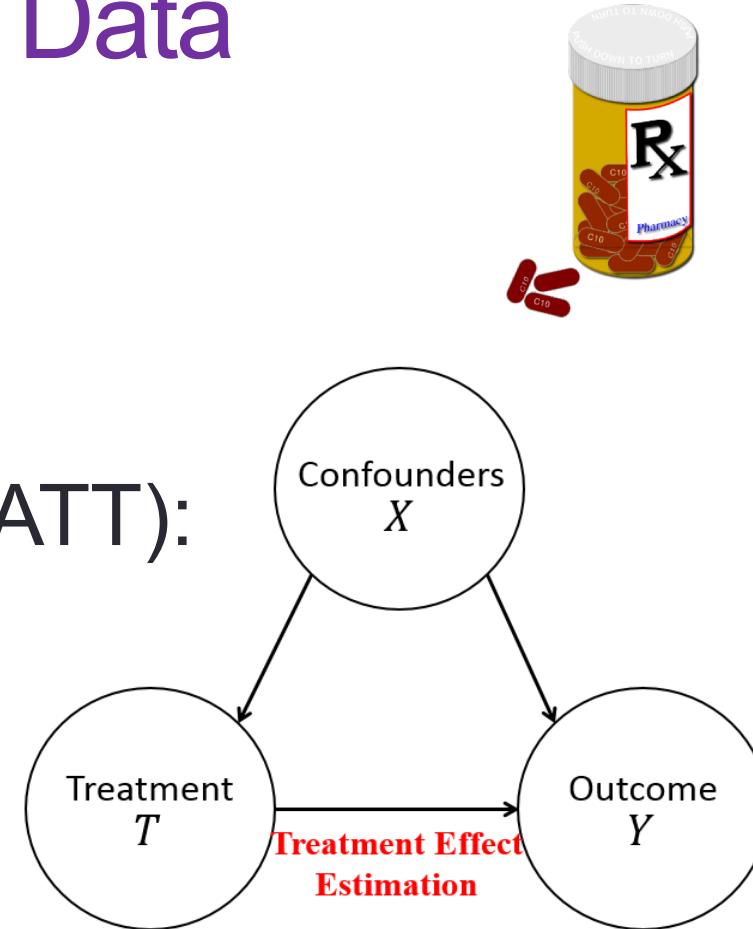
- Average Treatment Effect (ATE):

$$ATE = E[Y(T = 1) - Y(T = 0)]$$

- Average Treatment effect on the Treated (ATT):

$$ATT = E[Y(1)|T = 1] - E[Y(0)|T = 1]$$

- Two key points:
  - Changing T ( $T=1$  and  $T=0$ )
  - Keeping everything else (Confounder X) constant



# Causal Inference with Observational Data

- Average Treatment Effect (ATE):

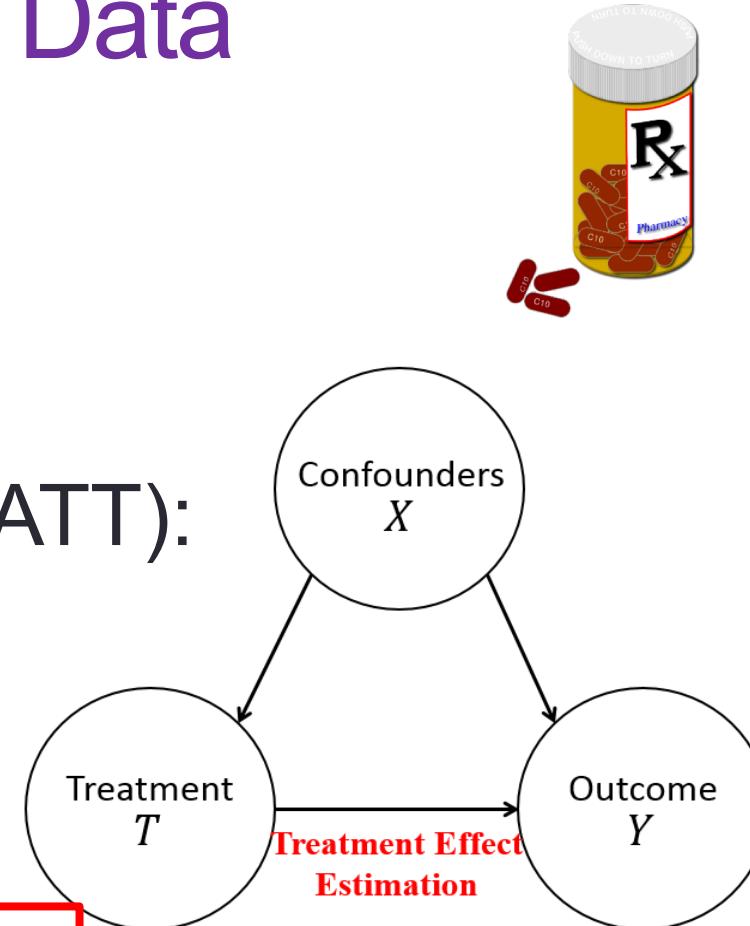
$$ATE = E[Y(T = 1) - Y(T = 0)]$$

- Average Treatment effect on the Treated (ATT):

$$ATT = E[Y(1)|T = 1] - E[Y(0)|T = 1]$$

- Two key points:

Balancing Confounders' Distribution



# Directly Confounder Balancing

- Recap: Propensity score based methods
  - Sample reweighting for **confounder balancing**
  - But, need propensity score model is correct
  - Weights would be very large if propensity score is close to 0 or 1
- Can we directly learn sample weight that can balance confounders' distribution between treated and control?

$$w_i = \frac{T_i}{e_i} + \frac{1 - T_i}{1 - e_i}$$

Yes!

# Directly Confounder Balancing

- **Motivation:** The collection of all the moments of variables uniquely determine their distributions.
- **Methods:** Learning sample weights by directly balancing confounders' moments as follows

$$\min_W \|\bar{\mathbf{X}}_t - \mathbf{X}_c^T W\|_2^2$$

The first moments of X  
on the **Treated Group**

The first moments of X  
on the **Control Group**

With moments, the sample weights can be learned  
without any model specification.

# Directly Confounder Balancing

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- **Methods:** Learning sample weights by directly balancing confounders' moments as follows

$$\min_W \|\bar{\mathbf{X}}_t - \mathbf{X}_c^T W\|_2^2$$

The first moments of X  
on the **Treated Group**

The first moments of X  
on the **Control Group**

- Estimating ATT by:  $\widehat{ATT} = \sum_{i:T_i=1} \frac{1}{n_t} Y(1) - \sum_{j:T_j=0} W_j Y(0)$

# Entropy Balancing

$$\begin{aligned} \min_W \quad & W \log(W) \\ s.t. \quad & \|\bar{\mathbf{X}}_t - \mathbf{X}_c^T W\|_2^2 = 0 \\ & \sum_{i=1}^n W_i = 1, W \succeq 0 \end{aligned}$$

- Maximum the entropy of sample weights  $W$
- Directly confounder balancing by sample weights  $W$
- But, treat all variables as confounders and balance them equally

# Approximate Residual Balancing

- 1. compute approximate balancing weights  $W$  as

$$W = \operatorname{argmin}_W \left\{ (1 - \zeta) \|W\|_2^2 + \zeta \left\| \bar{X}_t - \mathbf{X}_c^\top W \right\|_\infty^2 \text{ s.t. } \sum_{\{i:T_i=0\}} W_i = 1 \text{ and } W_i \geq 0 \right\}$$

- 2. Fit  $\beta_c$  in the linear model using a lasso or elastic net,

$$\hat{\beta}_c = \operatorname{argmin}_{\beta} \left\{ \sum_{\{i:W_i=0\}} \left( Y_i^{\text{obs}} - X_i \cdot \beta \right)^2 + \lambda ((1 - \alpha) \|\beta\|_2^2 + \alpha \|\beta\|_1) \right\}$$

- 3. Estimate the ATT as

$$\widehat{ATT} = \bar{Y}_t - \left( \bar{X}_t \cdot \hat{\beta}_c + \sum_{\{i:T_i=0\}} W_i (Y_i^{\text{obs}} - X_i \cdot \hat{\beta}_c) \right)$$

- Double Robustness: Exact confounder balancing or regression is correct.
- But, treats all variables as confounders and balance them equally

# Directly Confounder Balancing

- Recap:
  - *Entropy Balancing, Approximate Residual Balancing etc.*
  - Moments uniquely determine variables' distribution
  - Learning sample weights by balancing confounders' moments

$$\min_W \|\bar{\mathbf{X}}_t - \mathbf{X}_c^T W\|_2^2$$

The first moments of X  
on the **Treated Group**

The first moments of X  
on the **Control Group**

- But, treat all variables as confounders, and balance them equally
- Different confounders make different confounding bias

# Directly Confounder Balancing

- Recap:
    - *Entropy Balancing, Approximate Residual Balancing*, etc.
    - Moments uniquely determine variables'
    - Learning sample weights by moments
  - But, treat all variables as confounders, and balance them equally
  - Different confounders make different confounding bias
- How to differentiated confounders and their bias?
- The first moments of X on the **Control Group**

# Methods for Causal Inference

- **Matching**
- **Propensity Score Based Methods**
  - Propensity Score Matching
  - Inverse of Propensity Weighting (IPW)
  - Doubly Robust
  - Data-Driven Variable Decomposition (D<sup>2</sup>VD)
- **Directly Confounder Balancing**
  - Entropy Balancing
  - Approximate Residual Balancing
  - **Differentiated Confounder Balancing (DCB)**

# Differentiated Confounder Balancing

- **Ideas**: simultaneously learn *confounder weights*  $\beta$  and *sample weights*  $W$ .

$$\min \quad \underline{(\beta^T \cdot (\bar{\mathbf{X}}_t - \mathbf{X}_c^T W))}^2$$

- **Confounder weights** determine which variable is confounder and its contribution on confounding bias.
- **Sample weights** are designed for confounder balancing.

How to learn the these weights?

# Confounder Weights Learning

- General relationship among  $X$ ,  $T$ , and  $Y$ :

$$Y = f(\mathbf{X}) + T \cdot g(\mathbf{X}) + \epsilon \quad \rightarrow \quad \begin{aligned} ATT &= E(g(\mathbf{X}_t)) \\ Y(0) &= f(\mathbf{X}) + \epsilon \end{aligned}$$

$$\begin{aligned} f(\mathbf{X}) &= \mathbf{a}_1 \mathbf{X} + \sum_{ij} a_{ij} X_i X_j + \sum_{ijk} a_{ijk} X_i X_j X_k + \cdots + R_n(\mathbf{X}) \\ &= \alpha \mathbf{M}. \end{aligned} \quad \mathbf{M} = (\mathbf{X}, X_i X_j, X_i X_j X_k, \dots).$$

Confounder weights

Confounding bias

$$\widehat{ATT} = ATT + \sum_{k=1}^p \alpha_k \left( \sum_{i:T_i=1} \frac{1}{n_t} M_{i,k} - \sum_{j:T_j=0} W_j M_{j,k} \right) + \phi(\epsilon).$$

If  $\alpha_k = 0$ , then  $M_k$  is not confounder, no need to balance.  
 Different confounders have different confounding weights.

# Confounder Weights Learning

## Propositions:

- In observational studies, **not all** observed variables are confounders, and different confounders make **unequal** confounding bias on ATT with their own weights.
- The **confounder weights** can be learned by regressing potential outcome  $Y(0)$  on augmented variables  $M$ .

$$\mathbf{M} = (\mathbf{X}, X_i X_j, X_i X_j X_k, \dots).$$

# Sample Weights Learning

$$\mathbf{M} = (\mathbf{X}, X_i X_j, X_i X_j X_k, \dots).$$

- Any variable's distribution can be uniquely determined by the collection of all its **moments**.
- Learning the **sample weights  $W$**  by directly confounder balancing with confounders' moments.

$$\min \quad (\beta^T \cdot (\bar{\mathbf{M}}_t - \mathbf{M}_c^T W))^2$$

Confounders' moments  
on the **Treated Group**

Confounders' moments  
on the **Control Group**

With moments, the sample weights can be learned  
without any model specification.

# Differentiated Confounder Balancing

- Objective Function

$$\begin{aligned} \min \quad & \left( \beta^T \cdot (\bar{\mathbf{M}}_t - \mathbf{M}_c^T W) \right)^2 + \lambda \sum_{j:T_j=0} (1 + W_j) \cdot (Y_j - M_j \cdot \beta)^2, \\ \text{s.t.} \quad & \|W\|_2^2 \leq \delta, \quad \|\beta\|_2^2 \leq \mu, \quad \|\beta\|_1 \leq \nu, \quad \mathbf{1}^T W = 1 \quad \text{and} \quad W \succeq 0 \end{aligned}$$

The ENT[3] and ARB[4] algorithms are **special case** of our DCB algorithm by **setting the confounder weights as unit vector**.

**Our DCB algorithm is more generalize for treatment effect estimation.**

# Differentiated Confounder Balancing

- Algorithm

---

**Algorithm 1** Differentiated Confounder Balancing (DCB)

---

**Input:** Tradeoff parameters  $\lambda > 0$ ,  $\delta > 0$ ,  $\mu > 0$ ,  $\nu > 0$ , Augmented Variables Matrix on treat units  $\mathbf{M}_t$ , Augmented Variables Matrix on control units  $\mathbf{M}_c$  and Outcome  $Y$ .

**Output:** Confounder Weights  $\beta$  and Sample Weights  $W$

- 1: Initialize Confounder Weights  $\beta^{(0)}$  and Sample Weights  $W^{(0)}$
  - 2: Calculate the current value of  $\mathcal{J}(W, \beta)^{(0)} = \mathcal{J}(W^{(0)}, \beta^{(0)})$  with Equation (11)
  - 3: Initialize the iteration variable  $t \leftarrow 0$
  - 4: **repeat**
  - 5:     $t \leftarrow t + 1$
  - 6:    Update  $\beta^{(t)}$  by solving  $\mathcal{J}(\beta^{(t-1)})$  in Equation (12)
  - 7:    Update  $W^{(t)}$  by solving  $\mathcal{J}(W^{(t-1)})$  in Equation (13)
  - 8:    Calculate  $\mathcal{J}(W, \beta)^{(t)} = \mathcal{J}(W^{(t)}, \beta^{(t)})$
  - 9: **until**  $\mathcal{J}(W, \beta)^{(t)}$  converges or max iteration is reached
  - 10: **return**  $\beta, W$ .
- 

$$\begin{aligned}\mathcal{J}(\beta) &= (\beta^T \cdot (\bar{\mathbf{M}}_t - \mathbf{M}_c^T W))^2 + \mu \|\beta\|_2^2 + \nu \|\beta\|_1 \quad (12) \\ &\quad + \lambda \sum_{j:T_j=0} (1 + W_j) \cdot (Y_j - M_j \cdot \beta)^2\end{aligned}$$

$$\begin{aligned}\mathcal{J}(W) &= (\beta^T \cdot (\bar{\mathbf{M}}_t - \mathbf{M}_c^T W))^2 + \delta \|W\|_2^2 \quad (13) \\ &\quad + \lambda \sum_{j:T_j=0} (1 + W_j) \cdot (Y_j - M_j \cdot \beta)^2, \\ \text{s.t. } & \mathbf{1}^T W = 1 \text{ and } W \succeq 0.\end{aligned}$$



In each iteration, we first update  $\beta$  by fixing  $W$ , and then update  $W$  by fixing  $\beta$

- Training Complexity:  $O(np)$ 
  - $n$ : sample size,  $p$ : dimensions of variables

# Experiments

- Experimental Tasks:
  - Robustness Test (high-dimensional and noisy)
  - Accuracy Test (real world dataset)
  - Predictive Power Test (real ad application)

# Experiments

- Baselines:
  - **Directly Estimator**: comparing average outcome between treated and control units.
  - **IPW Estimator [1]**: reweighting via inverse of propensity score
  - **Doubly Robust Estimator [2]**: IPW + regression method
  - **Entropy Balancing Estimator [3]**: directly confounder balancing with entropy loss
  - **Approximate Residual Balancing [4]**: confounder balancing + regression
- Evaluation Metric:

$$\begin{aligned}
 Bias &= \left| \frac{1}{K} \sum_{k=1}^K \widehat{ATT}_k - ATT \right| \\
 SD &= \sqrt{\frac{1}{K} \sum_{k=1}^K (\widehat{ATT}_k - \frac{1}{K} \sum_{k=1}^K \widehat{ATT}_k)^2} \\
 MAE &= \frac{1}{K} \sum_{k=1}^K |\widehat{ATT}_k - ATT| \\
 RMSE &= \sqrt{\frac{1}{K} \sum_{k=1}^K (\widehat{ATT}_k - ATT)^2}
 \end{aligned}$$

# Experiments - Robustness Test

- Dataset

➤ Sample size:  $n = \{2000, 5000\}$

➤ Variables' dimensions:  $p = \{50, 100\}$

➤ Observed Variables:  $\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_p)$

$$\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_p \stackrel{iid}{\sim} \mathcal{N}(0, 1),$$

➤ Treatment: from logistic function  $T_{logit}$  and misspecified function  $T_{missp}$

$$T_{logit} \sim Bernoulli(1/(1 + \exp(-\sum_{i=1}^{p \cdot r_c} s_c \cdot x_i + \mathcal{N}(0, 1)))), \text{ and}$$

$$T_{missp} = 1 \text{ if } \sum_{i=1}^{p \cdot r_c} s_c \cdot x_i + \mathcal{N}(0, 1) > 0, \quad T_{missp} = 0 \text{ otherwise}$$

- Confounding rate  $r_c$ : the ratio of confounders to all observed variables.
- Confounding strength  $s_c$ : the bias strength of confounders

➤ Outcome: from linear function  $Y_{linear}$  and nonlinear function  $Y_{nonlin}$

$$Y_{linear} = T + \sum_{j=1}^p \{I(mod(j, 2) \equiv 0) \cdot (\frac{j}{2} + T) \cdot \mathbf{x}_j\} + \mathcal{N}(0, 3),$$

$$Y_{nonlin} = T + \sum_{j=1}^p \{I(mod(j, 2) \equiv 0) \cdot (\frac{j}{2} + T) \cdot \mathbf{x}_j\} + \mathcal{N}(0, 3) \\ + \sum_{j=1}^{p-1} \{I(mod(j, 10) \equiv 1) \cdot \frac{p}{2} \cdot (x_j^2 + x_j \cdot x_{j+1})\},$$

# Experiments - Robustness Test

More results see our paper!

| $r_c$       | $n/p$                 | $n = 2000, p = 50$   |              |              | $n = 2000, p = 100$  |              |              |
|-------------|-----------------------|----------------------|--------------|--------------|----------------------|--------------|--------------|
|             |                       | Estimator            | Bias (SD)    | MAE          | RMSE                 | Bias (SD)    | MAE          |
| $r_c = 0.8$ | $\widehat{ATT}_{dir}$ | 51.06 (3.725)        | 51.06        | 51.19        | 143.0 (9.389)        | 143.0        | 143.3        |
|             | $\widehat{ATT}_{IPW}$ | 29.99 (4.048)        | 29.99        | 30.26        | 98.24 (8.462)        | 98.24        | 98.60        |
|             | $\widehat{ATT}_{DR}$  | 0.345 (0.253)        | 0.367        | 0.428        | 4.492 (0.333)        | 4.492        | 4.504        |
|             | $\widehat{ATT}_{ENT}$ | 15.06 (1.745)        | 15.06        | 15.16        | 63.02 (4.551)        | 63.02        | 63.19        |
|             | $\widehat{ATT}_{ARB}$ | 0.231 (0.645)        | 0.553        | 0.685        | 2.909 (0.491)        | 2.909        | 2.951        |
|             | $\widehat{ATT}_{DCB}$ | <b>0.003</b> (0.127) | <b>0.102</b> | <b>0.127</b> | <b>0.020</b> (0.135) | <b>0.114</b> | <b>0.136</b> |

- **Directly estimator** fails in all settings, since it ignores confounding bias.
- **IPW and DR estimators** make huge error when facing high dimensional variables or the model specifications are incorrect.
- **ENT and ARB estimators** have poor performance since they balance all variables equally.

# Experiments - Robustness Test

More results see our paper!

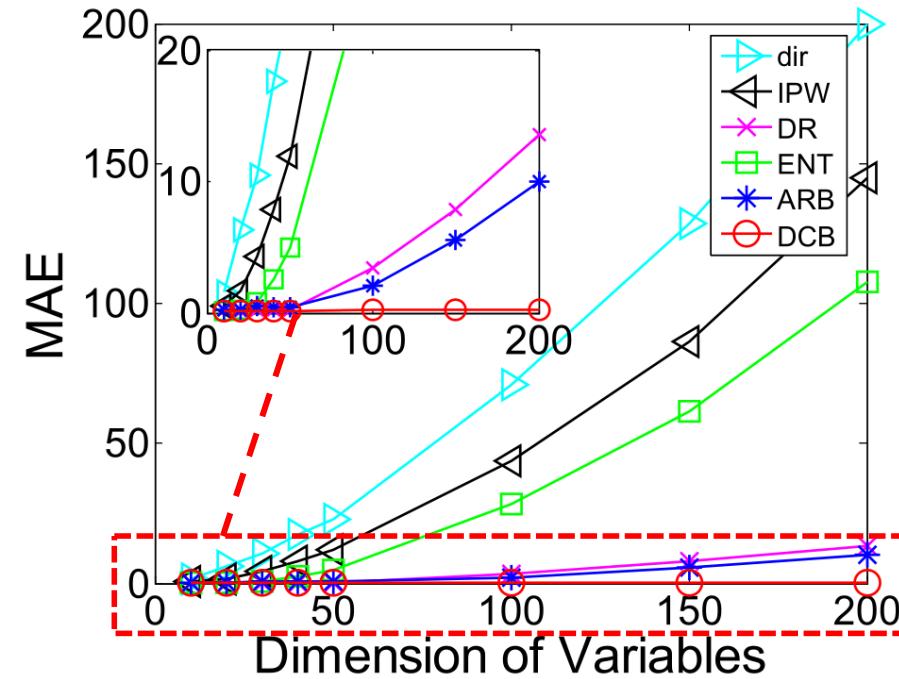
| $r_c$       | $n/p$                 | $n = 2000, p = 50$   |              |              | $n = 2000, p = 100$  |              |              |
|-------------|-----------------------|----------------------|--------------|--------------|----------------------|--------------|--------------|
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Our DCB estimator achieves significant improvements over the baselines in different settings.

Our DCB estimator is very **robust**!

# Experiments - Robustness Test

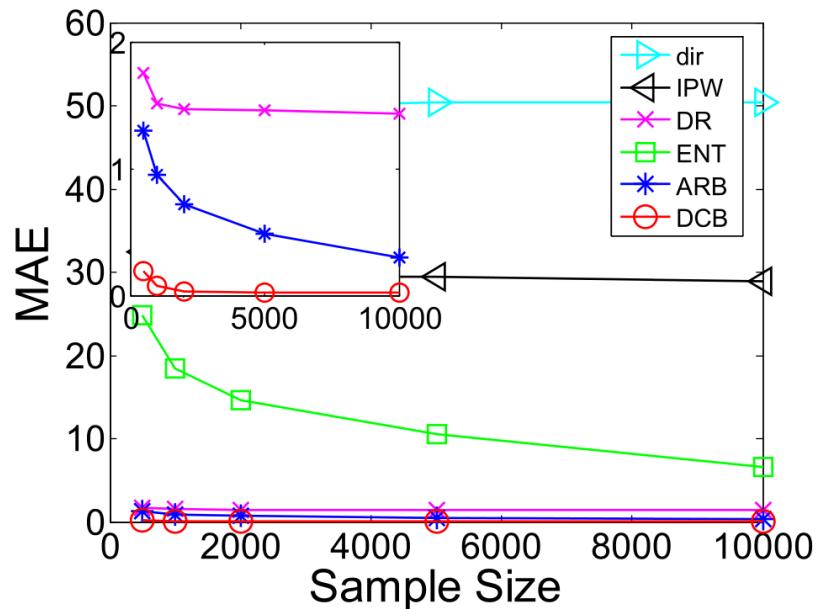
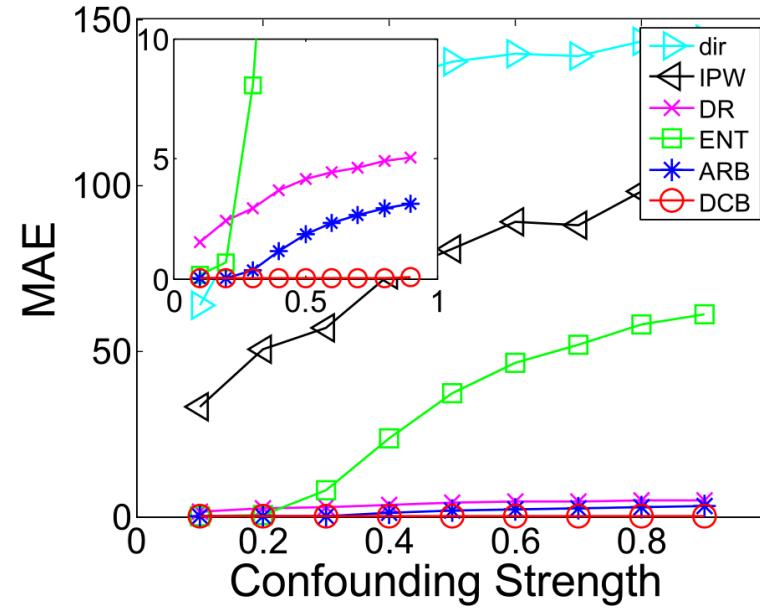
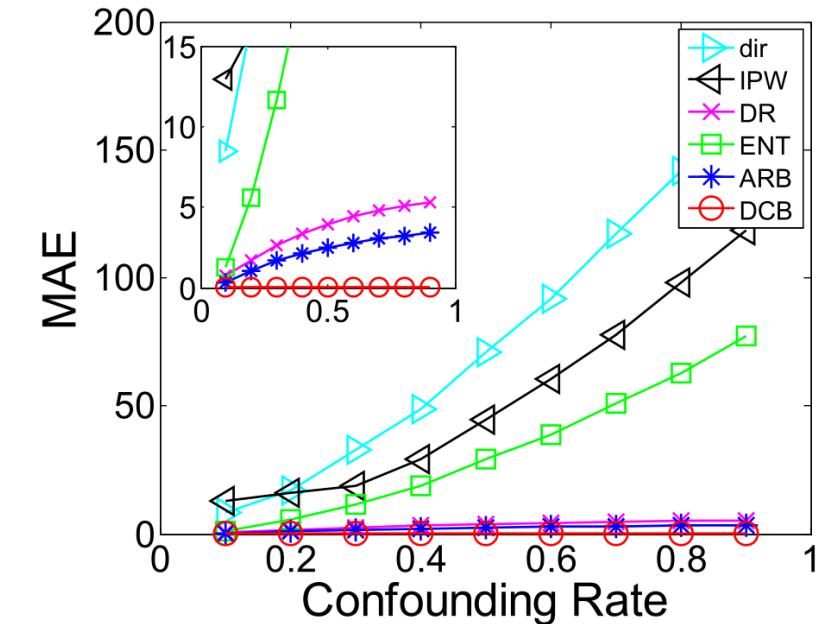
- Sample Size
- Dimension of variables
- Confounding rate
- Confounding strength



(b) dimension of variables  $p$

The MAE of our DCB estimator is consistent  
stable and small.

# Experiments - Robustness Test

(a) sample size  $n$ (d) confounding strength  $s_c$ (c) confounding rate  $r_c$ 

Our DCB algorithm is very **robust** for treatment effect estimation.

# Experiments - Accuracy Test

- LaLonde Dataset [5]: *Would the job training program increase people's earnings in the year of 1978?*
  - **Randomized experiments:** provide ground truth of treatment effect
  - **Observational studies:** check the performance of all estimators
- Experimental Setting:
  - **V-Raw:** variables set of 10 raw observed variables, including employment, education, age ethnicity and married status.
  - **V-INTERACTION:** variables set of raw variables, their pairwise one way interaction and their squared terms.

# Experiments - Accuracy Test

Results of ATT estimation

| Variables Set         | V-RAW           |             | V-INTERACTION   |             |
|-----------------------|-----------------|-------------|-----------------|-------------|
| Estimator             | $\widehat{ATT}$ | Bias (SD)   | $\widehat{ATT}$ | Bias (SD)   |
| $\widehat{ATT}_{dir}$ | -8471           | 10265 (374) | -8471           | 10265 (374) |
| $\widehat{ATT}_{IPW}$ | -4481           | 6275 (971)  | -4365           | 6159 (1024) |
| $\widehat{ATT}_{DR}$  | 1154            | 639 (491)   | 1590            | 204 (812)   |
| $\widehat{ATT}_{ENT}$ | 1535            | 259 (995)   | 1405            | 388 (787)   |
| $\widehat{ATT}_{ARB}$ | 1537            | 257 (996)   | 1627            | 167 (957)   |
| $\widehat{ATT}_{DCB}$ | 1958            | 164 (728)   | 1836            | 43 (716)    |

Our DCB estimator is more **accurate** than the baselines.

Our DCB estimator achieve a **better** confounder balancing under V-INTERACTION setting.

# Experiments - Predictive Power

2015



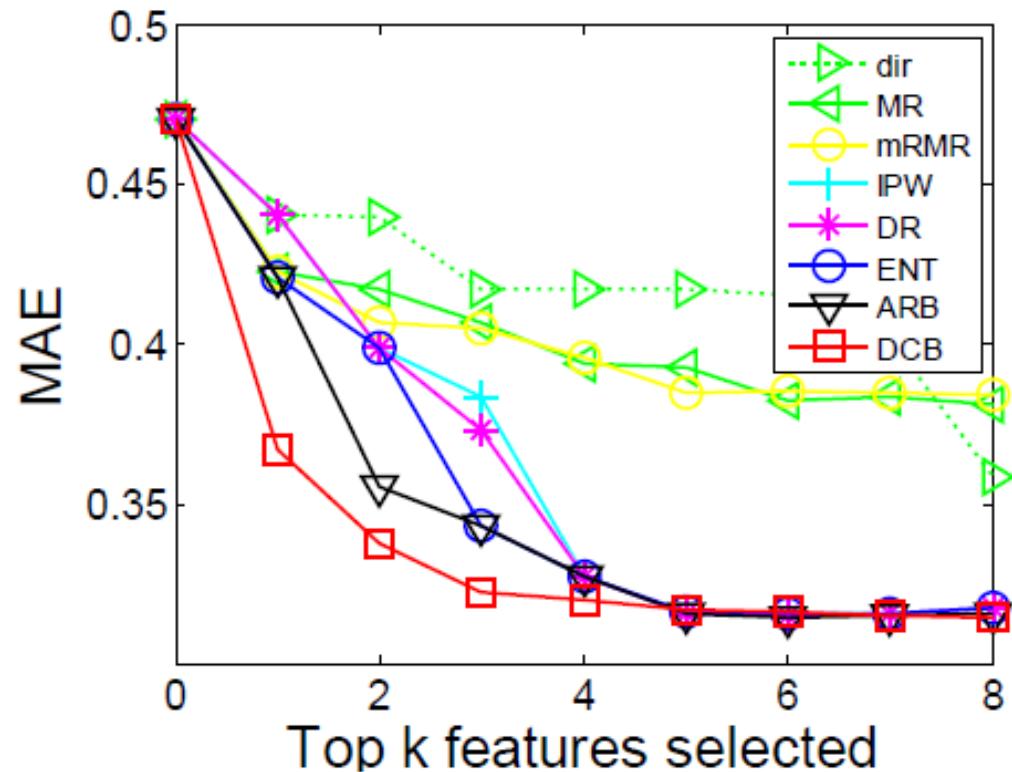
- Dataset Description:
  - Online advertising campaign (LONGCHAMP)
  - Users Feedback: 14,891 LIKE; 93,108 DISLIKE
  - 56 Features for each user
    - Age, gender, #friends, device, user setting on WeChat
- Experimental Setting:
  - Outcome Y: users feedback
  - Treatment T: one feature



$Y = 1$ , if LIKE  
 $Y = 0$ , if DISLIKE

Select the top k features with high causal effect for prediction

# Experiments - Predictive Power



- Two correlation-based feature selection baselines:
  - **MRel [6]**: maximum relevance
  - **mRMR [7]**: Maximum relevance and minimum redundancy.

- Our DCB estimator achieves the best prediction accuracy.
- Correlation based methods perform worse than causal methods.

# Summary: Directly Confounder Balancing

- **Motivation:** Moments can uniquely determine distribution
- Entropy Balancing
  - Confounder balancing with maximizing entropy of sample weights
- Approximate Residual Balancing
  - Combine confounder balancing and regression for doubly robust
- Treat all variables as confounders, and balance them equally
- But different confounders make different bias
- **Differentiated Confounder Balancing (DCB)**
  - Theoretical proof on the necessary of differentiation on confounders
  - Improving the accuracy and robust on treatment effect estimation

# Summary: Methods for Causal Inference

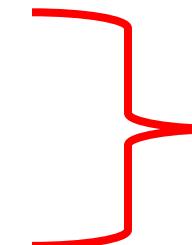
- **Matching** Limited to low-dimensional settings

- **Propensity Score Based Methods**

- Propensity Score Matching
- Inverse of Propensity Weighting (IPW)
- Doubly Robust
- Data-Driven Variable Decomposition (D<sup>2</sup>VD)

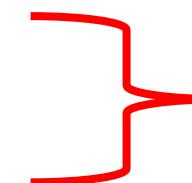
- **Directly Confounder Balancing**

- Entropy Balancing
- Approximate Residual Balancing
- Differentiated Confounder Balancing (DCB)



Treat all observed variables as confounder

Not all observed variables are confounders



Balance all confounder equally

Different confounders make different bias

# OUTLINE

PART I. Introduction to Causal Inference

PART II. Methods for Causal Inference

**PART III. Causally Regularized Machine Learning**

PART IV. Benchmark and Open Datasets

PART V. Conclusion and Discussion

# OUTLINE

PART I. Introduction to Causal Inference

PART II. Methods for Causal Inference

**PART III. Causally Regularized Machine Learning**

**Causal Inference for Stable Prediction**

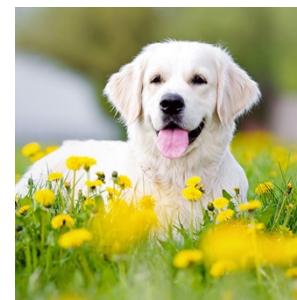
**Causal Inference for Offline Policy Evaluation**

PART IV. Benchmark and Open Datasets

PART V. Conclusion and Discussion

# Causal Inference for Stable Prediction

- CAN and CANNOT of predictive models



Yes



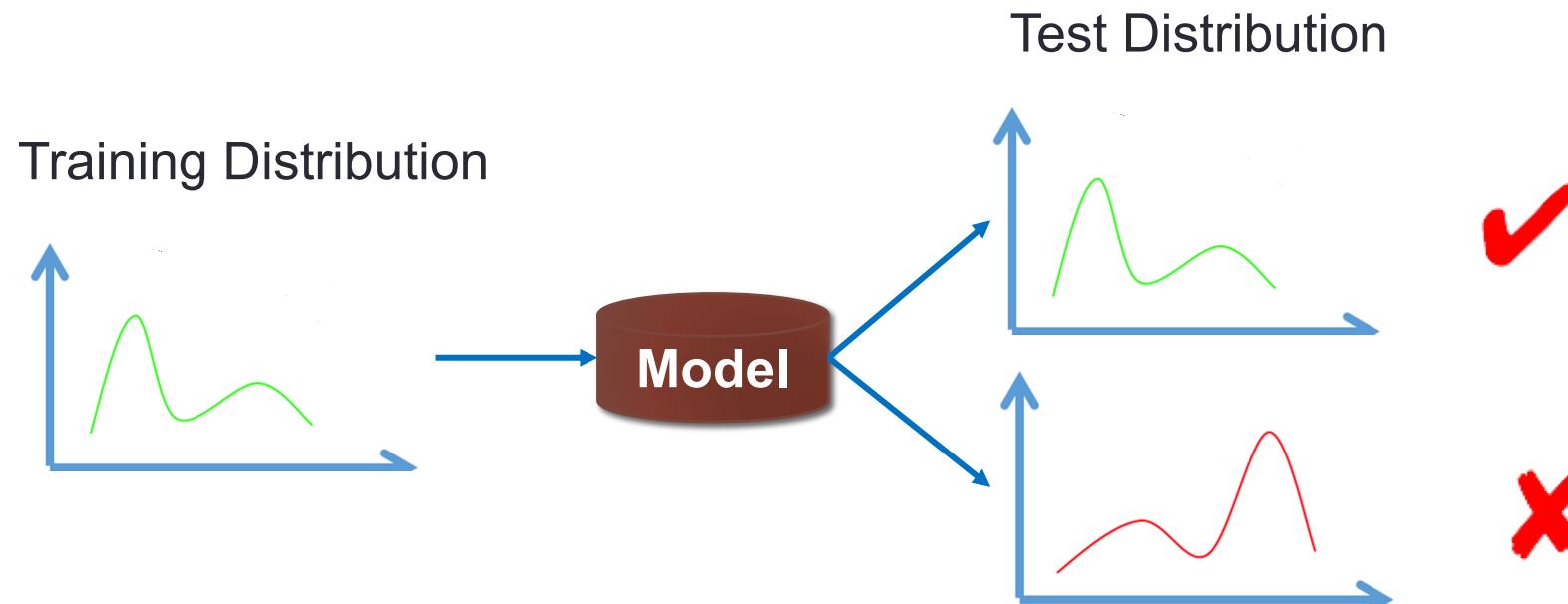
Maybe



No

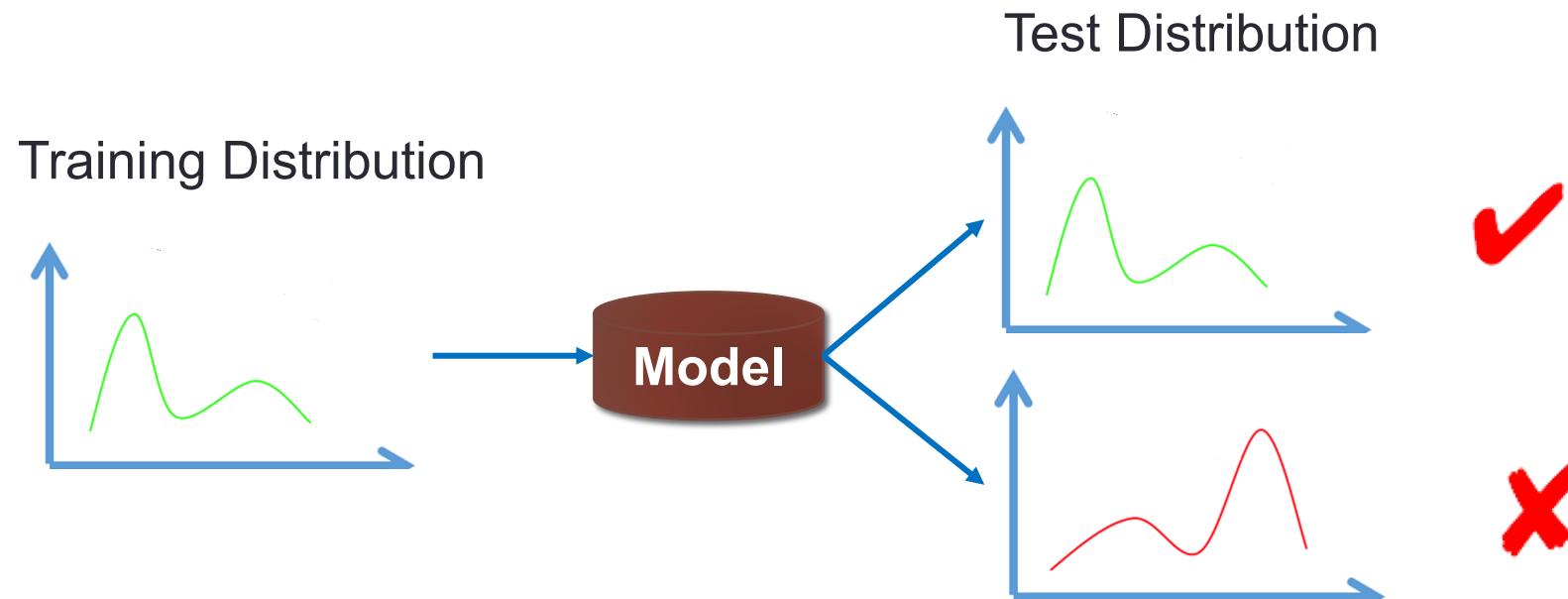
# Why they fail?

- The fault of Data
  - IID hypothesis (violated often)
  - Sample selection bias result in distribution shift
  - More serious in small-sample learning
  - We CANNOT control the generation of testing data



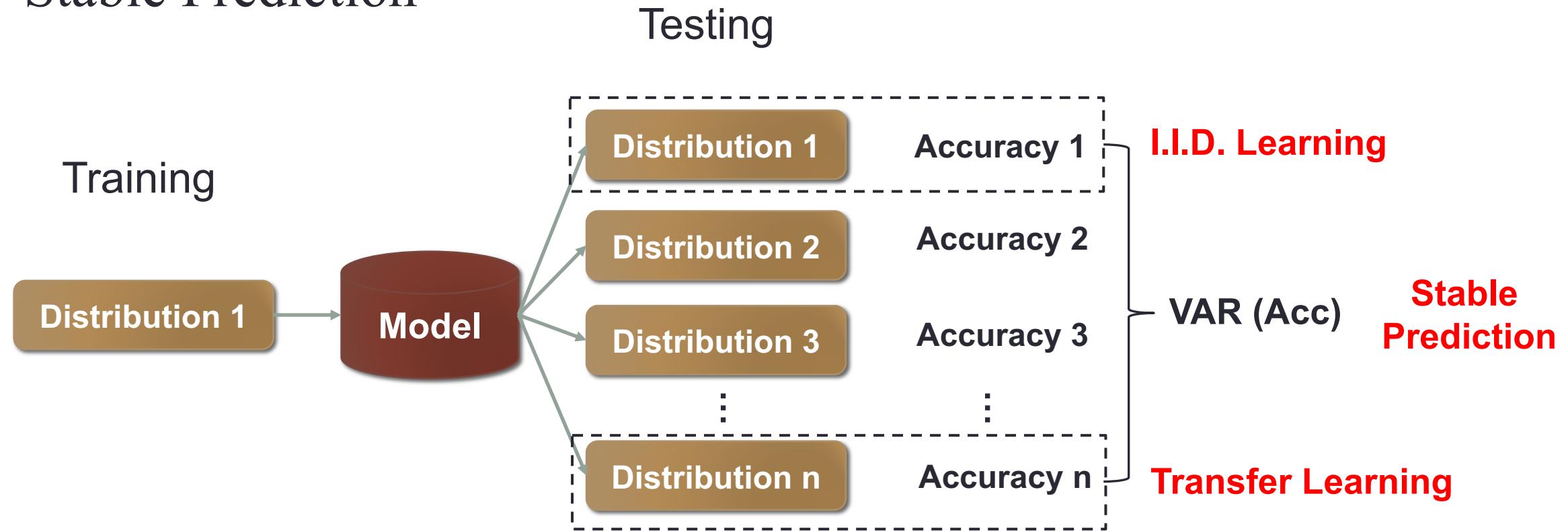
# Why they fail?

- The fault of Model
  - Correlation based model
  - Three sources of correlation: **Causation**, **Confounding**, and **Selection Bias** (**Invariant Causation** and **Spurious Correlation**)
  - Idea: Causally Regularized Stable Learning



# Stable Prediction

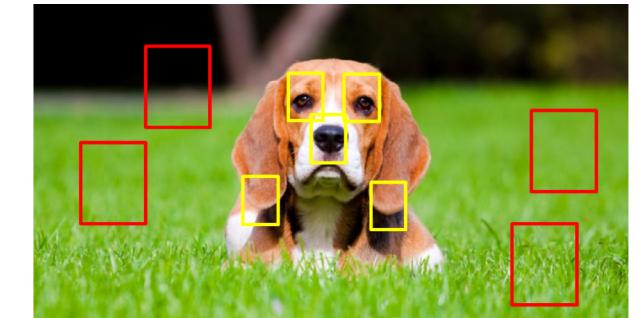
- Stable Prediction



Stable Prediction across Unknown Testing Data

# Why would a predictive model not be stable?

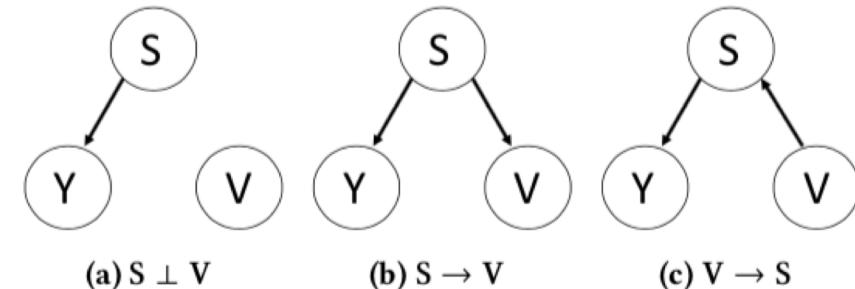
- Prediction / Classification
  - $X$ : vector of features;  $Y = \{0,1\}$
  - Environment: joint distribution of  $X$  and  $Y$ , denoted as  $P(XY)$
- Suppose  $X = \{S, V\}$ , and  $Y = f(S) + \varepsilon$ 
  - $S$ : set of **stable (causal) features**
  - $V$ : set of **non-causal features**
  - $P(Y|S)$  is stable, but  $P(Y|V)$  is not stable
- **Why would a predictive model not be stable?**
  - **Dependence issue**,  $Y$  is not independent with  $V$  (**Spurious Correlation**)
  - **Environment shift issue**,  $P(XY)_{training} \neq P(XY)_{testing}$



# Why would a predictive model not be stable?

- **Dependence issue**

- $X = \{S, V\}$ , and  $Y = f(S) + \varepsilon$
- Diagram (b) & (c):
  - $Y$  is not independent with  $V$
- Diagram (a):  $Y \perp V$ 
  - Selection bias, leading to  $Y$  is not independent with  $V$
  - **Some  $v \subseteq V$  would be learned as important predictors**



**Figure 1: Three diagrams for stable features  $S$ , noisy features  $V$ , and response variable  $Y$ .**

- **Environment shift issue**

- $P(XY) = P(Y|X)P(X) = P(Y|S)P(X)$  (assume  $P(Y|S)$  is stable)
- Selection bias  $\rightarrow P(X)_{training} \neq P(X)_{testing}$   
 $Y$  is not independent with  $V$   $\Rightarrow$   **$Corr(V_{training}, Y_{training}) \neq Corr(V_{testing}, Y_{testing})$**

# Related Work – address env. shift problem

- Covariate shift
  - Kernel mean matching [1], maximum entropy [2], robust bias-aware [3]
  - Importance weights: mimic the distribution of testing data to training data

$$\begin{aligned} & \lim_{n \rightarrow \infty} \min_h \mathbb{E}_{f_{\text{training}}^{(n)}(x) \tilde{f}(y|x)} \left[ \frac{f_{\text{testing}}(\mathbf{X})}{f_{\text{training}}(\mathbf{X})} (Y - h(\mathbf{X}))^2 \right] \\ &= \min_h \mathbb{E}_{f_{\text{testing}}(x) \tilde{f}(y|x)} [(Y - h(\mathbf{X})^2)] \end{aligned}$$

- These methods require prior knowledge of testing data
- These methods ignore the dependence issue

# Related Work

- Invariant Component Learning
  - Invariant prediction [4], domain generalization [5]
  - Assume  $P(Y|S)$  is stable across environments
  - Finding a subset/representation of features  $S'$ , such that  $P(Y|S')$  is invariant across all observed **multiple** environments
- Their performance depends on the diversity of their training data
- They could still have dependence issue on  $V'$ , if  $P(Y|V')$  is also invariant across observed environments

# Challenges

- **Dependence challenge**
  - $Y$  is not independent with  $V$
  - **Some  $v \subseteq V$  would be learned as important predictors**
- **Environment shift challenge**
  - The joint distribution  $P(XY)$  is different across environments.
  - **$\text{Corr}(V_{\text{training}}, Y_{\text{training}}) \neq \text{Corr}(V_{\text{testing}}, Y_{\text{testing}})$**
  - Can be addressed if  $V \perp Y$  on training environment
- **Unknown testing environments challenge**
  - No prior knowledge on future testing data.
  - Can be addressed if  $V \perp Y$  on training environment

# Challenges

- **Dependence challenge**
  - $Y$  is not independent with  $V$
  - **Some  $v \subseteq V$  would be learned as important predictors**
- **Environment shift challenge**
  - The joint distribution  $P(XY)$  is different across environments.
  - **$\text{Corr}(V_{\text{training}}, Y_{\text{training}}) \neq \text{Corr}(V_{\text{testing}}, Y_{\text{testing}})$**
  - Can be addressed if  $V \perp Y$  on training environment
- **Unknown testing environments challenge**

Key Challenge: How to make  $V \perp Y$

# Linking to Causality

- Outcome generating mechanism
  - $Y = f(S) + \varepsilon, X = \{S, V\}$
- Difference between S and V
  - $S$  has causal effect on  $Y$ ,
  - but  $V$  has no causal effect on  $Y$ .
- **Our idea:** Recover causation between  $X$  and  $Y$ , such that  $V \perp Y$ , and only  $S$  is correlated with  $Y$

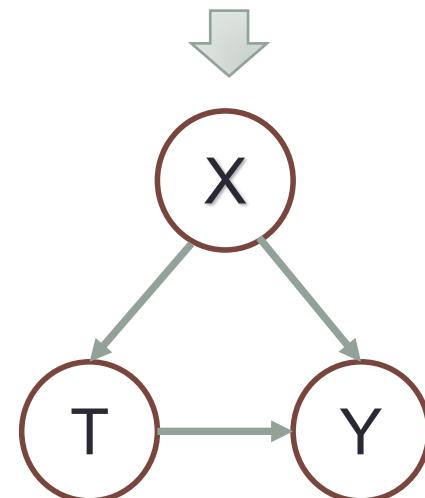
# Towards stable prediction

- Discard spurious correlation and embrace causality.



Typical Correlation Framework

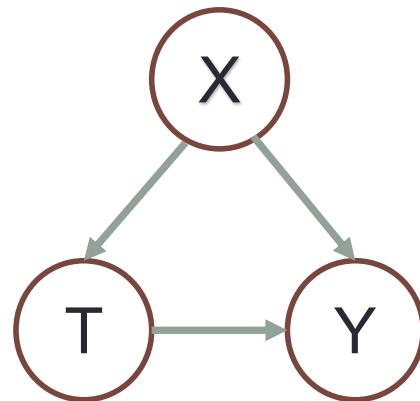
Estimate the **correlation effect** of variable **T** and output **Y** without evaluating the relationships between **X** and **T**



Typical Causal Framework

Estimate the **causal effect** of variable **T** on output **Y** With balanced confounder **X** (A/B Testing)

# Causal Inference by Exactly Matching



Typical Causal Framework

## Analogy of A/B Testing

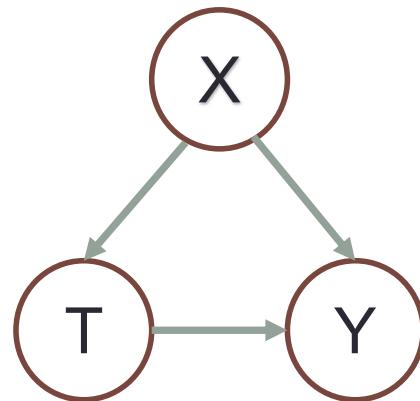
Given a feature T

**Find out the sample pairs that one contains T while the other don't, but they are similar in all other features.**

Calculate the difference of Y distribution in treated and controlled groups. (correlation between T and Y)

The requirement is too strong and we can hardly find satisfied groups of samples.

# Causal Inference by Confounder Balancing



Typical Causal Framework

## Analogy of A/B Testing

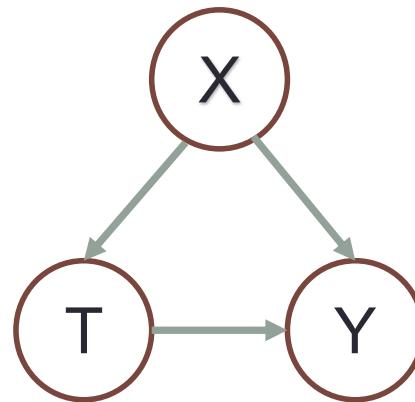
Given a feature T

Assign different weights to samples so that the samples with T and the samples without T have similar distributions in X

Calculate the difference of Y distribution in treated and controlled groups. (correlation between T and Y)

Too many parameters. For N samples and K features, we need to learn  $K \times N$  parameters. Not learning-friendly.

# Global Balancing: bridging causality and prediction



Typical Causal Framework

## Analogy of A/B Testing

Given **ANY** feature T

Assign **global sample weights** to samples so that the samples with T and the samples without T have similar distributions in X

Calculate the difference of Y distribution in treated and controlled groups. (correlation between T and Y)

Reduce the parameter number from  $K^N$  to  $N$ .

# Causal Regularizer and Theoretical Guarantee

- **Causal Regularizer** (Approximate global balancing)
  - Making any two variables in  $\mathbf{X}$  become independent by learning a global sample weights  $W$ :

$$\sum_{j=1}^p \left\| \frac{\mathbf{X}_{\cdot,-j}^T \cdot (W \odot \mathbf{X}_{\cdot,j})}{W^T \cdot \mathbf{X}_{\cdot,j}} - \frac{\mathbf{X}_{\cdot,-j}^T \cdot (W \odot (1 - \mathbf{X}_{\cdot,j}))}{W^T \cdot (1 - \mathbf{X}_{\cdot,j})} \right\|_2^2, \quad (4)$$

  
 ↓  
 0

PROPOSITION 3.3. If  $0 < \hat{P}(\mathbf{X}_i = x) < 1$  for all  $x$ , where  $\hat{P}(\mathbf{X}_i = x) = \frac{1}{n} \sum_i \mathbb{I}(\mathbf{X}_i = x)$ , there exists a solution  $W^*$  satisfies equation (4) equals 0 and variables in  $\mathbf{X}$  are independent after balancing by  $W^*$ .

# Causally Regularized Logistic Regression

- Global Balancing Regression (GBR) Algorithm

$$\begin{aligned}
 & \min \quad \sum_{i=1}^n W_i \cdot \log(1 + \exp((1 - 2Y_i) \cdot (\mathbf{X}_i \beta))), \\
 & \text{s.t.} \quad \sum_{j=1}^p \left\| \frac{\mathbf{X}_{\cdot,-j}^T \cdot (W \odot \mathbf{X}_{\cdot,j})}{W^T \cdot \mathbf{X}_{\cdot,j}} - \frac{\mathbf{X}_{\cdot,-j}^T \cdot (W \odot (1 - \mathbf{X}_{\cdot,j}))}{W^T \cdot (1 - \mathbf{X}_{\cdot,j})} \right\|_2^2 \leq \lambda_1, \quad W \geq 0, \\
 & \quad \|W\|_2^2 \leq \lambda_2, \quad \|\beta\|_2^2 \leq \lambda_3, \quad \|\beta\|_1 \leq \lambda_4, \quad (\sum_{k=1}^n W_k - 1)^2 \leq \lambda_5
 \end{aligned} \tag{5}$$

Sample re-weighted logistic loss

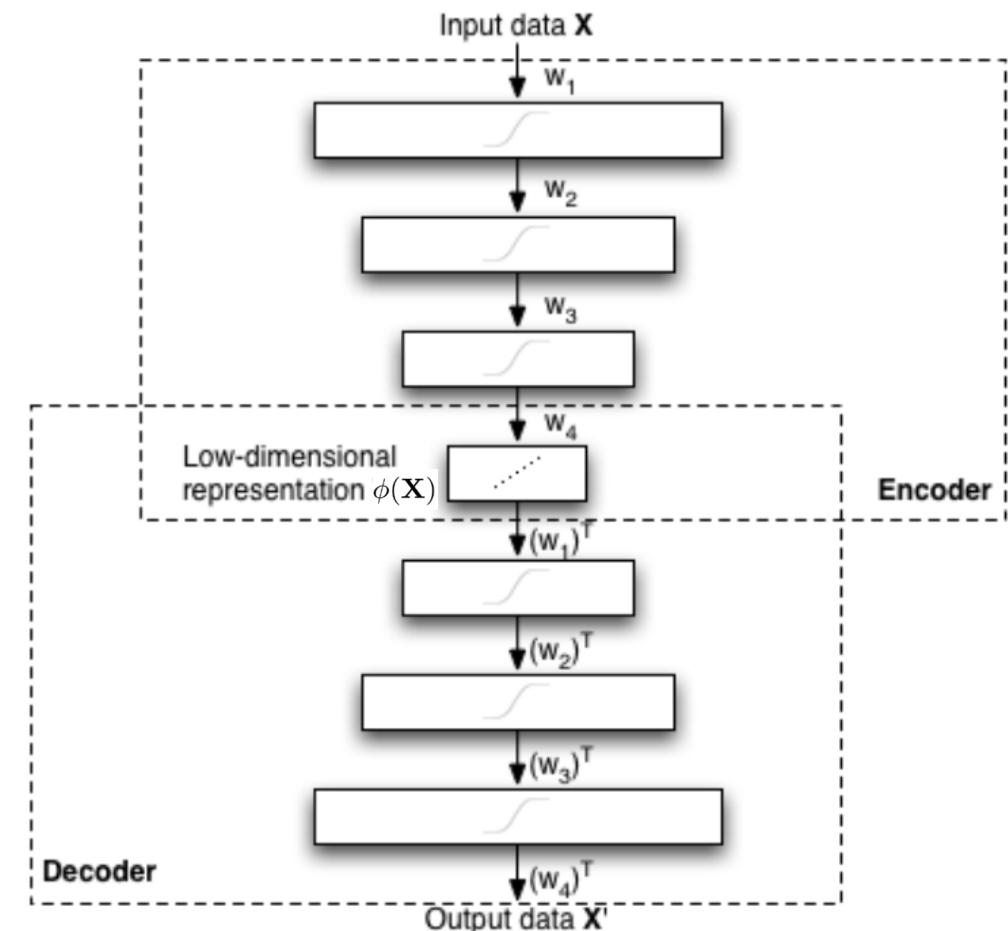
Causal Regularizer

Causality Coefficients

- Causality Coefficients: explainable and stable
- Linear model

# Challenges from the Wild Big Data Era

- High dimensional predictors
  - Hundred and thousand variables
  - Dimension reduction
- Non-linear predictions
  - Non-linear relationship between predictors and outcome variable
  - Non-linear function
- Deep Auto-Encoder



# From Shallow to Deep - DGBR

- Deep Global Balancing Regression Algorithm

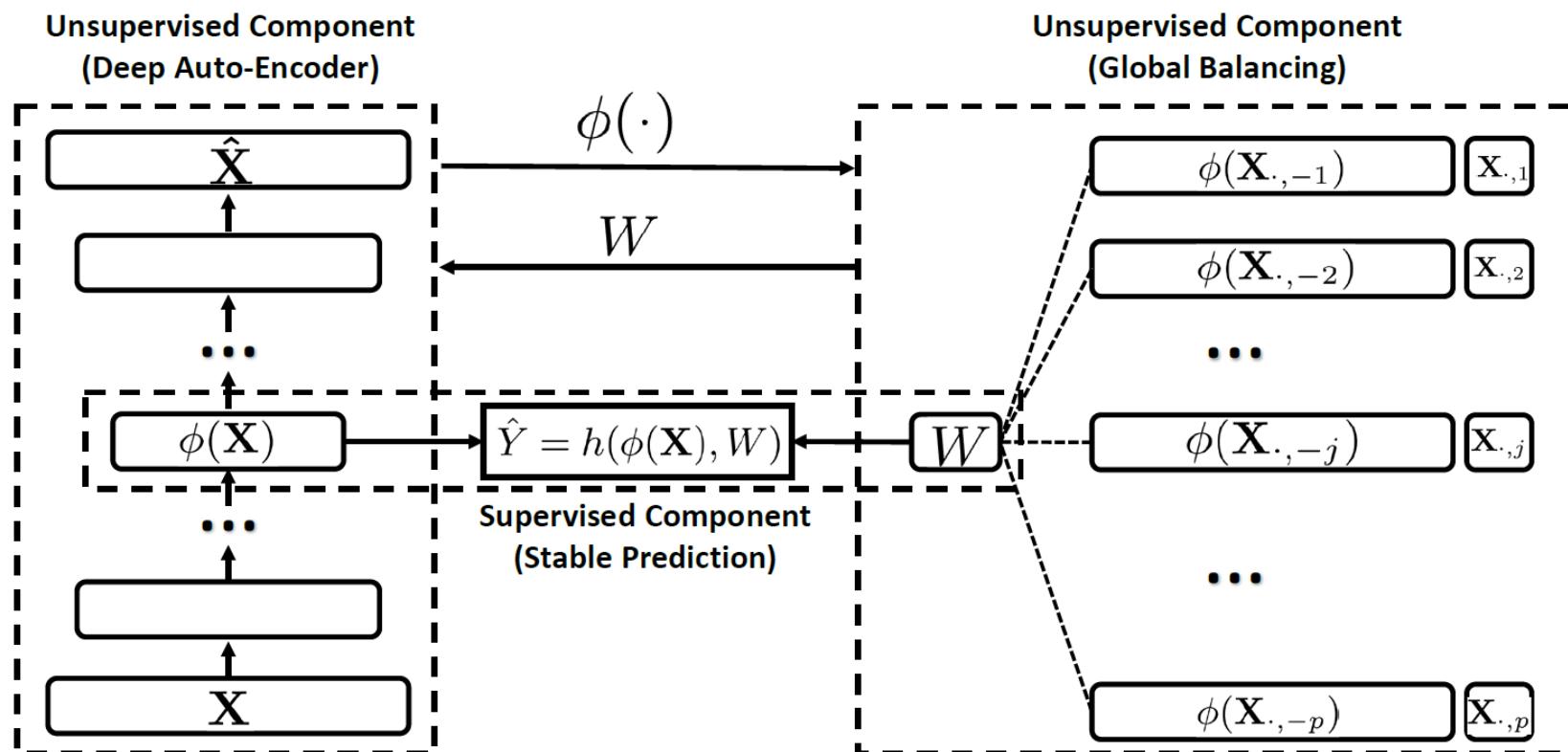


Figure 2: The framework of our proposed DGBR model.

# Theoretical Analysis

$$\sum_{j=1}^p \left\| \frac{\mathbf{X}_{\cdot,-j}^T \cdot (W \odot \mathbf{X}_{\cdot,j})}{W^T \cdot \mathbf{X}_{\cdot,j}} - \frac{\mathbf{X}_{\cdot,-j}^T \cdot (W \odot (1-\mathbf{X}_{\cdot,j}))}{W^T \cdot (1-\mathbf{X}_{\cdot,j})} \right\|_2^2, \quad (4)$$

- The components of  $\mathbf{X}$  could be mutually independent in the reweighted data.

PROPOSITION 1 . If  $0 < \hat{P}(\mathbf{X}_i = x) < 1$  for all  $x$ , where  $\hat{P}(\mathbf{X}_i = x) = \frac{1}{n} \sum_i \mathbb{I}(\mathbf{X}_i = x)$ , *there exists a solution  $W^*$  satisfies equation (4) equals 0 and variables in  $\mathbf{X}$  are independent after balancing by  $W^*$ .*

- Our GBR algorithm can make  $V \perp Y$

PROPOSITION 2 . If  $0 < \hat{P}(\mathbf{X}_i^e = x) < 1$  for all  $x$  in environment  $e$ ,  $Y^{e'}$  and  $\mathbf{V}^{e'}$  are independent when the joint probability mass function of  $(\mathbf{X}^{e'}, Y^{e'})$  is given by reweighting the distribution from environment  $e$  using weights  $W^*$ , so that  $p^{e'}(x, y) = p^e(x) \cdot (1/|\mathcal{X}|)$ .

# Theoretical Analysis

$$\sum_{j=1}^p \left\| \frac{\mathbf{X}_{\cdot,-j}^T \cdot (W \odot \mathbf{X}_{\cdot,j})}{W^T \cdot \mathbf{X}_{\cdot,j}} - \frac{\mathbf{X}_{\cdot,-j}^T \cdot (W \odot (1-\mathbf{X}_{\cdot,j}))}{W^T \cdot (1-\mathbf{X}_{\cdot,j})} \right\|_2^2, \quad (4)$$

- The components of  $\mathbf{X}$  could be mutually independent in the reweighted data.

PROPOSITION 1 . If  $0 < \hat{P}(\mathbf{X}_i = x) < 1$  for all  $x$ , where  $\hat{P}(\mathbf{X}_i = x) = \frac{1}{n} \sum_i \mathbb{I}(\mathbf{X}_i = x)$ , there exists a solution  $W^*$  satisfies equation (4) equals 0 and variables in  $\mathbf{X}$  are independent after balancing by  $W^*$ .

- Our GBR algorithm can make  $V \perp Y$

PROPOSITION 2 . If  $0 < \hat{P}(\mathbf{X}_i^e = x) < 1$  for all  $x$  in environ-

Propositions 1&2 suggest that our GBR algorithm can make a stable prediction across unknown environments

# Theoretical Analysis

- Our DGBR algorithm can preserve all properties of the GBR algorithm while making the overlap property easier to satisfy and reducing the variance of balancing weights.
- Our DGBR algorithm can enable more accurate estimation of  $P(Y|S)$ .
- More details could be found in our paper.

# Experiments

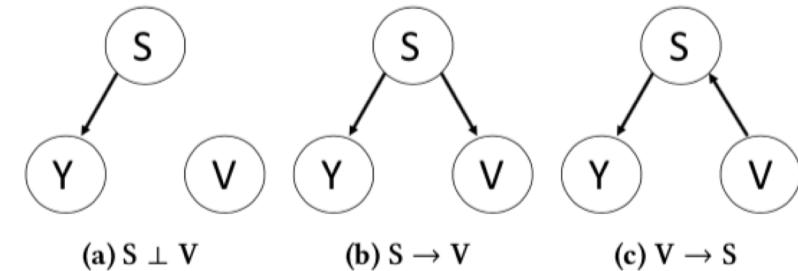
- Baselines:
  - Logistic Regression (LR)
  - Deep Logistic Regression (DLR): LR + Deep Auto Encoder
- Evaluation Metric:
  - RMSE, Average\_Error, Stability\_Error

$$\text{Average\_Error} = \frac{1}{|\mathcal{E}|} \sum_{e \in \mathcal{E}} \text{Error}(D^e), \quad (1)$$

$$\text{Stability\_Error} = \sqrt{\frac{1}{|\mathcal{E}|-1} \sum_{e \in \mathcal{E}} (\text{Error}(D^e) - \text{Average\_Error})^2}, \quad (2)$$

# Experiments on Synthetic Data

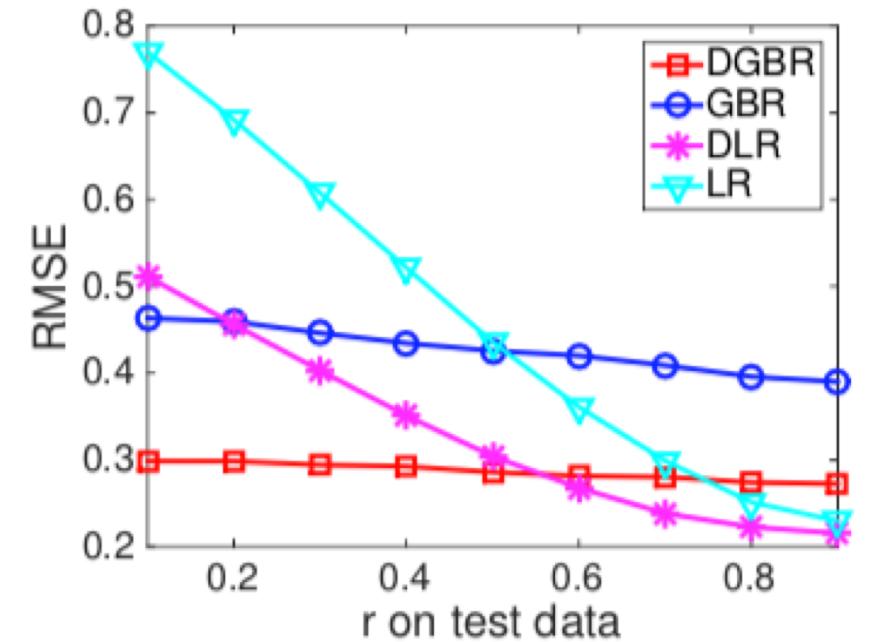
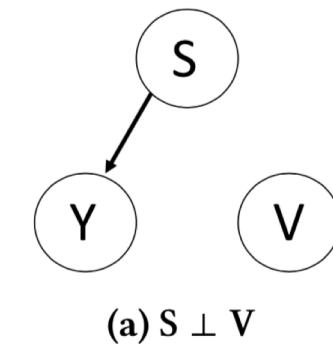
- Data generating
  - $X = \{S, V\}$  is binary.
  - $Y = h(f(S) + \epsilon)$  is also binary.
- Environments generating
  - Changing  $P_{XY}$  by sample selection with the **bias rate:  $r$**
  - Varying  $P(Y|V)$ :
    - if  $V = Y$ , then  $p(selected) = r$ , otherwise  $p(selected) = 1 - r$ .
  - **Different  $r$  means different environments**
  - Note that:  $r > 0.5$  implies  $\text{Corr}(V, Y)$  is positive



**Figure 1: Three diagrams for stable features  $S$ , noisy features  $V$ , and response variable  $Y$ .**

# Experiments on Synthetic Data

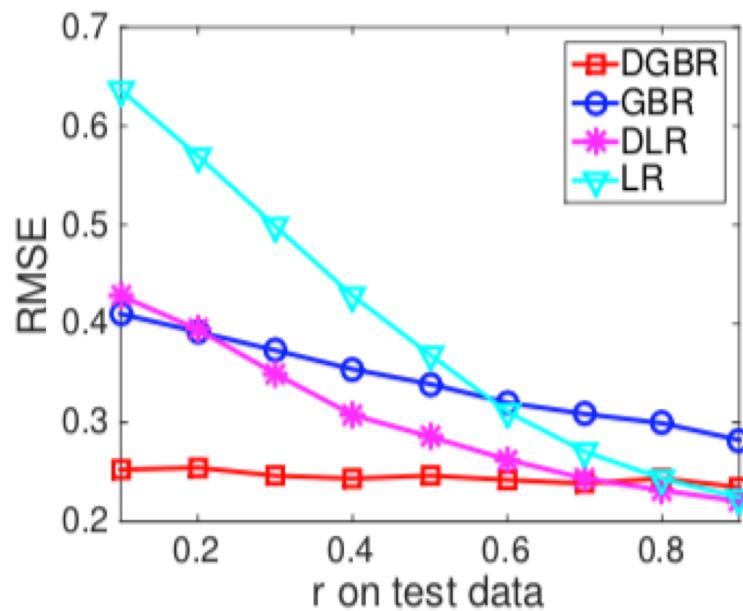
- Setting  $S \perp V$ 
  - Trained on one environment  $r = 0.85$ , and tested on all environments  $r = \{0.1, \dots, 0.9\}$
  - Different  $r$  means different environment
  - $r > 0.5$  implies  $\text{Corr}(V, Y)$  is positive
- Traditional LR and DLR failed
- GBR (dark blue) is more stable than LR
- DGBR (Red) is more stable than DLR
- DGBR is more stable and precise than GBR



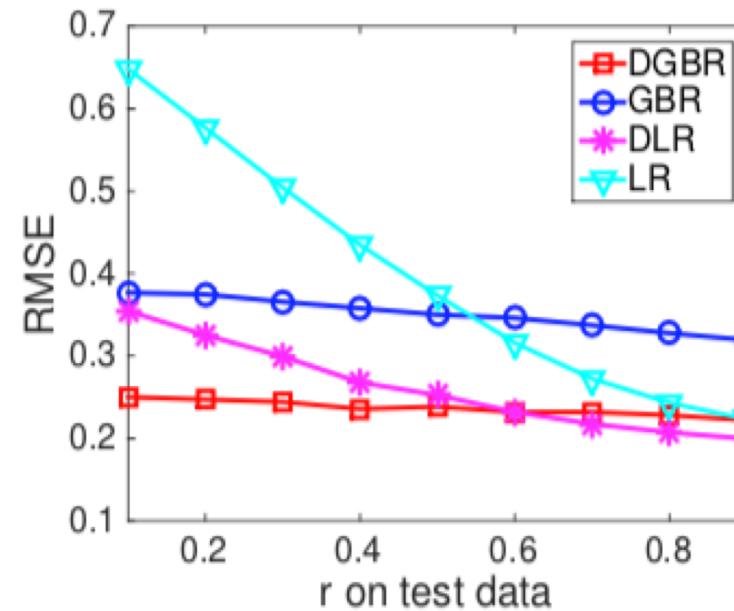
(f) Trained on  $n = 2000$ ,  $p = 20$ ,  $r = 0.85$

# Experiments on Synthetic Data

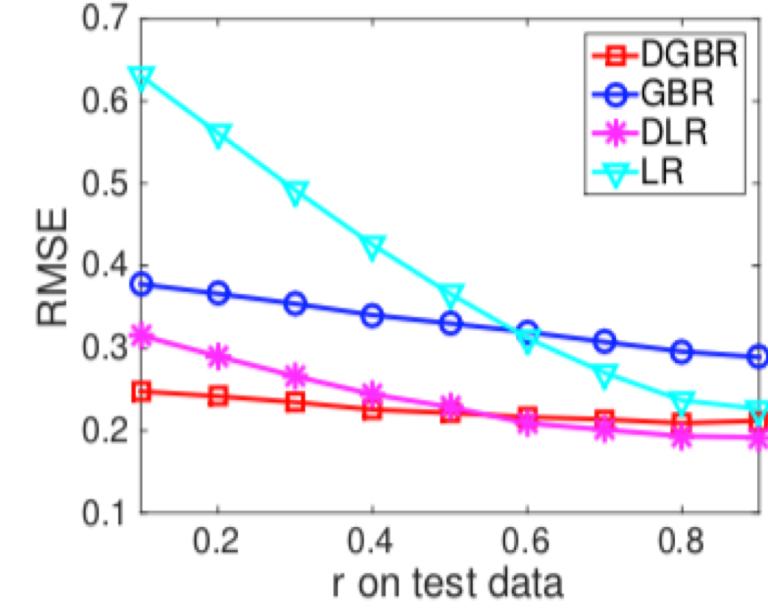
- More settings: varying  $n$ ,  $p$ , and  $r$



(b) Trained on  $n = 1000$ ,  $p = 20$ ,  $r = 0.75$



(e) Trained on  $n = 2000$ ,  $p = 20$ ,  $r = 0.75$

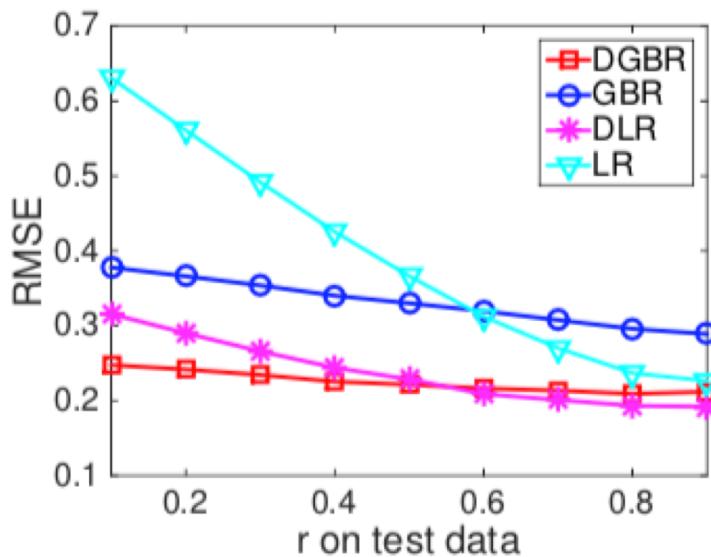


(h) Trained on  $n = 4000$ ,  $p = 20$ ,  $r = 0.75$

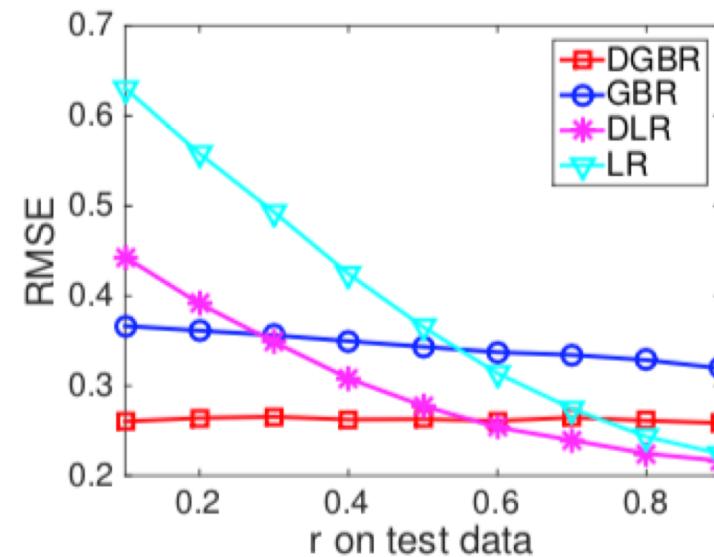
Vary sample size  $n$

# Experiments on Synthetic Data

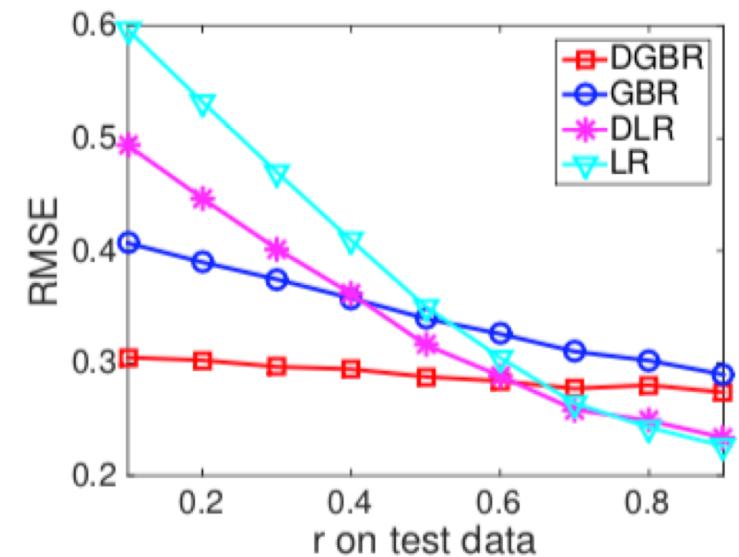
- More settings: varying  $n$ ,  $p$ , and  $r$



(a) Trained on  $n = 4000$ ,  $p = 20$ ,  $r = 0.75$



(b) Trained on  $n = 4000$ ,  $p = 40$ ,  $r = 0.75$

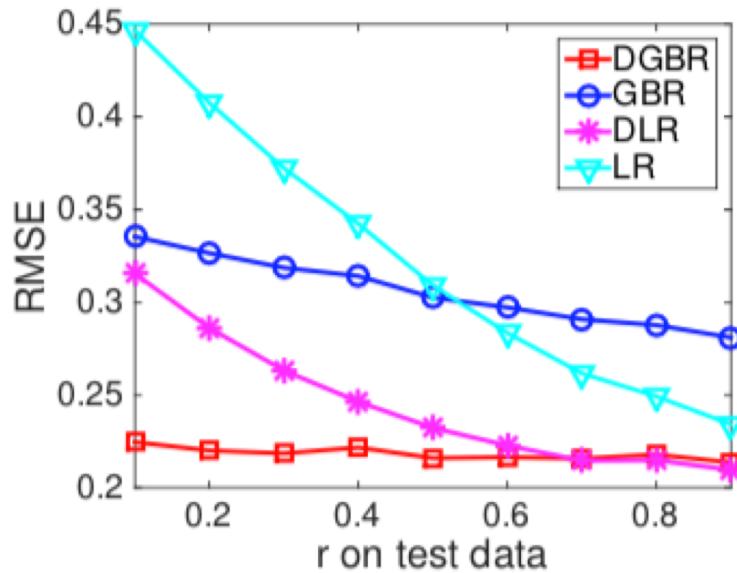


(c) Trained on  $n = 4000$ ,  $p = 80$ ,  $r = 0.75$

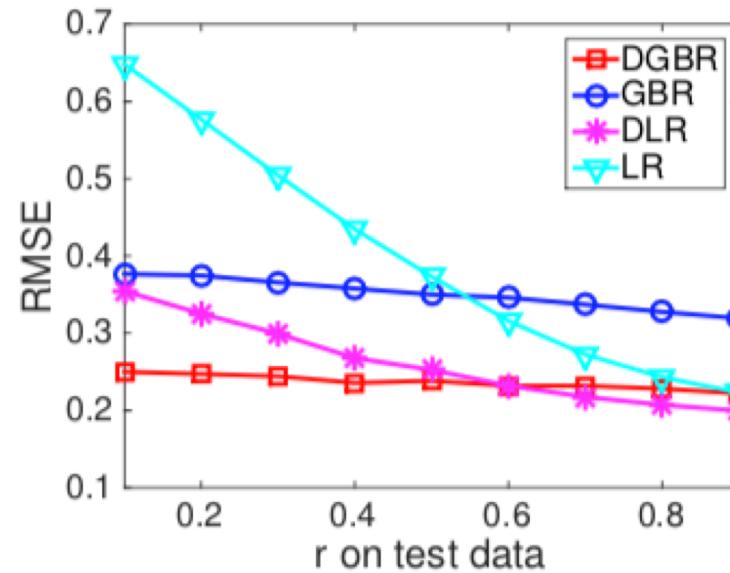
Vary variables' dimension  $p$

# Experiments on Synthetic Data

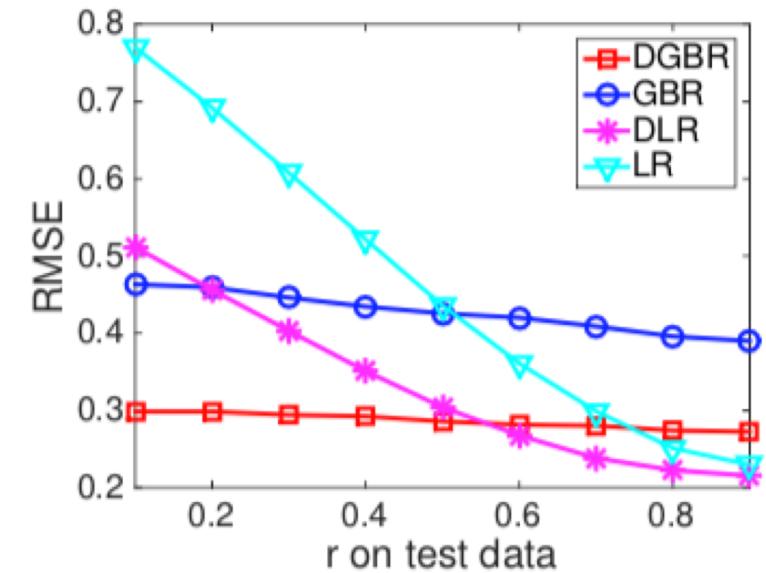
- More settings: varying  $n$ ,  $p$ , and  $r$



(d) Trained on  $n = 2000, p = 20, r = 0.65$



(e) Trained on  $n = 2000, p = 20, r = 0.75$

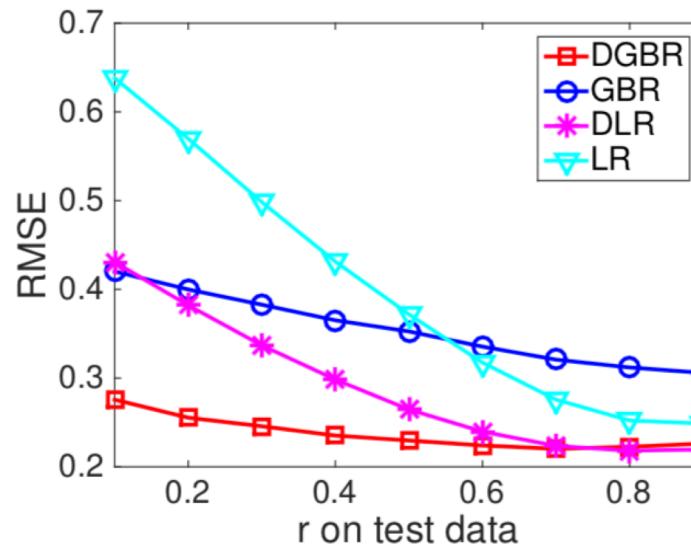
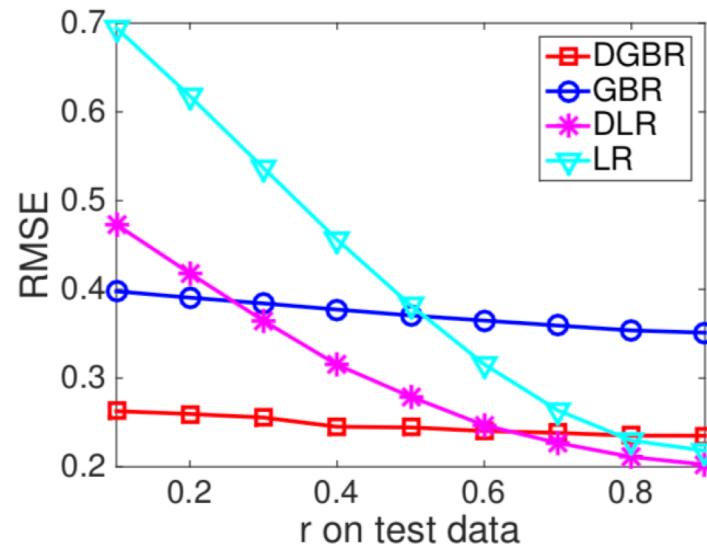
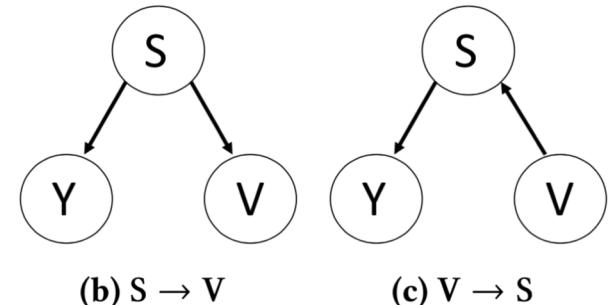


(f) Trained on  $n = 2000, p = 20, r = 0.85$

Vary bias rate  $r$  on training environment

# Experiments on Synthetic Data

- More settings: setting  $S \rightarrow V$  ( $S$  is the cause of  $V$ )  
setting  $V \rightarrow S$  ( $V$  is the cause of  $S$ )



The RMSE of DGBR is consistently stable and small across environments under all settings.

# Experiments on online advertising

2015



- Dataset Description:
  - Online advertising campaign (LONGCHAMP)
  - Users Feedback: 14,891 LIKE; 93,108 DISLIKE
  - 56 Features for each user
    - Age, gender, #friends, device, user setting on WeChat
- Experimental Setting:
  - Outcome Y: users feedback  $\leftarrow$  Y = 1, if LIKE  
Y = 0, if DISLIKE
  - Setting: generating environment with users' age.

# Experiments on online advertising

- Environments generating:
  - Separate the whole dataset into 4 environments by users' age, including  $Age \in [20,30)$ ,  $Age \in [30,40)$ ,  $Age \in [40,50)$ , and  $Age \in [50,100)$ .

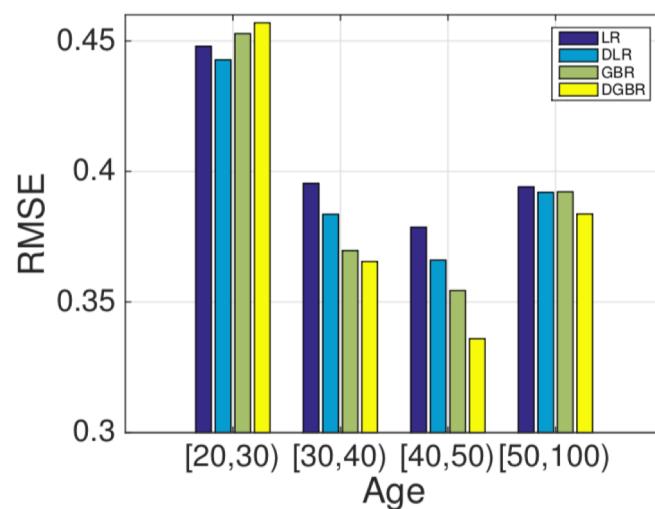


Fig. 15: Prediction across environments separated by age. The models are trained on dataset where users'  $Age \in [20, 30)$ , but tested on various datasets with different users' age range.

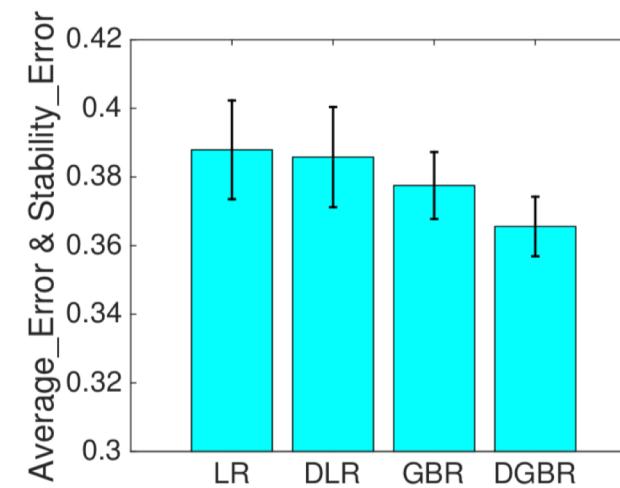
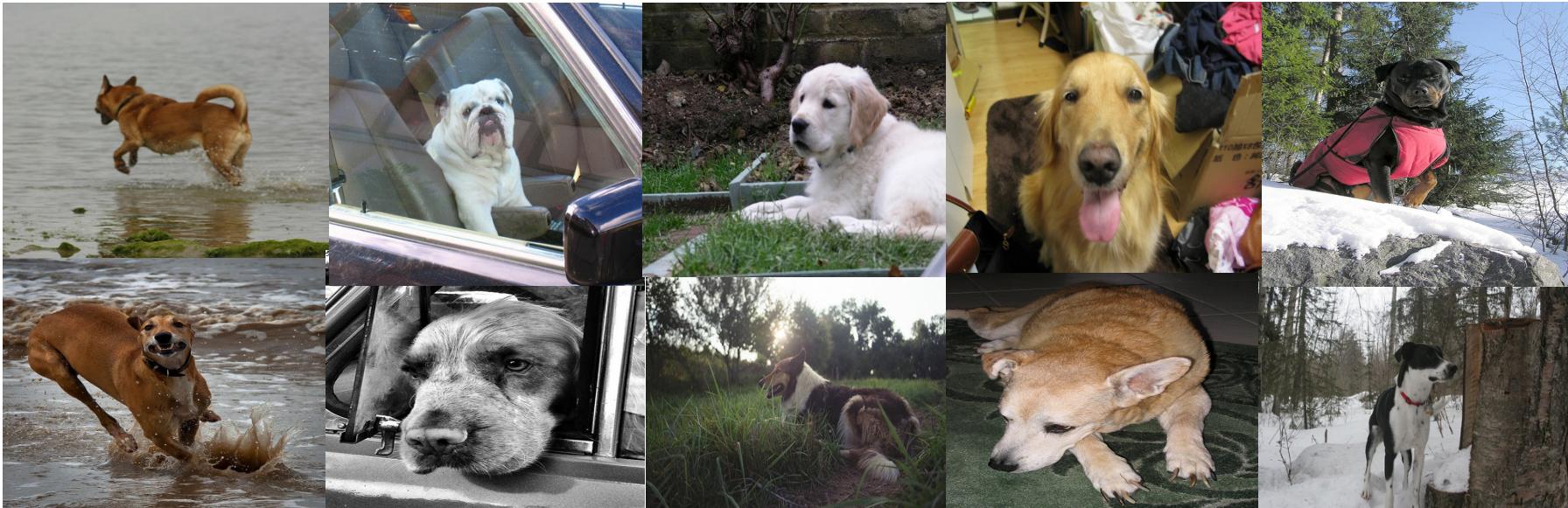


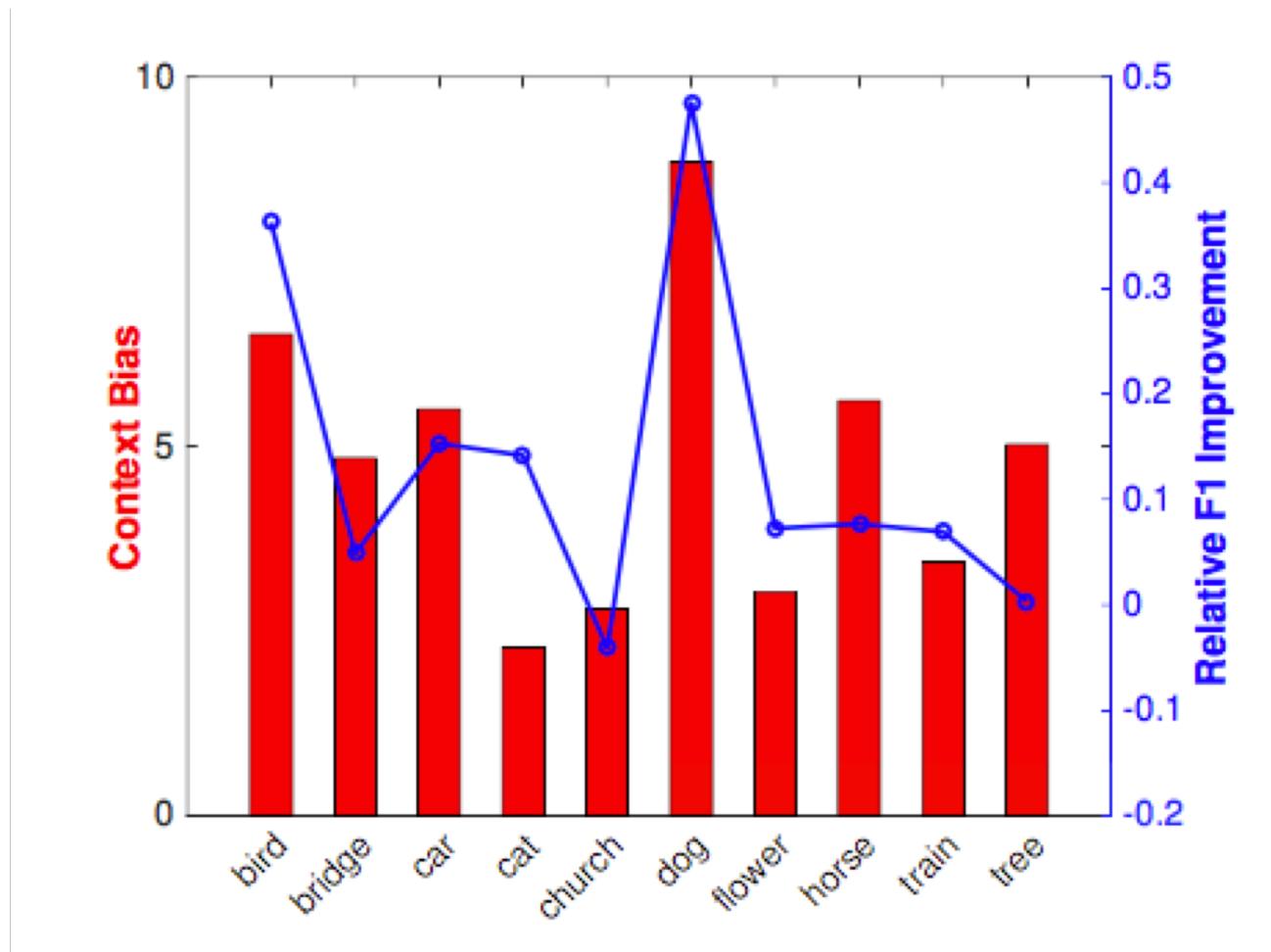
Fig. 16: *Average\_Error* and *Stability\_Error* of all algorithms across environments after fixing  $P(Y)$  as the same with its value on global dataset.

# Experiments on image classification

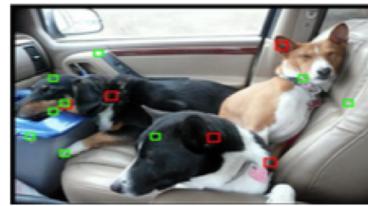
- Source: *YFCC100M*
- Type: multi-tags and high-resolution
- Scale: 10-category, each with nearly 1000 images
- Method: one *major object tag* (as category label) and 5 *context tags* which are frequently co-occurred with the major tag



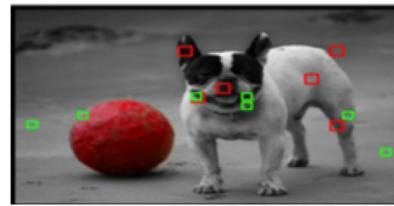
# Experiments on image classification



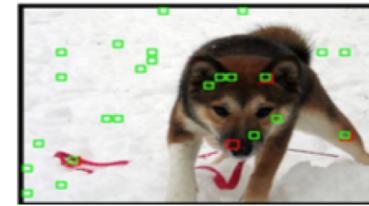
# Experiments on image classification



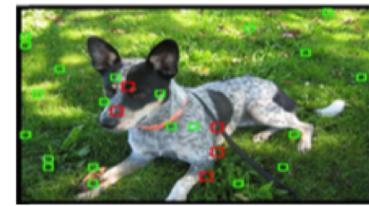
(a)



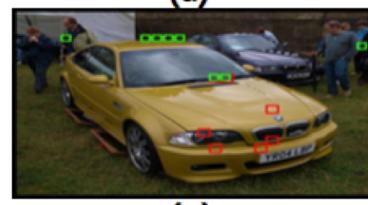
(b)



(c)



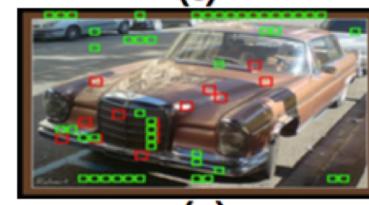
(d)



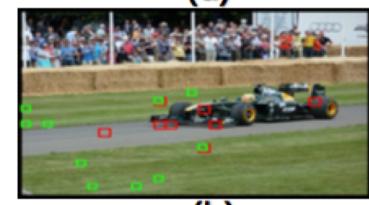
(e)



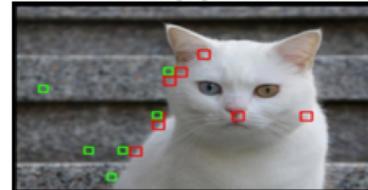
(f)



(g)



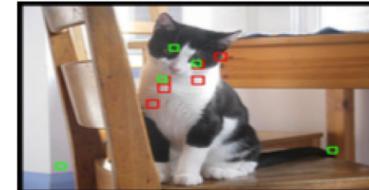
(h)



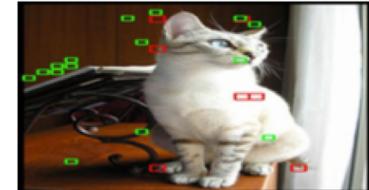
(i)



(j)



(k)



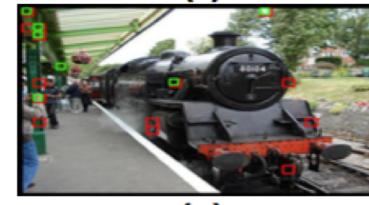
(l)



(m)



(n)



(o)



(p)

# Summary: Causally Regularized Stable Learning

- Today's Machine Learning:
  - Correlation Based
  - Correlation: causation, confounding, selection bias (Spurious Correlation)
  - To know the hows but not the whys
  - 知其然，但不知其所以然
- Causally Regularized Stable Learning
  - Causal regularizer
  - Recover causation from correlation
  - Causation based stable learning
  - Improving interpretability and stability on prediction

# OUTLINE

PART I. Introduction to Causal Inference

PART II. Methods for Causal Inference

**PART III. Causally Regularized Machine Learning**

Causal Inference for Stable Prediction

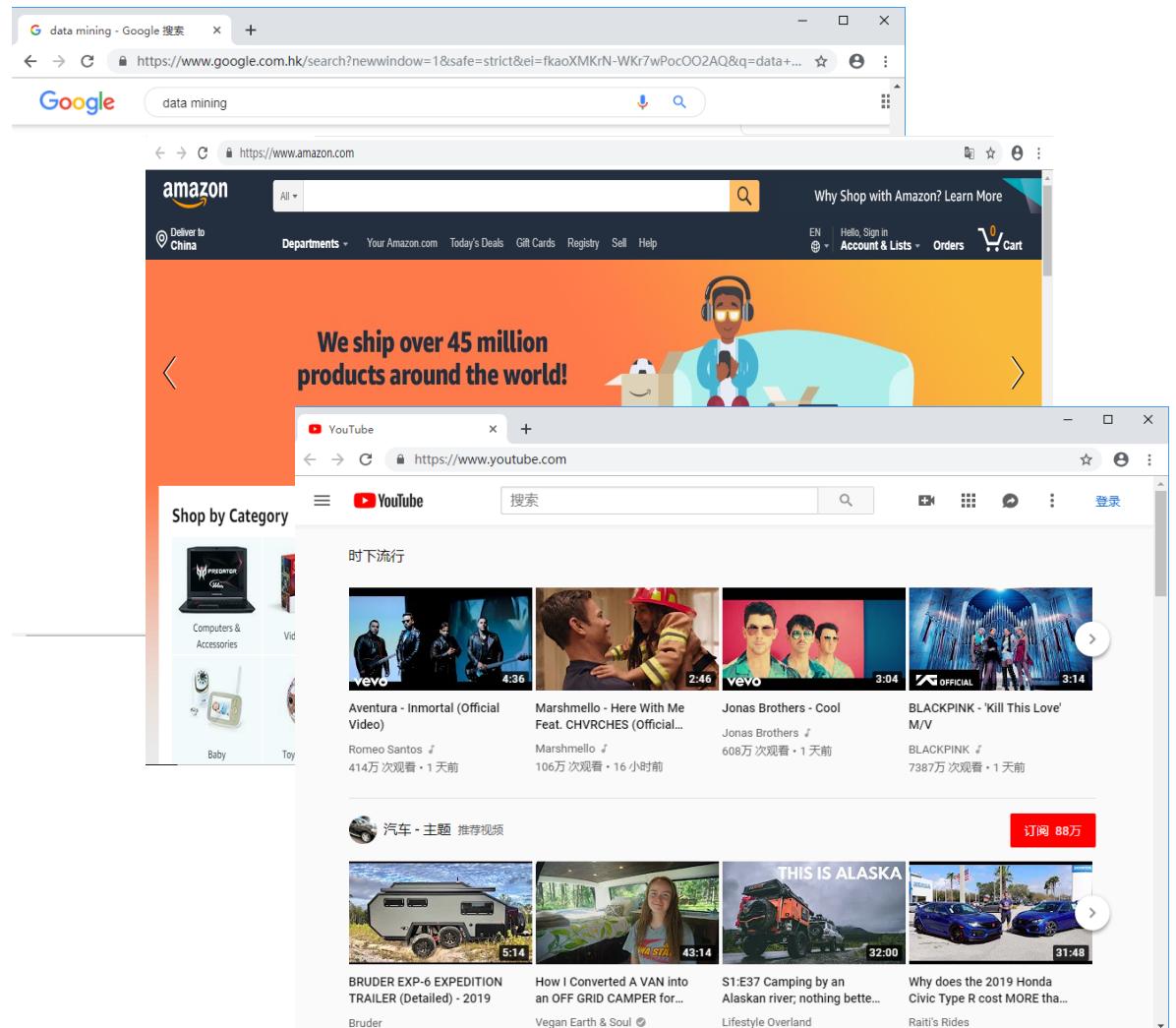
**Causal Inference for Offline Policy Evaluation**

PART IV. Benchmark and Open Datasets

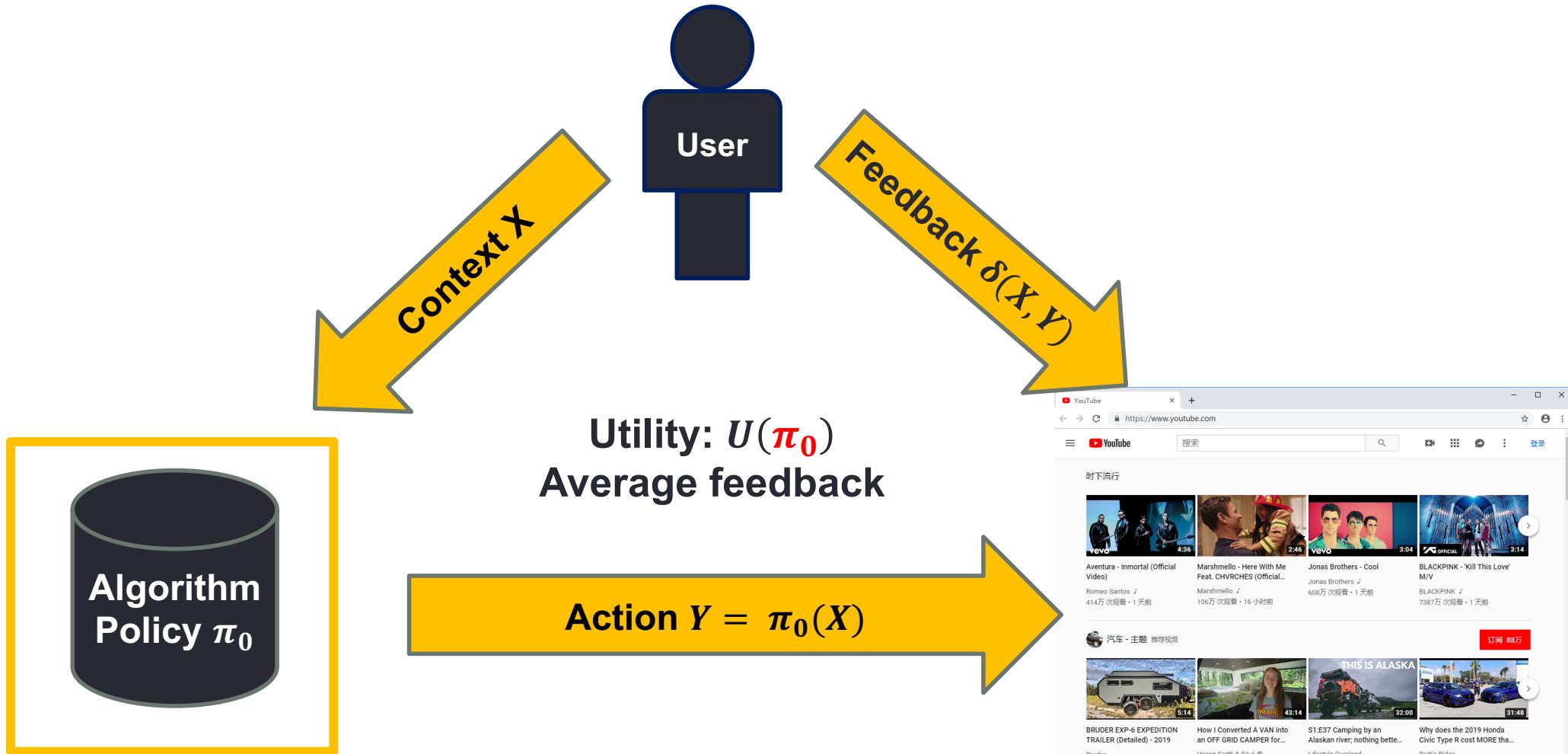
PART V. Conclusion and Discussion

# User Interactive systems

- Examples:
  - Search engines
  - Ads-placement systems
  - Videos recommender systems
- Policy: recommended algorithm
- Logs of user behavior for policy evaluation
  - Evaluate the system performance
  - Improve the policy in the system

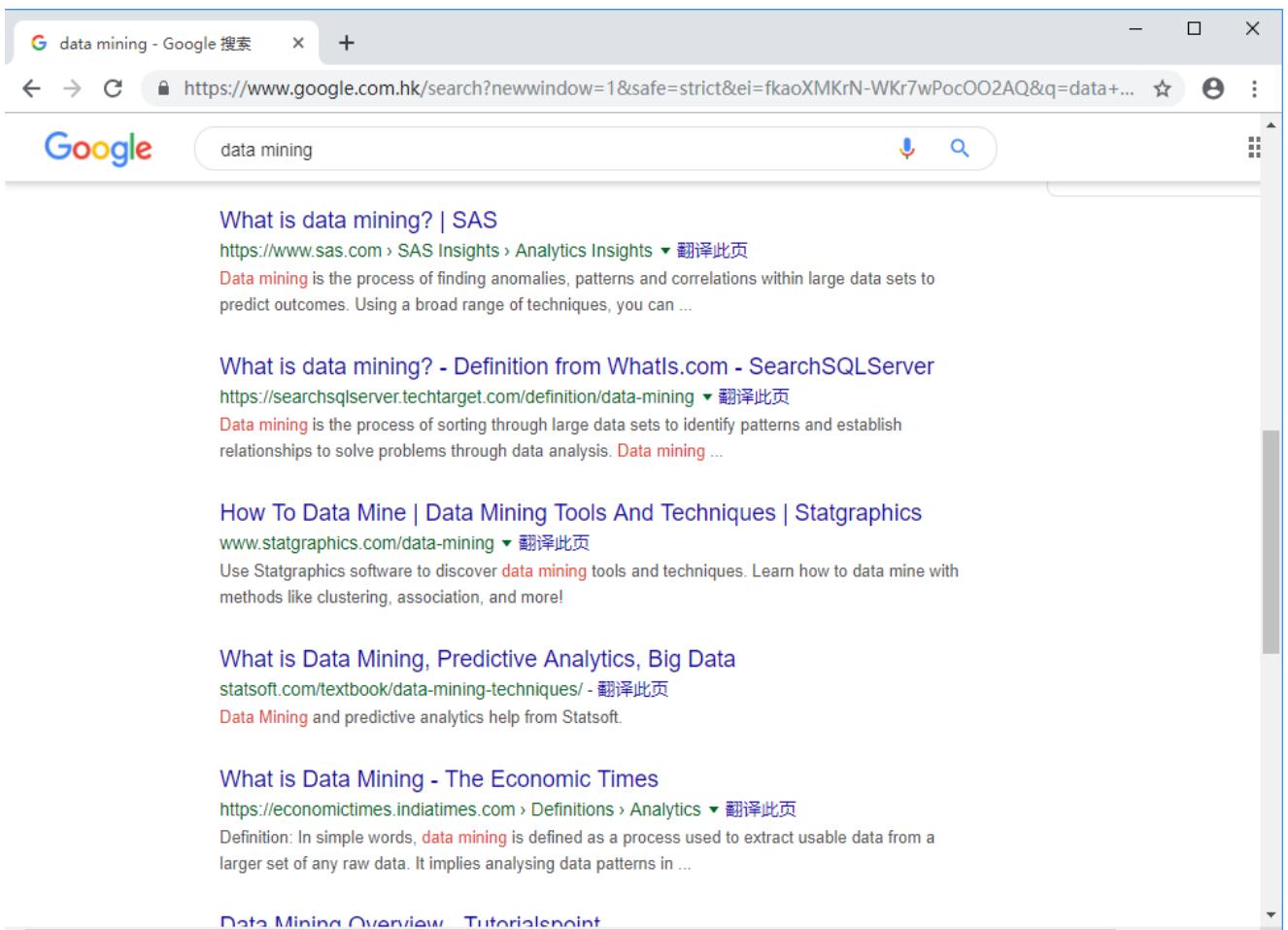


# Interactive System Schema



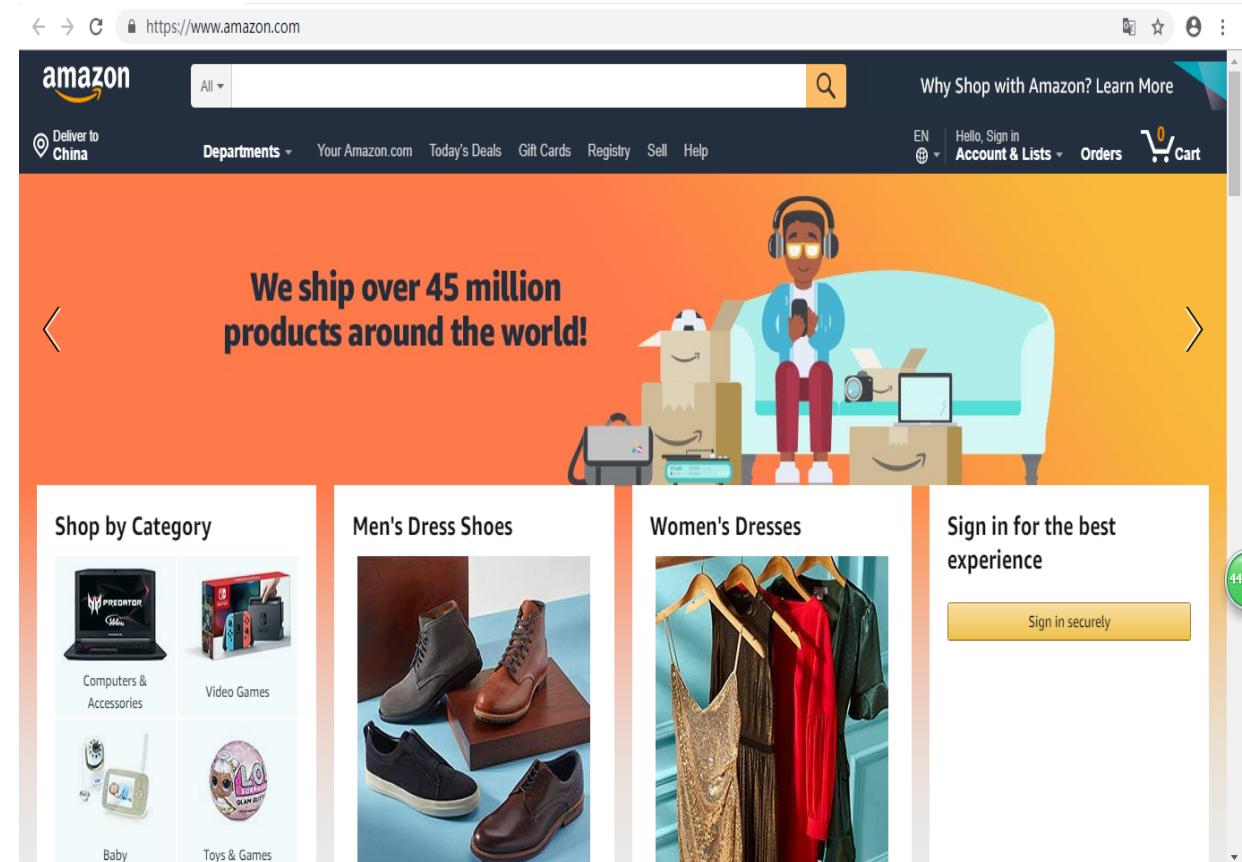
# Search engine

- Context  $X$ :
  - Query
- Action  $Y = \pi_0(X)$ :
  - Top-k ranking results
- Feedback  $\delta(X, Y)$ :
  - Click or not



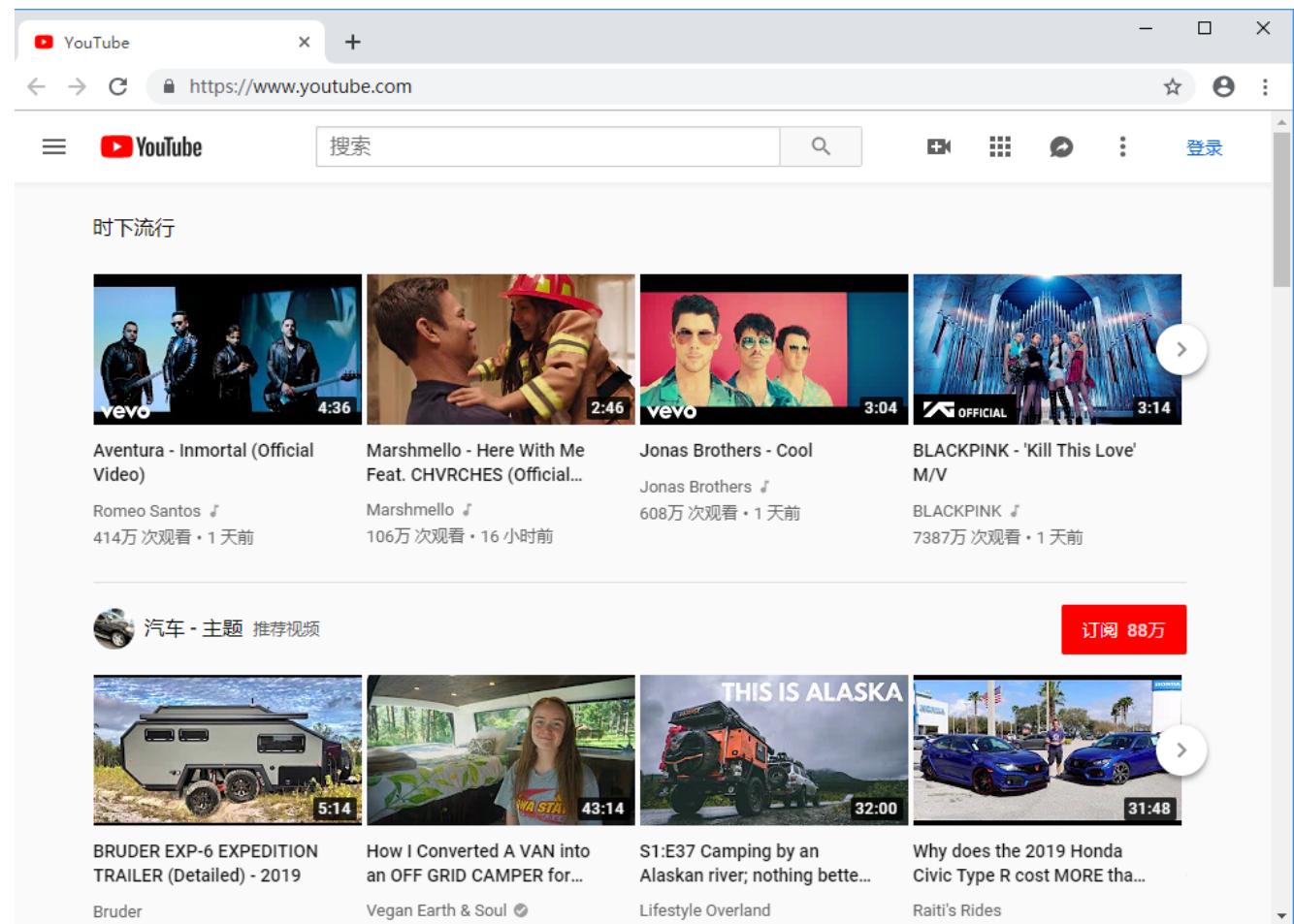
# Ads-placement systems

- Context  $X$ :
  - Users' features
- Action  $Y = \pi_0(X)$ :
  - Ads placed
- Feedback  $\delta(X, Y)$ :
  - Click or not
  - Buy or not



# Video Recommender System

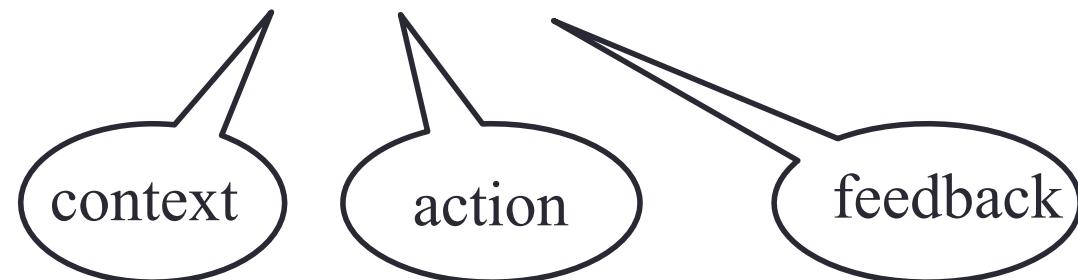
- Context  $X$ :
  - User features
- Action  $Y = \pi_0(X)$ :
  - Videos recommend
- Feedback  $\delta(X, Y)$ :
  - Click or not
  - Watching time



# Offline Policy Evaluation

- Log Data from  $\pi_0$ : samples indexed by  $1, 2, \dots, n$

$$S = ((X_1, Y_1, \delta_1), (X_2, Y_2, \delta_2), \dots, (X_n, Y_n, \delta_n))$$



- Properties
  - Contexts  $X_i$  are drawn i.i.d from unknown  $\Pr(X)$
  - Actions  $Y_i$  are decided by the existing policy  $\pi_0: X \rightarrow Y$
  - Feedback  $\delta_i$  are from unknown feedback function  $\delta: X \times Y \rightarrow R$

How to evaluate a **new policy**  $\pi$  ?

# Policy Evaluation: Online A/B Testing

- A/B Testing:
  - Deploy a new policy  $\pi$  in the interactive systems
  - Draw  $\mathbf{X} \sim Pr(\mathcal{X})$ , select  $\mathbf{Y} \sim \pi(\mathcal{Y}|\mathbf{X})$ , and get  $\delta(\mathbf{X}, \mathbf{Y})$
- Drawbacks:
  - Long turn-around time
  - Costly, number of A/B Testing limited
  - May be detrimental to the user experience
- Big Data Era
  - Lots of logged data

How to evaluate a new policy  $\pi$  **offline** with logged data ?

# Offline Policy Evaluation

- Given the logged data from a past (existing) policy  $\pi_0$ :

$$S = ((X_1, Y_1, \delta_1), (X_2, Y_2, \delta_2), \dots, (X_n, Y_n, \delta_n))$$

- Goal: to estimate the utility of a new policy  $\pi$ :

$$U(\pi) = \mathbb{E}_{\mathbf{X} \sim Pr(\mathbf{X}), Y \sim \pi(\mathcal{Y}|\mathbf{X})} [\delta(\mathbf{X}, Y)]$$

- Utility: the average feedback of policy over the population

$$U(\pi) = \mathbb{E}_{X \sim Pr(X), Y \sim \pi(Y|X)} [\delta(X, Y)]$$

# Challenges of Offline Policy Evaluation

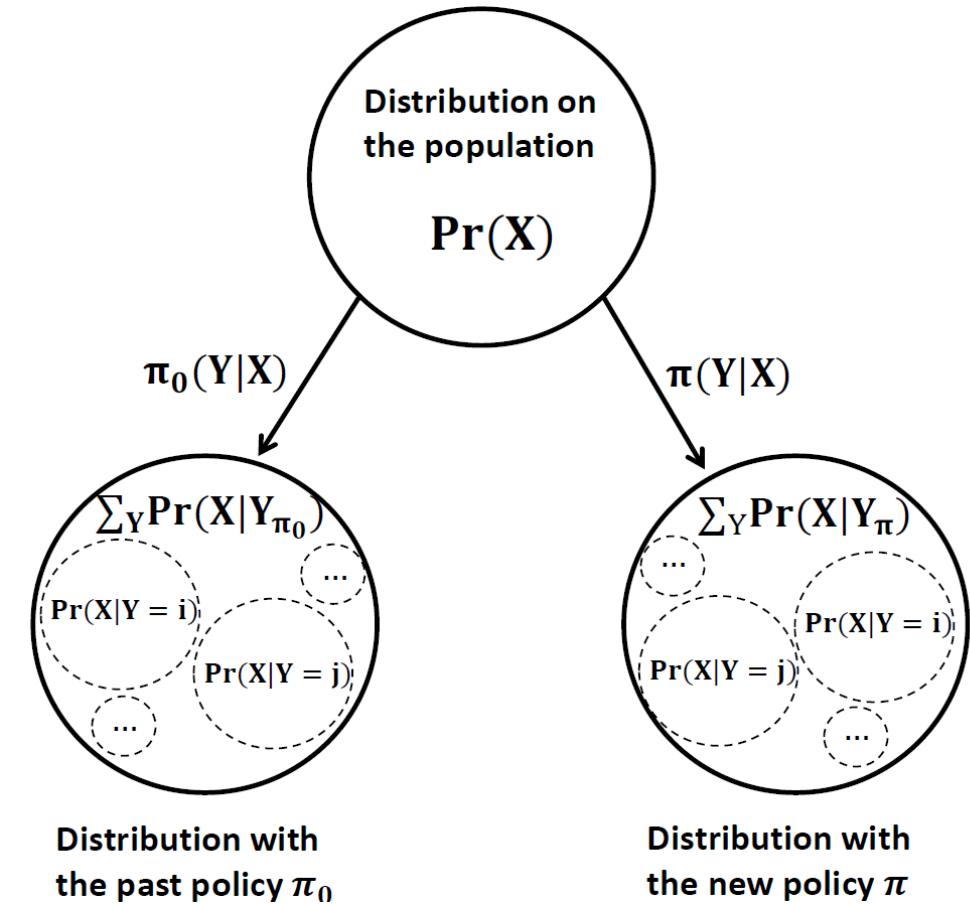
- **Distribution shift** induced by the past policy  $\pi_0$ 
  - $Y$  is assigned based on  $X$  through  $\pi_0(Y|X)$

$$Pr(X|Y_{\pi_0} = i) \neq Pr(X|Y_{\pi_0} = j) \neq Pr(X)$$

- **Action discrepancy** induced by the new policy  $\pi(Y|X)$ :  $Y$  is assigned through  $\pi(Y|X)$

$$\pi(Y = i|X) \neq \pi(Y = j|X)$$

$\pi(Y = k|X) \approx 0$  : No context  $X$  will be assigned to  $Y=k$  under  $\pi$ , hence distribution shift from action  $Y=k$  does not affect results



**Focus on the action group with high value of  $\pi(Y = i|X)$**

# Related Work

- Direct method (DM) directly estimate the feedback function  $\hat{\delta}(\mathbf{X}, \mathbf{Y})$  by utilizing the logged data to predict the feedbacks of actions chosen by the new policy  $\pi$ .

$$\hat{U}_{DM}(\pi) = \frac{1}{n} \sum_{i=1}^n \sum_{Y_j \in \mathcal{Y}} \hat{\delta}(X_i, Y_j) \pi(Y_j | X_i)$$

- Direct method is unbiased if the feedback model is correct.
- But we hardly know the real underlying feedback function, and it ignores the distribution shift induced by the past policy.

# Related Work

- Inverse propensity score (IPS) estimator use the propensity score (the probability of the chosen action  $\hat{\pi}_0(Y|X)$ ) to reweight sample:

$$\widehat{U}_{IPS}(\pi) = \frac{1}{n} \sum_{i=1}^n \delta_i \frac{\pi(Y_i|X_i)}{\widehat{\pi}_0(Y_i|X_i)}$$

- IPS is **unbiased** if propensity score model is correct.
- **But** we have no prior knowledge on propensity score model
- High variance if propensity score is close to 0 and 1
- Ignoring the **action discrepancy** induced by new policy  $\pi$

# Related Work

- Doubly Robust (DR) estimator combined IPS estimator and direct method:

$$\widehat{U}_{DR}(\pi) = \frac{1}{n} \sum_{i=1}^n \sum_{Y \in \mathcal{Y}} \pi(Y|X_i) \left[ \widehat{\delta}(X_i, Y) + \frac{I(Y = Y_i)}{\widehat{\pi}_0(Y_i|X_i)} (\delta_i - \widehat{\delta}(X_i, Y)) \right]$$

- DR estimator is unbiased if either propensity score model or feedback model is correct
- But one cannot guarantee the specified model is correct
- Moreover, it still ignores the action discrepancy induced by new policy  $\pi$

# Summary on Related Work

- Distribution shift induced by the past policy  $\pi_0$ 
  - $Y$  is assigned based on  $\pi_0(Y|X)$

$$Pr(X|Y_{\pi_0} = i) \neq Pr(X)$$

- Action discrepancy induced by the new policy  $\pi(Y|X)$

$$\pi(Y = i|X) \neq \pi(Y = j|X)$$

$\pi(Y = k|X) \approx 0$  : No  $X$  will be assigned with  $Y=k$  under  $\pi$ , hence distribution shift from action  $Y=k$  does not affect results

**Focus on the action group with high  $\pi(Y = i|X)$**

## Related Work

## Remain Challenges

## Models dependency

# Context Balancing

- Context Balancing: a non-parametric method based on directly covariate balancing to correct the distribution shift induced by the past policy
- Learning sample weights  $W$  in each action group  $k$  as follows:

$$W_{Y=k} = \arg \min_{W_{Y=k}} \left\| \frac{1}{n} \sum_{i=1}^n \mathbf{M}_i - \sum_{j | Y_j=k} W_j \cdot \mathbf{M}_j \right\|_2^2,$$

The distribution  
on the population

$\mathbf{M} = \{\mathbf{X}, \mathbf{X}^2, \mathbf{X}_i \mathbf{X}_j, \mathbf{X}^3, \mathbf{X}_i \mathbf{X}_j \mathbf{X}_k, \dots\}$

The corrected  
distribution

- With sample weights  $W = \{W_{Y=1}, W_{Y=2}, \dots, W_{Y=K}\}$ , CB estimator is

$$\widehat{U}_{CB}(\pi) = \sum_{i=1}^n \pi(Y_i | X_i) W_i \delta_i$$

Remove the model dependency  
But ignore action discrepancy

# Focused Context Balancing (FCB) estimator

- **Context Balancing:** learning sample weights by directly variables balancing

$$W_{Y=k} = \arg \min_{W_{Y=k}} \left\| \frac{1}{n} \sum_{i=1}^n \mathbf{M}_i - \sum_{j: Y_j=k} W_j \cdot \mathbf{M}_j \right\|_2^2$$

- **Focused Context Balancing:** focusing on the action group with high probability when learning sample weights:

$$W_{Y=k} = \arg \min_{W_{Y=k}} \left\| \sum_{i=1}^n \frac{1}{n} \pi(Y = k | \mathbf{X}_i) \mathbf{M}_i - \sum_{i: Y_i=k} W_i \pi(Y = k | \mathbf{X}_i) \mathbf{M}_i \right\|_2^2$$

Focused Component

# Theoretical Analysis

- Taylor's expansion of feedback function on the context:

$$\delta(\mathbf{X}, Y = k) = \alpha_{Y=k} \cdot \mathbf{M} \text{ where } \mathbf{M} = \{\mathbf{X}, \mathbf{X}^2, \mathbf{X}_i \mathbf{X}_j, \mathbf{X}^3, \mathbf{X}_i \mathbf{X}_j \mathbf{X}_k, \dots\}$$

$$\begin{aligned}\widehat{U}(\pi) &= \sum_{i=1}^n W_i \pi(Y = Y_i | \mathbf{X}_{i,}) \delta(\mathbf{X}_{i,}, Y_i) \\ &= \sum_{k \in \mathcal{Y}} \alpha_{Y=k} \sum_{i: Y_i=k} W_i \pi(Y = k | \mathbf{X}_{i,}) \mathbf{M}_{i,} \\ &= \sum_{k \in \mathcal{Y}} \alpha_{Y=k} \left[ \sum_{i: Y_i=k} W_i \pi(Y = k | \mathbf{X}_{i,}) \mathbf{M}_{i,} - \frac{1}{n} \sum_{i=1}^n \pi(Y = k | \mathbf{X}_{i,}) \mathbf{M}_{i,} \right] \\ &\quad + \sum_{k \in \mathcal{Y}} \alpha_{Y=k} \frac{1}{n} \sum_{i=1}^n \pi(Y = k | \mathbf{X}_{i,}) \mathbf{M}_{i,} \\ &= \sum_{k \in \mathcal{Y}} \alpha_{Y=k} B_k + \frac{1}{n} \sum_{i=1}^n \sum_{k \in \mathcal{Y}} \delta(\mathbf{X}_{i,}, Y = k) \pi(Y = k | \mathbf{X}_{i,}) \\ &= \sum_{k \in \mathcal{Y}} \alpha_{Y=k} B_k + U(\pi)\end{aligned}$$

Distribution shift induced by past policy  
Action discrepancy from new policy

$$B_k = \boxed{\sum_{i: Y_i=k} W_i \pi(Y = k | \mathbf{X}_{i,}) \mathbf{M}_{i,}} - \boxed{\frac{1}{n} \sum_{i=1}^n \pi(Y = k | \mathbf{X}_{i,}) \mathbf{M}_{i,}}$$

The adjusted distribution

Focused Component

The target distribution

# Focused Context Balancing algorithm

- Objective Function:

Focused Component

$$\begin{aligned}
 & \min_{W_{Y=k}} \left\| \sum_{i:Y_i=k} W_i \pi(Y = k | \mathbf{X}_{i,}) \mathbf{M}_i - \sum_{i=1}^n \frac{1}{n} \pi(Y = k | \mathbf{X}_{i,}) \mathbf{M}_i \right\|_2^2 \\
 & s.t. \quad \sum_{i:Y_i=k} W_i^2 \leq \lambda \quad \sum_{i:Y_i=k} W_i = 1 \quad and \quad W \geq 0,
 \end{aligned} \tag{7}$$

- Policy Evaluation:

$$\widehat{U}_{FCB}(\pi) = \sum_{i=1}^n \pi(Y_i | X_i) W_i \delta_i.$$

# Experiment

- Baselines:
  - Direct Method: regressing on an estimated feedback function to evaluate the effect of new policy.
  - R-IPS: IPS estimator + roughly estimated propensity score not associated with context.
  - E-IPS: IPS estimator with estimated propensity score
  - T-IPS: IPS estimator with the true propensity score
  - SN-IPS: IPS estimator with estimated propensity score + Normalized sample weights
  - Doubly Robust: IPS estimator with estimated propensity score + Direct Method
  - CB: covariate balancing to learn sample weights + ignoring distribution shift induced by new policy.
- Evaluation Metric:

$$\begin{aligned}
 Bias &= \left| \frac{1}{T} \sum_{i=1}^T \widehat{U}(\pi)_i - U(\pi) \right| \\
 SD &= \sqrt{\frac{1}{T} \sum_{i=1}^T (\widehat{U}(\pi)_i - \frac{1}{T} \sum_{i=1}^T \widehat{U}(\pi)_i)^2} \\
 MAE &= \frac{1}{T} \sum_{i=1}^T |\widehat{U}(\pi)_i - U(\pi)| \\
 RMSE &= \sqrt{\frac{1}{T} \sum_{i=1}^T (\widehat{U}(\pi)_i - U(\pi))^2}
 \end{aligned}$$

# Experiment - Simulations

- Dataset

- Sample size:  $n = \{5,000, 10,000\}$
- Context dimension:  $p = \{50, 100\}$
- Observed context:  $\mathbf{X} = (x_1, x_2, \dots, x_p) \quad x_1, x_2, \dots, x_p \stackrel{iid}{\sim} Bernoulli(0.5)$
- Policy to be evaluated: from sigmoid function

$$\pi_{sig}(Y = 1 | \mathbf{X}) = 1 / \left( 1 + e^{-\sum_{i=1}^p (x_i - 0.5)} \right)$$

- Logged policy: from inverse proportional function, constant function and linear function

$$\pi_{inv}(Y = 1 | \mathbf{X}) = 1 / (1 + 3 \sum_i x_i / p) + \mathcal{N}(0, 0.1)$$

$$\pi_{uni}(Y = 1 | \mathbf{X}) = 0.5 + \mathcal{N}(0, 0.1)$$

$$\pi_{lin}(Y = 1 | \mathbf{X}) = \sum_i x_i / p + \mathcal{N}(0, 0.1)$$

- Feedback function: from linear and non-linear function

$$\delta_{linear} = Y + \sum_{i=1}^p \{ I(i \bmod 2 = 0) \cdot (\frac{i}{2} + Y) x_i \} + \mathcal{N}(0, 3)$$

$$\begin{aligned} \delta_{nonlin} = & Y + \sum_{i=1}^p \{ I(i \bmod 2 = 0) \cdot (\frac{i}{2} + Y) x_i \} + \mathcal{N}(0, 3) \\ & + \sum_{i=1}^{p-1} \{ I(i \bmod 5 = 0) \cdot (\frac{i}{5} + Y) x_i x_{i+1} \} \end{aligned}$$

# Experiments on Synthetic Data

- Part of simulation results:

| Setting 1: $\delta = \delta_{linear}$ |                                 |                  |       |       |                   |       |       |                   |       |       |                    |       |       |
|---------------------------------------|---------------------------------|------------------|-------|-------|-------------------|-------|-------|-------------------|-------|-------|--------------------|-------|-------|
|                                       | n/p                             | n = 5000, p = 50 |       |       | n = 5000, p = 100 |       |       | n = 10000, p = 50 |       |       | n = 10000, p = 100 |       |       |
| $\pi_0$                               | Estimator                       | Bias(SD)         | MAE   | RMSE  | Bias(SD)          | MAE   | RMSE  | Bias(SD)          | MAE   | RMSE  | Bias(SD)           | MAE   | RMSE  |
| $\pi_{inv}$                           | $\widehat{U}_{R-IPS}(\pi)$      | 7.306(1.632)     | 7.305 | 7.486 | 21.03(6.842)      | 21.03 | 22.11 | 7.083(1.399)      | 7.083 | 7.220 | 20.31(6.726)       | 20.31 | 21.40 |
|                                       | $\widehat{U}_{DM}(\pi)$         | 2.168(0.505)     | 2.168 | 2.226 | 3.612(1.274)      | 3.612 | 3.832 | 1.953(0.302)      | 1.953 | 1.975 | 3.439(1.104)       | 3.439 | 3.620 |
|                                       | $\widehat{U}_{E-IPS}(\pi)$      | 0.120(0.923)     | 0.787 | 0.927 | 0.577(3.865)      | 2.983 | 3.905 | 0.102(0.742)      | 0.641 | 0.746 | 0.012(3.015)       | 2.346 | 3.012 |
|                                       | $\widehat{U}_{T-IPS}(\pi)$      | 0.111(1.837)     | 1.496 | 1.839 | 0.058(7.736)      | 5.911 | 7.741 | 0.197(1.769)      | 1.486 | 1.780 | 0.360(7.382)       | 5.885 | 7.395 |
|                                       | $\widehat{U}_{E-IPS}^{SN}(\pi)$ | 0.074(0.654)     | 0.540 | 0.659 | 0.013(1.696)      | 1.252 | 1.691 | 0.032(0.438)      | 0.350 | 0.438 | 0.430(1.299)       | 1.176 | 1.415 |
|                                       | $\widehat{U}_{DR}(\pi)$         | 0.056(0.576)     | 0.476 | 0.581 | 0.031(1.531)      | 1.079 | 1.512 | 0.021(0.398)      | 0.312 | 0.393 | 0.364(1.118)       | 0.974 | 1.197 |
|                                       | $\widehat{U}_{CB}(\pi)$         | 0.058(0.938)     | 0.755 | 0.942 | 0.093(3.363)      | 2.739 | 3.348 | 0.164(0.596)      | 0.499 | 0.620 | 0.256(2.681)       | 2.153 | 2.709 |
|                                       | $\widehat{U}_{FCB}(\pi)$        | 0.008(0.492)     | 0.404 | 0.494 | 0.128(1.250)      | 0.904 | 1.295 | 0.014(0.345)      | 0.285 | 0.357 | 0.213(0.935)       | 0.775 | 0.972 |

**Estimated propensity score is better than true propensity score.**  
**True propensity score is closer to 0 or 1, leading to high variance.**

# Experiments on Synthetic Data

- Part of simulation results:

| Setting 1: $\delta = \delta_{linear}$ |                                 |                      |              |              |                      |              |              |                      |              |              |                      |              |              |
|---------------------------------------|---------------------------------|----------------------|--------------|--------------|----------------------|--------------|--------------|----------------------|--------------|--------------|----------------------|--------------|--------------|
|                                       | n/p                             | n = 5000, p = 50     |              |              | n = 5000, p = 100    |              |              | n = 10000, p = 50    |              |              | n = 10000, p = 100   |              |              |
| $\pi_0$                               | Estimator                       | Bias(SD)             | MAE          | RMSE         |
| $\pi_{inv}$                           | $\widehat{U}_{R-IPS}(\pi)$      | 7.306(1.632)         | 7.305        | 7.486        | 21.03(6.842)         | 21.03        | 22.11        | 7.083(1.399)         | 7.083        | 7.220        | 20.31(6.726)         | 20.31        | 21.40        |
|                                       | $\widehat{U}_{DM}(\pi)$         | 2.168(0.505)         | 2.168        | 2.226        | 3.612(1.274)         | 3.612        | 3.832        | 1.953(0.302)         | 1.953        | 1.975        | 3.439(1.104)         | 3.439        | 3.620        |
|                                       | $\widehat{U}_{E-IPS}(\pi)$      | 0.120(0.923)         | 0.787        | 0.927        | 0.577(3.865)         | 2.983        | 3.905        | 0.102(0.742)         | 0.641        | 0.746        | <b>0.012</b> (3.015) | 2.346        | 3.012        |
|                                       | $\widehat{U}_{T-IPS}(\pi)$      | 0.111(1.837)         | 1.496        | 1.839        | 0.058(7.736)         | 5.911        | 7.741        | 0.197(1.769)         | 1.486        | 1.780        | 0.360(7.382)         | 5.885        | 7.395        |
|                                       | $\widehat{U}_{E-IPS}^{SN}(\pi)$ | 0.074(0.654)         | 0.540        | 0.659        | <b>0.013</b> (1.696) | 1.252        | 1.691        | 0.032(0.438)         | 0.350        | 0.438        | 0.430(1.299)         | 1.176        | 1.415        |
|                                       | $\widehat{U}_{DR}(\pi)$         | 0.056(0.576)         | 0.476        | 0.581        | 0.031(1.531)         | 1.079        | 1.512        | 0.021(0.398)         | 0.312        | 0.393        | 0.364(1.118)         | 0.974        | 1.197        |
|                                       | $\widehat{U}_{CB}(\pi)$         | 0.058(0.938)         | 0.755        | 0.942        | 0.093(3.363)         | 2.739        | 3.348        | 0.164(0.596)         | 0.499        | 0.620        | 0.256(2.681)         | 2.153        | 2.709        |
|                                       | $\widehat{U}_{FCB}(\pi)$        | <b>0.008</b> (0.492) | <b>0.404</b> | <b>0.494</b> | 0.128(1.250)         | <b>0.904</b> | <b>1.295</b> | <b>0.014</b> (0.345) | <b>0.285</b> | <b>0.357</b> | 0.213(0.935)         | <b>0.775</b> | <b>0.972</b> |

**CB estimator performs not very well.**  
 Because it ignores the action discrepancy from the new policy

# Experiments on Synthetic Data

- Part of simulation results:

| Setting 1: $\delta = \delta_{linear}$ |                                 |                      |              |              |                      |              |              |                      |              |              |                      |              |              |
|---------------------------------------|---------------------------------|----------------------|--------------|--------------|----------------------|--------------|--------------|----------------------|--------------|--------------|----------------------|--------------|--------------|
|                                       | n/p                             | $n = 5000, p = 50$   |              |              | $n = 5000, p = 100$  |              |              | $n = 10000, p = 50$  |              |              | $n = 10000, p = 100$ |              |              |
| $\pi_0$                               | Estimator                       | Bias(SD)             | MAE          | RMSE         |
| $\pi_{inv}$                           | $\widehat{U}_{R-IPS}(\pi)$      | 7.306(1.632)         | 7.305        | 7.486        | 21.03(6.842)         | 21.03        | 22.11        | 7.083(1.399)         | 7.083        | 7.220        | 20.31(6.726)         | 20.31        | 21.40        |
|                                       | $\widehat{U}_{DM}(\pi)$         | 2.168(0.505)         | 2.168        | 2.226        | 3.612(1.274)         | 3.612        | 3.832        | 1.953(0.302)         | 1.953        | 1.975        | 3.439(1.104)         | 3.439        | 3.620        |
|                                       | $\widehat{U}_{E-IPS}(\pi)$      | 0.120(0.923)         | 0.787        | 0.927        | 0.577(3.865)         | 2.983        | 3.905        | 0.102(0.742)         | 0.641        | 0.746        | <b>0.012</b> (3.015) | 2.346        | 3.012        |
|                                       | $\widehat{U}_{T-IPS}(\pi)$      | 0.111(1.837)         | 1.496        | 1.839        | 0.058(7.736)         | 5.911        | 7.741        | 0.197(1.769)         | 1.486        | 1.780        | 0.360(7.382)         | 5.885        | 7.395        |
|                                       | $\widehat{U}_{E-IPS}^{SN}(\pi)$ | 0.074(0.654)         | 0.540        | 0.659        | <b>0.013</b> (1.696) | 1.252        | 1.691        | 0.032(0.438)         | 0.350        | 0.438        | 0.430(1.299)         | 1.176        | 1.415        |
|                                       | $\widehat{U}_{DR}(\pi)$         | 0.056(0.576)         | 0.476        | 0.581        | 0.031(1.531)         | 1.079        | 1.512        | 0.021(0.398)         | 0.312        | 0.393        | 0.364(1.118)         | 0.974        | 1.197        |
|                                       | $\widehat{U}_{CB}(\pi)$         | 0.058(0.938)         | 0.755        | 0.942        | 0.093(3.363)         | 2.739        | 3.348        | 0.164(0.596)         | 0.499        | 0.620        | 0.256(2.681)         | 2.153        | 2.709        |
| $\widehat{U}_{FCB}(\pi)$              | $\widehat{U}_{FCB}(\pi)$        | <b>0.008</b> (0.492) | <b>0.404</b> | <b>0.494</b> | 0.128(1.250)         | <b>0.904</b> | <b>1.295</b> | <b>0.014</b> (0.345) | <b>0.285</b> | <b>0.357</b> | 0.213(0.935)         | <b>0.775</b> | <b>0.972</b> |

With considering the action discrepancy, Our FCB estimator can consistently improve the performance of policy evaluation.

# Experiment - Classifier evaluation

- A classifier can be defined as a **policy** based on a given dataset
  - Features of samples~ **context**  $\mathbf{X}$
  - Predicted label of samples ~ **action**  $\hat{Y}$  predicted by the classifier
  - **Feedback function:**  $\delta(\mathbf{X}, Y) = I(Y = Y^t)$ . ( $Y^t$  is the true label)
  - The **policy evaluation** is equivalent to the evaluation of the **classifier accuracy**
- Datasets: several multiclass classification bench-mark from UCI-repository.
- The new policy to be evaluated
  - **Logistic regression model** trained on the training set
- The past policy:
  - A simple function **based on one feature variable**

# Experiments - Classifier evaluation

| Estimator                              | Dataset:glass        |              |       | Dataset:wilt         |              |       | Dataset:pageblock    |              |              | Dataset:particle     |              |              |
|--|----------------------|--------------|-------|----------------------|--------------|-------|----------------------|--------------|--------------|----------------------|--------------|--------------|
|  | Bias(SD)             | MAE          | RMSE  | Bias(SD)             | MAE          | RMSE  | Bias(SD)             | MAE          | RMSE         | Bias(SD)             | MAE          | RMSE         |
| $\widehat{U}_{R\text{-}IPS}(\pi)$      | 0.711(7.805)         | 5.961        | 7.837 | 0.750(1.090)         | 1.112        | 1.323 | 42.19(2.711)         | 42.19        | 42.28        | 4.093(0.432)         | 4.093        | 4.116        |
| $\widehat{U}_{DM}(\pi)$                | 8.810(4.164)         | 8.810        | 9.744 | 0.096(0.380)         | 0.309        | 0.391 | 2.224(0.444)         | 2.224        | 2.267        | 0.741(0.228)         | 0.741        | 0.776        |
| $\widehat{U}_{E\text{-}IPS}(\pi)$      | 1.648(5.707)         | 4.739        | 5.940 | 0.128(0.323)         | 0.267        | 0.347 | 4.723(3.991)         | 5.788        | 6.184        | 0.230(0.281)         | 0.287        | 0.362        |
| $\widehat{U}_{T\text{-}IPS}(\pi)$      | 1.488(6.162)         | 4.866        | 6.339 | 0.175(1.205)         | 0.983        | 1.217 | <b>0.324</b> (2.327) | 1.794        | 2.348        | <b>0.012</b> (0.553) | 0.447        | 0.554        |
| $\widehat{U}_{E\text{-}IPS}^{SN}(\pi)$ | 0.315(5.455)         | 4.447        | 5.465 | 0.121(0.322)         | 0.265        | 0.343 | 1.539(2.326)         | 2.247        | 2.788        | 0.091(0.277)         | 0.222        | 0.293        |
| $\widehat{U}_{CB}(\pi)$                | <b>0.094</b> (6.364) | 5.028        | 6.365 | 0.165(0.337)         | 0.318        | 0.372 | 4.660(2.810)         | 5.014        | 5.442        | 0.277(0.325)         | 0.347        | 0.429        |
| $\widehat{U}_{DR}(\pi)$                | 1.035(5.334)         | 4.420        | 5.434 | 0.129(0.323)         | 0.269        | 0.347 | 1.734(1.978)         | 2.152        | 2.630        | 0.124(0.276)         | 0.228        | 0.303        |
| $\widehat{U}_{FCB}(\pi)$               | 0.562(5.242)         | <b>4.098</b> | 5.273 | <b>0.024</b> (0.329) | <b>0.250</b> | 0.328 | 0.747(0.617)         | <b>0.791</b> | <b>0.968</b> | 0.080(0.261)         | <b>0.215</b> | <b>0.272</b> |

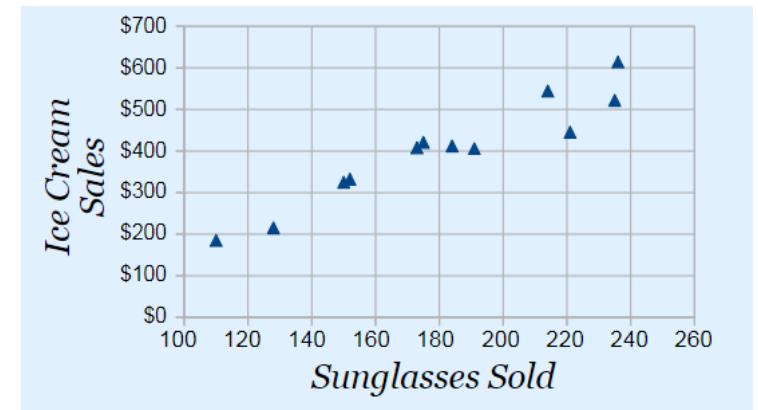
By simultaneously considering the **distribution shift** and **action discrepancy**, Our FCB algorithm performs the best for offline policy evaluation.

# Summary: Causal Inference for Offline Policy Evaluation

- Challenges of offline policy evaluation:
  - Distribution shift induced by the past policy ← **Related work**
  - Action discrepancy induced by the new policy
  - Model dependency
- **Focused Context Balancing**
  - To remove the model dependency
  - Simultaneously consider distribution shift and action discrepancy
  - Significantly improve the accuracy on policy evaluation
  - **Supporting for decision making, which policy is the best to deploy**

# Summary: Causally Regularized Machine Learning

- We have highly accurate predictions, but they are not enough for:
  - Interpretable prediction
  - Stable/Robust prediction in the future
  - Decision making



Algorithm A



Algorithm B



# Summary: Causally Regularized Machine Learning

- Causal Inference with Observational Data
  - Recover causation from observed correlation
  - Estimating causal effect for improving **interpretability**
- Causal Inference for Stable Prediction
  - Disrupt spurious correlation, embrace causation
  - **Interpretable and Stable prediction** in the future
- Causal Inference for Offline Policy Evaluation
  - Evaluating a new policy based on the log data from a past policy
  - Support **decision making** with the effect of new policies

# OUTLINE

PART I. Introduction to Causal Inference

PART II. Methods for Causal Inference

PART III. Causally Regularized Machine Learning

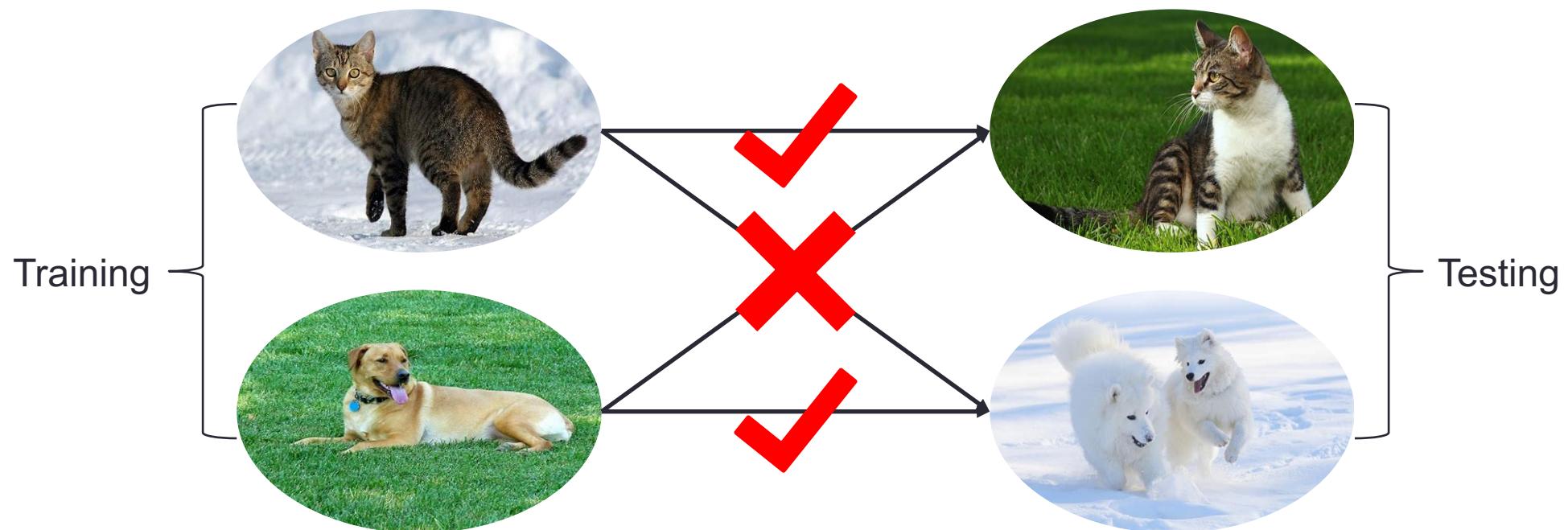
**PART IV. Benchmark and Open Datasets**

PART V. Conclusion and Discussion

# TOWARDS NON-I.I.D. IMAGE CLASSIFICATION: A DATASET AND BASELINES

Correlation V.S. Causation

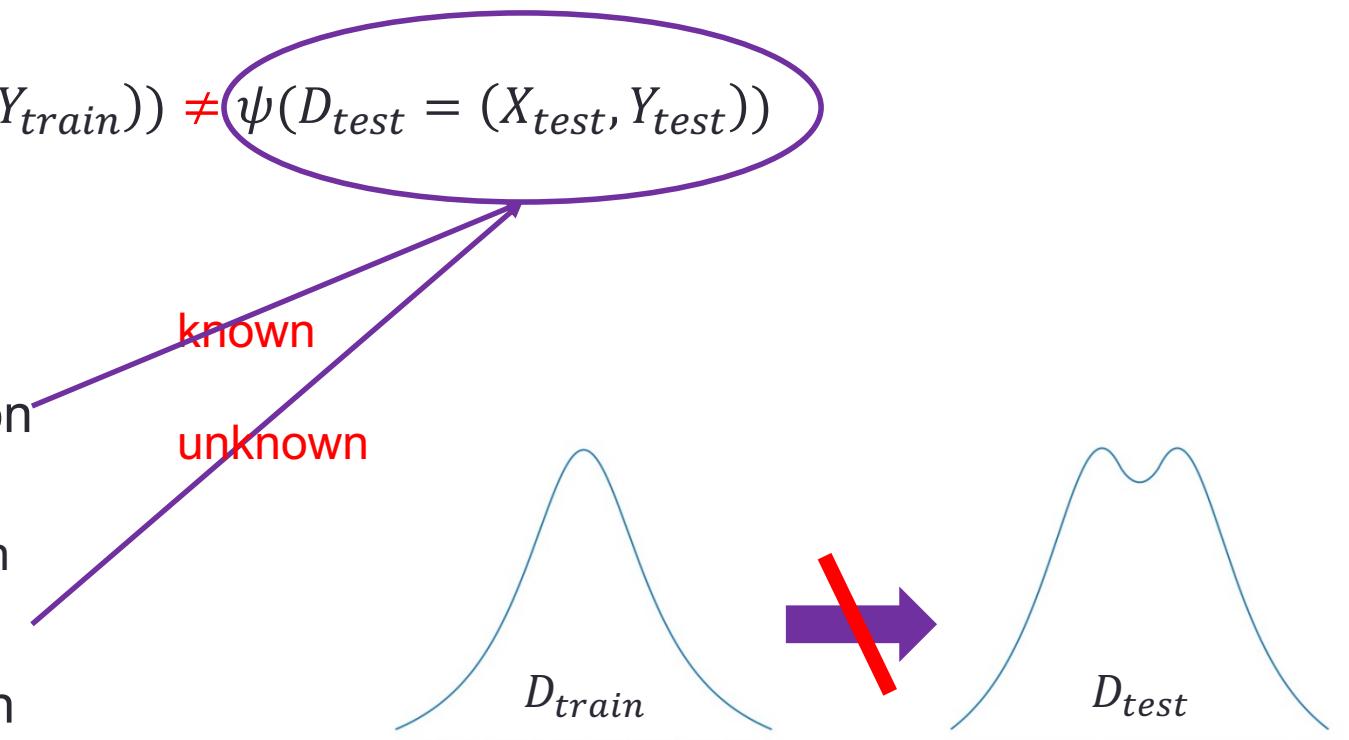
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# Non-I.I.D. Image Classification

- Non I.I.D. Image Classification

- Two tasks
  - Targeted Non-I.I.D. Image Classification
    - Have prior knowledge on testing data
    - e.g. transfer learning, domain adaptation
  - General Non-I.I.D. Image Classification
    - Testing is unknown, no prior
    - more practical & realistic



# Existence of Non-I.I.Dness

- One metric (NI) for Non-I.I.Dness

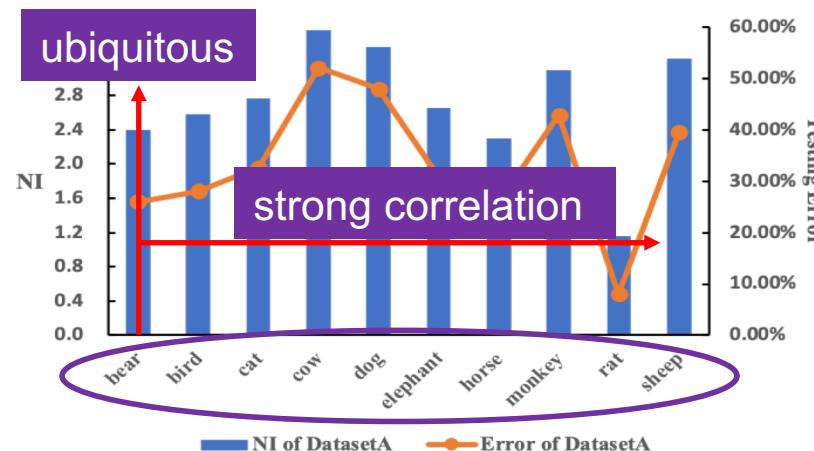
**Definition 1 Non-I.I.D. Index (NI)** Given a feature extractor  $g_\varphi(\cdot)$  and a class  $C$ , **the degree of distribution shift** between training data  $D_{train}^C$  and testing data  $D_{test}^C$  is defined as:

$$NI(C) = \frac{\left\| \overline{g_\varphi(X_{train}^C)} - \overline{g_\varphi(X_{test}^C)} \right\|_2}{\sigma(g_\varphi(X_{train}^C \cup X_{test}^C))},$$

**Distribution shift**

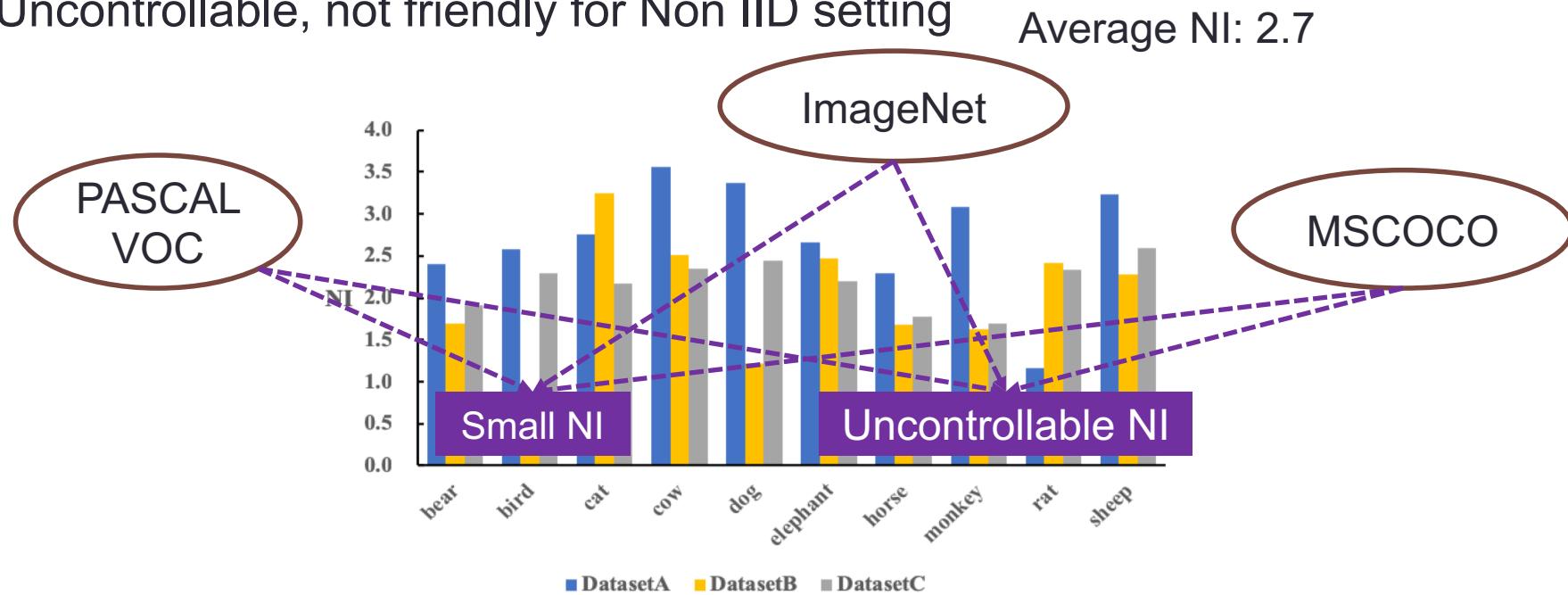
**For normalization**

- Existence of Non-I.I.Dness on Dataset consisted of 10 subclasses from ImageNet
- For each class
  - Training data
  - Testing data
  - CNN for prediction



# Related Datasets

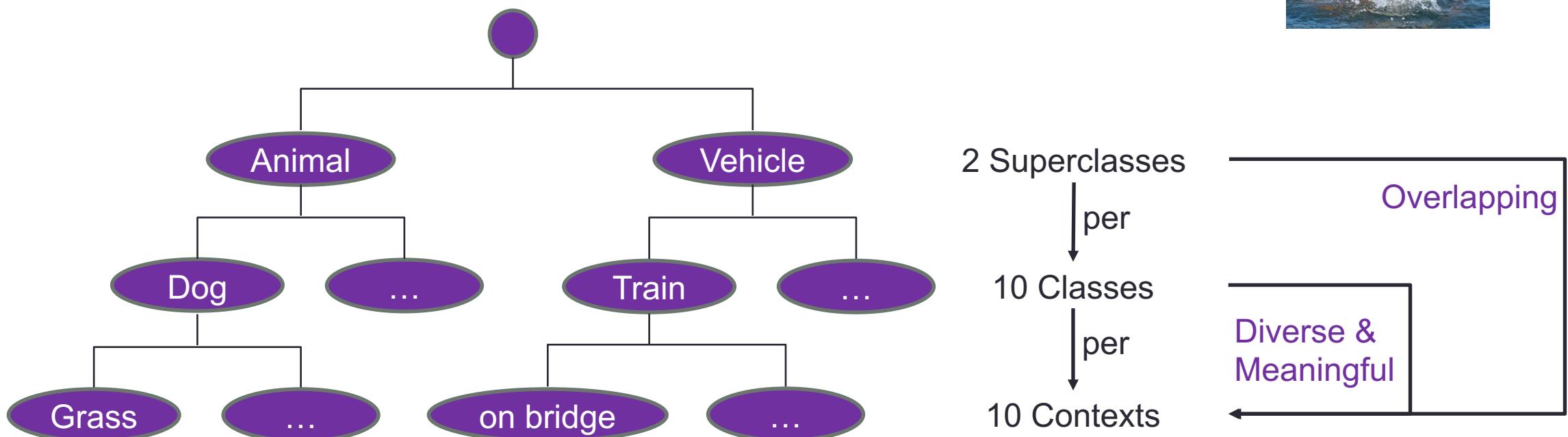
- DatasetA & DatasetB & DatasetC
  - NI is ubiquitous, but small on these datasets
  - NI is Uncontrollable, not friendly for Non IID setting



A dataset for Non-I.I.D. image classification is demanded.

# NICO - Non-I.I.D. Image Dataset with Contexts

- **NICO** Datasets:
- Object label: e.g. dog
- Contextual labels (Contexts)
  - the background or scene of a object, e.g. grass/water
- Structure of NICO



# NICO - Non-I.I.D. Image Dataset with Contexts

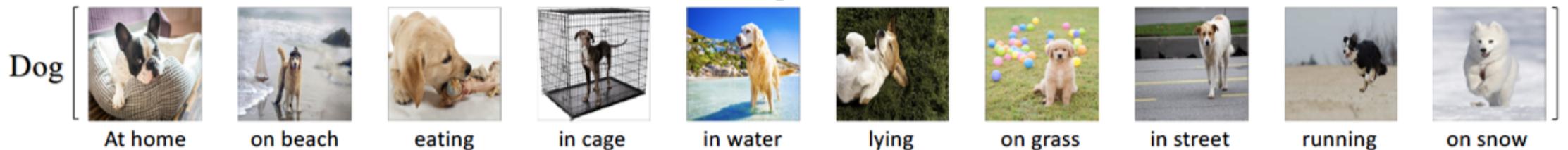
- Data size of each class in NICO
  - Sample size: thousands for each class
  - Each superclass: 10,000 images
  - Sufficient for some basic neural networks (CNN)
- Samples with contexts in NICO

| <i>Animal</i> | DATA SIZE | <i>Vehicle</i> | DATA SIZE |
|---------------|-----------|----------------|-----------|
| BEAR          | 1609      | AIRPLANE       | 930       |
| BIRD          | 1590      | BICYCLE        | 1639      |
| CAT           | 1479      | BOAT           | 2156      |
| COW           | 1192      | BUS            | 1009      |
| DOG           | 1624      | CAR            | 1026      |
| ELEPHANT      | 1178      | HELICOPTER     | 1351      |
| HORSE         | 1258      | MOTORCYCLE     | 1542      |
| MONKEY        | 1117      | TRAIN          | 750       |
| RAT           | 846       | TRUCK          | 1000      |
| SHEEP         | 918       |                |           |



# Controlling NI on NICO Dataset

- Minimum Bias (comparing with ImageNet)
- Proportional Bias (controllable)
  - Number of samples in each context
- Compositional Bias (controllable)
  - Number of contexts that observed



# Minimum Bias

- In this setting, the way of random sampling leads to minimum distribution shift between training and testing distributions in dataset, which simulates **a nearly i.i.d. scenario**.
  - 8000 samples for training and 2000 sample for testing in each superclass (ConvNet)

|         | Average NI | Testing Accuracy |
|---------|------------|------------------|
| Animal  | 3.85       | 49.6%            |
| Vehicle | 3.20       | 63.0%            |

Average NI on ImageNet: 2.7

Images in our NICO  
are with **rich contextual  
information**

more **challenging** for  
image classification

Our NICO data is more Non-iid, more challenging

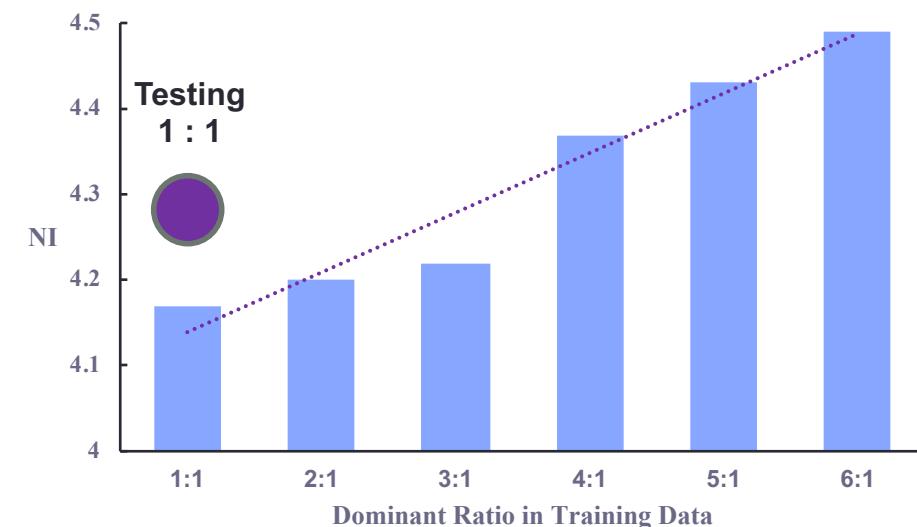
# Proportional Bias

- Given a class, when sampling positive samples, we use **all contexts** for both training and testing, but the **percentage of each context** is different between training and testing dataset.



$$\text{Dominant Ratio} = \frac{N_{dominant}}{N_{minor}}$$

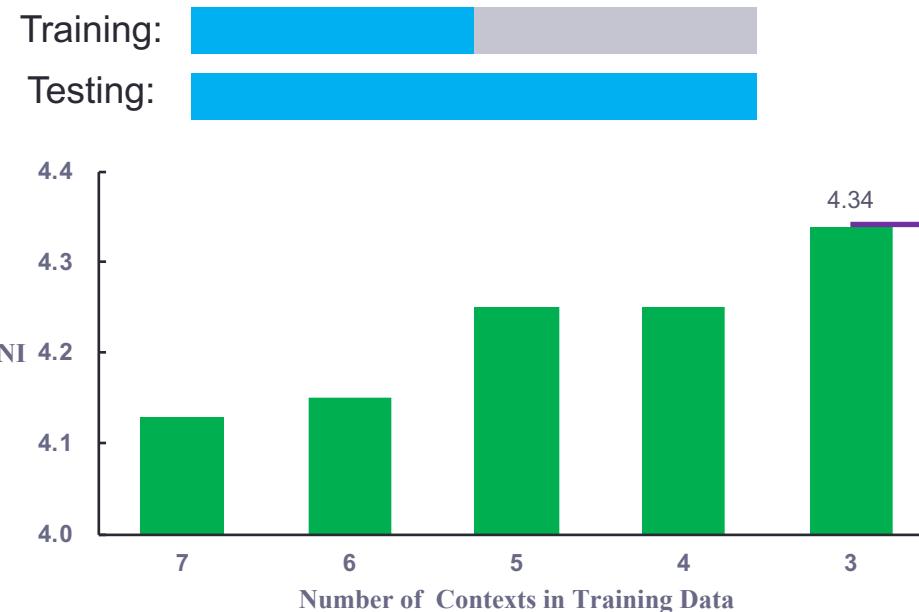
We can control NI by varying dominate ratio



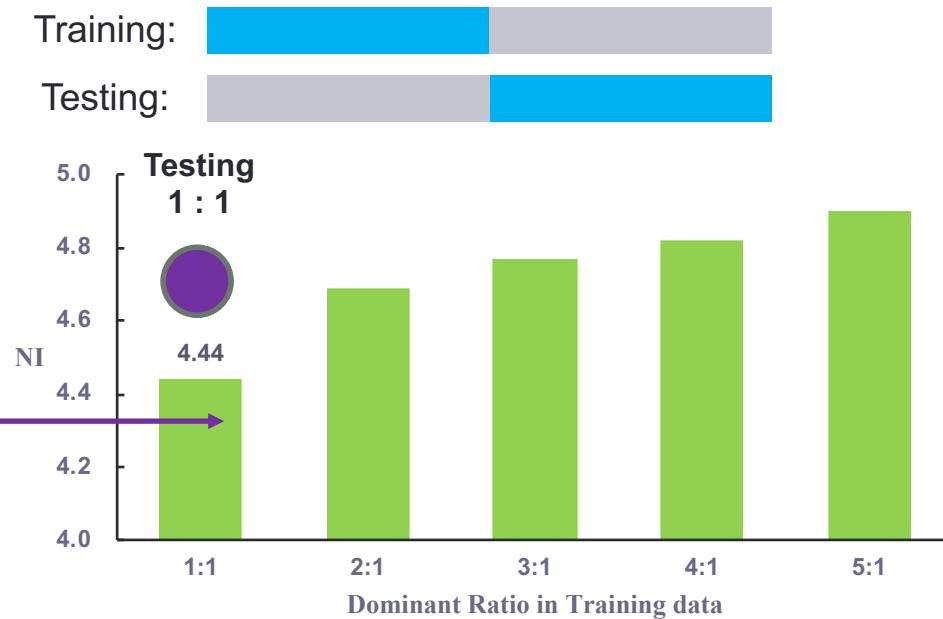
# Compositional Bias

$$\text{Dominant Ratio} = \frac{N_{\text{dominant}}}{N_{\text{minor}}}$$

- Given a class, the observed contexts are different between training and testing data.



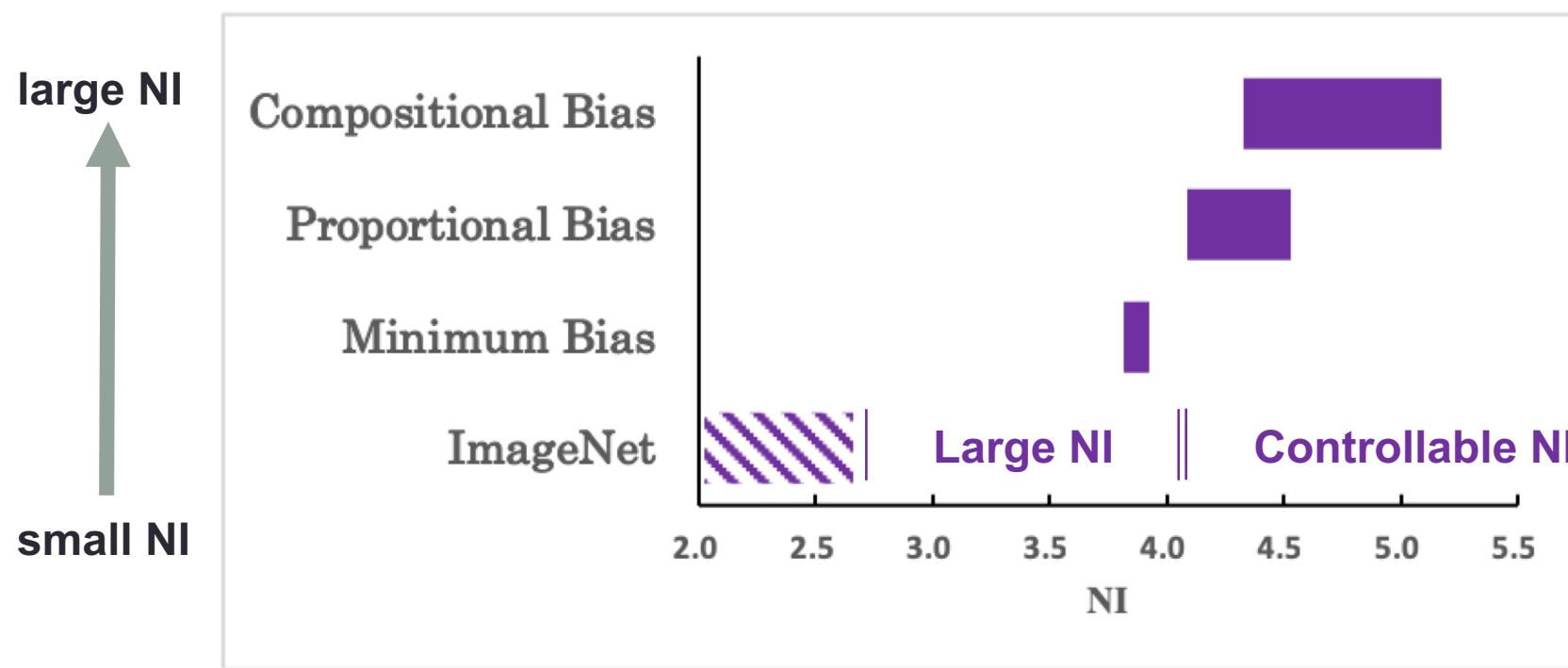
Moderate setting  
(Overlap)



Radical setting  
(No Overlap & Dominant ratio)

# NICO - Non-I.I.D. Image Dataset with Contexts

- Summary on Non-iidness on our dataset
- Range of NI value for each method
- Large and controllable NI

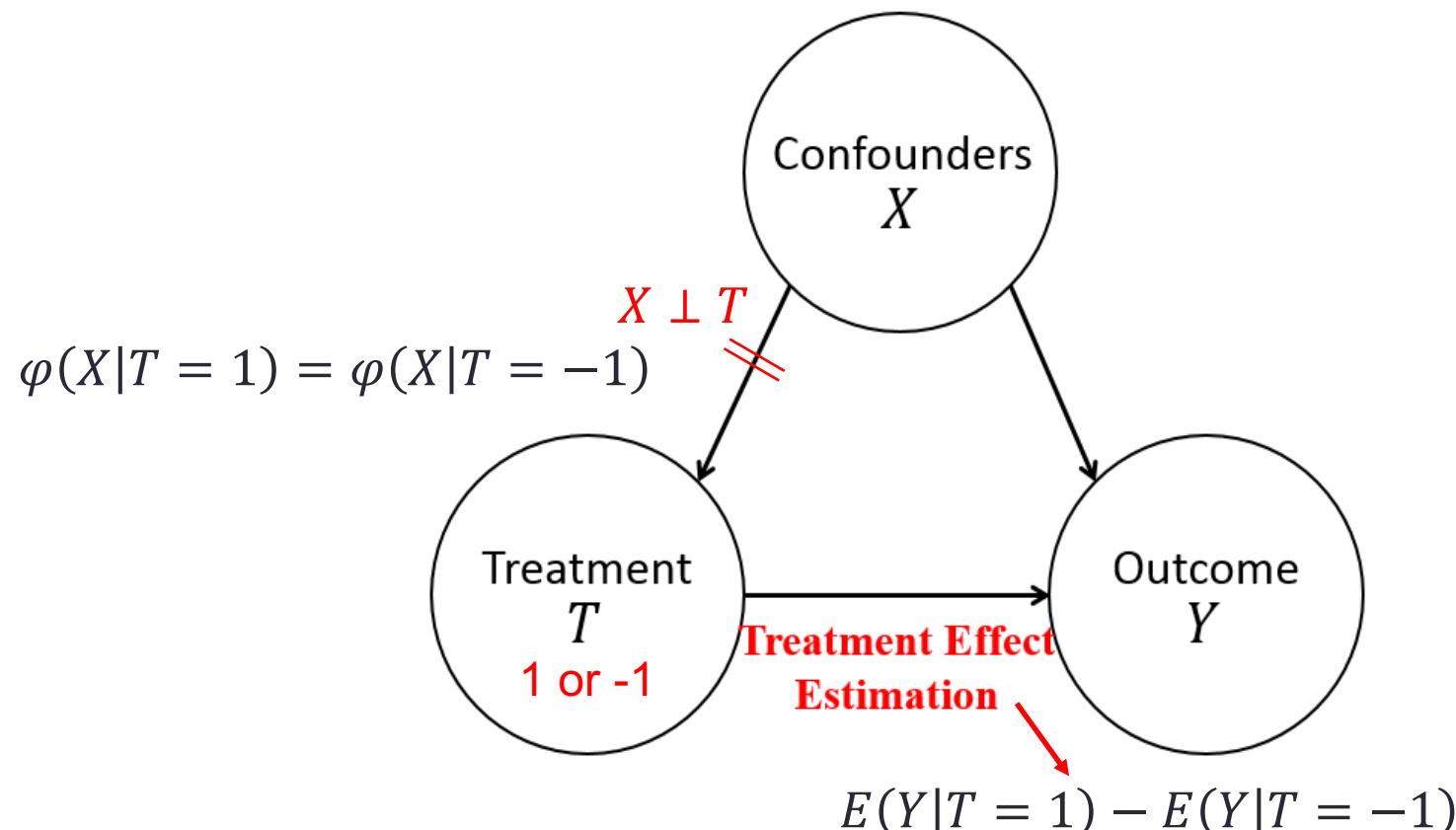


Targeted/General Non-I.I.D.  
Image Classification

Global Balancing Method

# ConvNet with Batch Balancing (CNBB)

- Confounder Balancing in the literature of Causal Inference

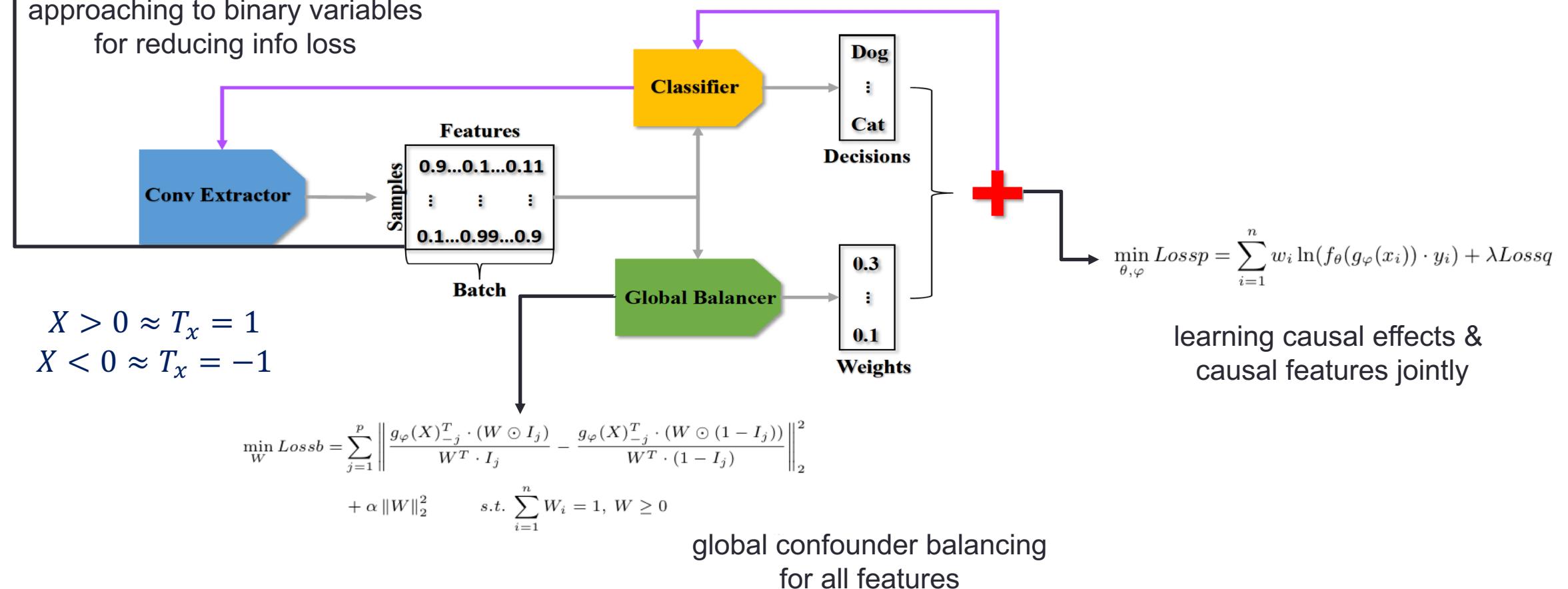


CNBB = Confounder balancing + ConvNet

# ConvNet with Batch Balancing (CNBB)

$$\text{Loss}_{\text{sq}} = - \sum_{i=1}^n \|g_\varphi(x_i)\|_2^2$$

approaching to binary variables  
for reducing info loss



# Experiments

- We design four experiments according to the supported Non-I.I.D. settings of NICO:
  - Minimum bias (Exp 1)
    - **Nearly I.I.D.** in NICO (average improvement **0.33%**)
  - Proportional bias (Exp2)
    - **Different dominate ratio**
    - fix dominant ratio of training to 5:1
    - vary dominant ratio of testing from 1:5 to 4:1
  - Compositional bias (Exp3)
    - **Different observed contexts**
    - Testing: with all contexts
    - Training: vary observed contexts from 3 to 7
  - Combined Proportional & Compositional bias (Exp4)
    - **No overlap on the observed contexts**
    - **Different dominate ratio**
    - fix dominant ratio of testing to 1:1
    - vary dominant ratio of training from 1:1 to 5:1

always  
superior

| Exp2        | 1 : 5        | 1 : 1        | 2 : 1        | 3 : 1        | 4 : 1        |
|-------------|--------------|--------------|--------------|--------------|--------------|
| CNN         | 37.17        | 37.80        | 41.46        | 42.50        | 43.23        |
| CNN+BN      | 38.70        | <b>39.60</b> | 41.64        | 42.00        | 43.85        |
| <b>CNBB</b> | <b>39.06</b> | <b>39.60</b> | <b>42.12</b> | <b>43.33</b> | <b>44.15</b> |

Table 1. Performances of different methods on test accuracy (%) for proportional bias in *Animal* superclass.

| Exp3        | 3            | 4            | 5            | 6            | 7            |
|-------------|--------------|--------------|--------------|--------------|--------------|
| CNN         | 40.61        | 42.32        | 43.34        | 44.03        | 44.03        |
| CNN+BN      | <b>41.98</b> | 38.85        | 43.12        | 44.71        | 44.31        |
| <b>CNBB</b> | 41.41        | <b>43.34</b> | <b>44.54</b> | <b>45.96</b> | <b>45.16</b> |

Table 2. Performances of different methods on test accuracy (%) for compositional bias in *Vehicle* superclass.

| Exp4        | 1 : 1        | 2 : 1        | 3 : 1        | 4 : 1        | 5 : 1        |
|-------------|--------------|--------------|--------------|--------------|--------------|
| CNN         | 37.07        | 35.20        | 34.53        | 34.13        | 33.73        |
| CNN+BN      | 33.87        | 32.93        | 31.20        | 30.93        | 30.67        |
| <b>CNBB</b> | <b>38.98</b> | <b>36.89</b> | <b>35.87</b> | <b>35.33</b> | <b>35.02</b> |

Table 3. Performances of different methods of test accuracy (%) for combined proportional & compositional bias in *Vehicle* superclass.

# Summary on Experimental Results

- The range of NI with respect to the average improvement of performance to CNN

| Experiment | Improvement  | NI          |
|------------|--------------|-------------|
| Exp1       | 0.33%        | 3.81 - 3.93 |
| Exp2       | 1.22% more   | 4.17 - 4.53 |
| Exp3       | 1.22% effect | 4.13 - 4.34 |
| Exp4       | 1.49%        | 4.44 - 4.90 |

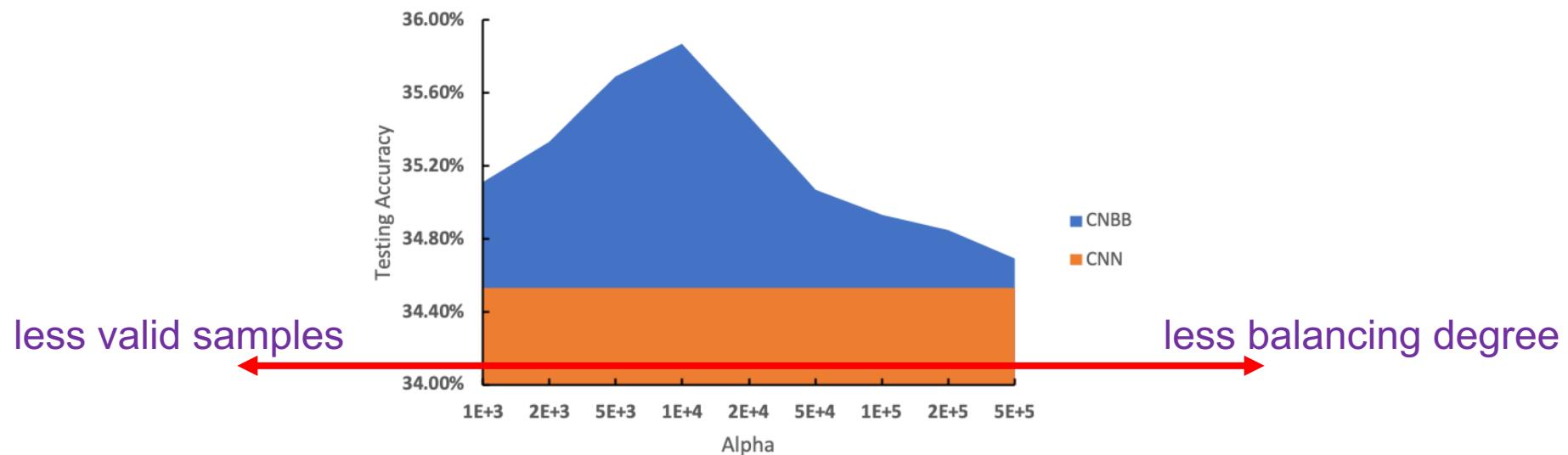
more bias

# Analysis

- Insight of Batch Balancing Mechanism

$$\min_W Loss_{sb} = \sum_{j=1}^p \left\| \frac{g_\varphi(X)_{-j}^T \cdot (W \odot I_j)}{W^T \cdot I_j} - \frac{g_\varphi(X)_{-j}^T \cdot (W \odot (1 - I_j))}{W^T \cdot (1 - I_j)} \right\|_2^2$$

$$+ \alpha \|W\|_2^2 \quad s.t. \quad \sum_{i=1}^n W_i = 1, \quad W \geq 0$$



# Summary: NICO for Non-iid Image Classification

- **NICO**: Non-iid image classification dataset
  - Non-iid Index (NI) to describe the distribution shift
  - Three ways to control NI in NICO Dataset
  - Benchmark for Non-iid image classification
- The performance of benchmark is not so exciting, more work need to do.
- How to use causal knowledge for Non-iid prediction

# OUTLINE

**PART I. Introduction to Causal Inference**

**PART II. Methods for Causal Inference**

**PART III. Causally Regularized Machine Learning**

**PART IV. Benchmark and Open Datasets**

**PART V. Conclusion and Discussion**

# Conclusion

- Correlation-based machine learning are not enough for
  - Interpretable learning
  - Decision making
  - Stable/Robust prediction in the future
- Correlation: causation, confounding, selection bias
  - Causation: Invariant and Stable across environments
  - Confounding / Selection bias: Spurious correlation, changeable
- Causally Regularized Machine Learning:
  - Causal regularizer
  - Recover causation from correlation
  - Causation-based machine learning

# Conclusion

- Causally Regularized Machine Learning: Causation-based
  - **Causal Inference** for Interpretable learning
  - **Policy Evaluation** for Decision making
  - **Causally Regularized Stable Prediction** in the future
- **NICO**: Non-iid image classification dataset
  - **Non-iid Index (NI)** to describe the distribution shift
  - Three ways to **control NI** in NICO Dataset
  - **Benchmark** for Non-iid image classification

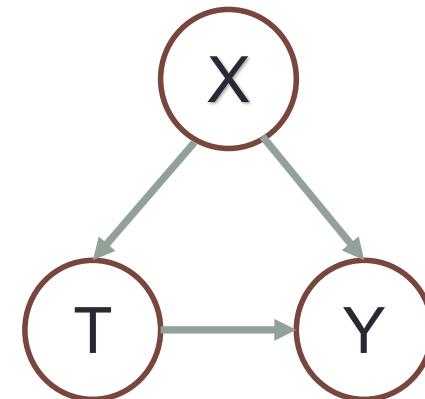
# Future Work and Discussion

- Correlation



Correlation Framework

- Causation



Causal Framework

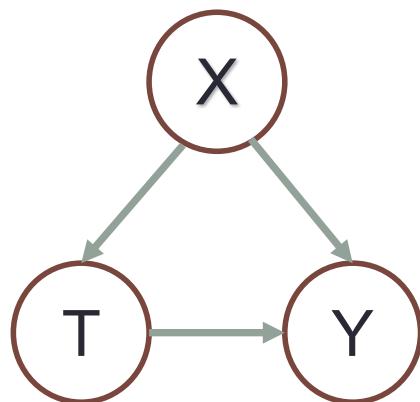
Recover causation from the observed correlation!

# Future Work and Discussion

- With Causality, we can do:
  - Recover causation for **interpretability**
  - Help to guide **decision making (actionable)**
  - Make **stable and robust prediction** in the future
  - Prevent algorithmic bias (**Fairness**)
- **Discard spurious correlation and embrace causality**
- **Do interpretable, actionable, stable, fairness prediction**

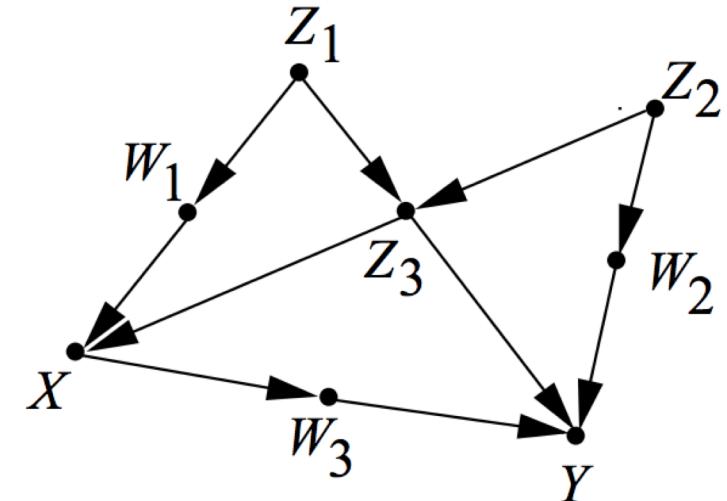
# Future Work and Discussion

- Potential Outcome Framework
  - Rubin
- Structural Causal Model (SCM)
  - Pearl



Potential Outcome  
Framework

Many untestable assumptions



SCM

Strong prior knowledge

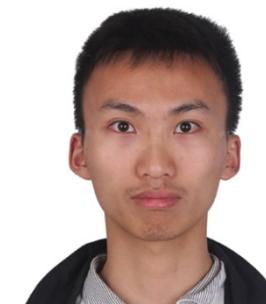
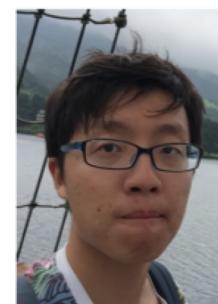
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# Acknowledgement



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Thank You!