

# Estimating Individual Treatment Effect: Generalization Bounds and Algorithms

Uri Shalit · Fredrik D Johansson · David Sontag

Presenters: Vahid & Tom

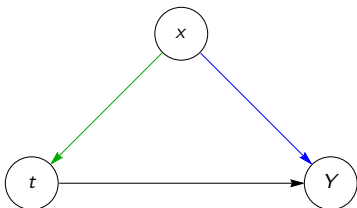
November 19, 2021

## Recall: Potential Outcomes

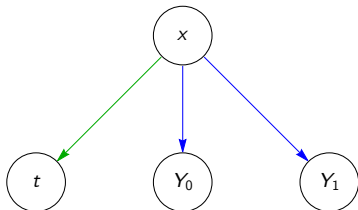
### Potential Outcomes

For covariates  $X$  and binary treatment  $T$ , potential outcomes  $Y_0(x)$  and  $Y_1(x)$  are defined as

$$Y_i(x) = \mathbb{E}[Y|X = x, do(T = i)]$$



(a) Causal graph for treatment-effect



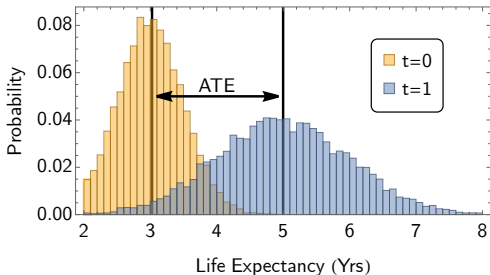
(b) Causal graph after replacing  $Y$  with  $Y_0$  and  $Y_1$

# Recall: Average Treatment Effect

## Average Treatment Effect (ATE)

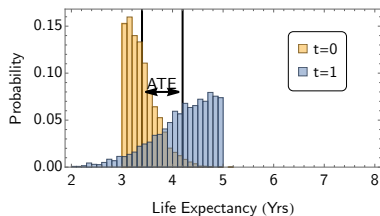
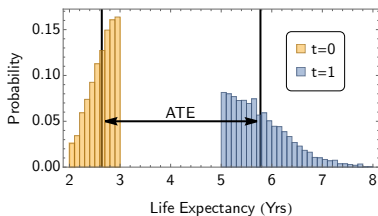
ATE is the difference in mean potential outcomes, i.e.,

$$\text{ATE} \triangleq \mathbb{E}_x[Y_1(x)] - \mathbb{E}_x[Y_0(x)]$$



# ATE with Selection Bias

Selection bias may occur when treatment and control groups are not chosen randomly

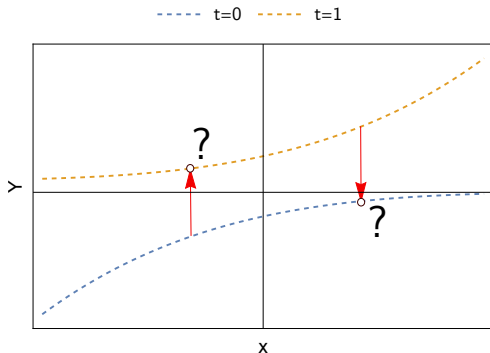


# Individual Treatment Effect

## Individual Treatment Effect (ITE)

Answers the question of how well does an **individual**  $x$  respond to a treatment

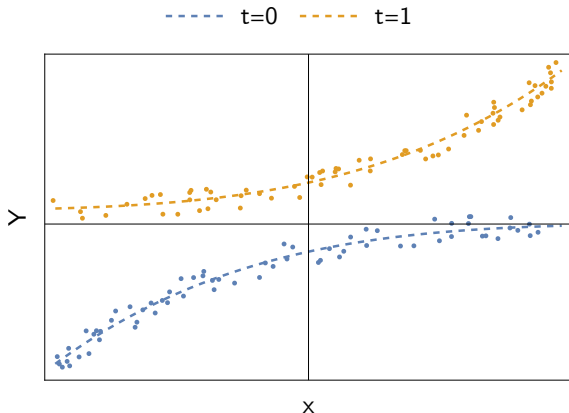
$$\text{ITE} \triangleq \mathbb{E}[Y_1|x] - \mathbb{E}[Y_0|x]$$



# Learning ITE

Learn  $m_1(x) = \hat{Y}_1(x)$  and  $m_0(x) = \hat{Y}_0(x)$  using supervised learning:

$$\widehat{\text{ITE}} = m_1(x) - m_0(x)$$



## Learning ITE: Problems

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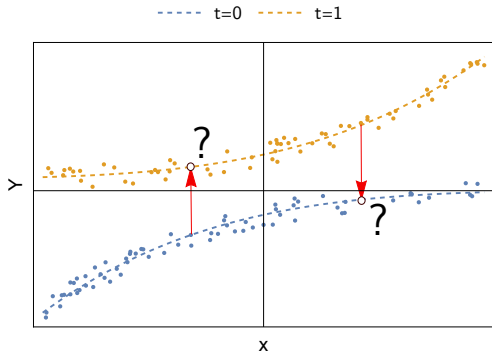
- ▶ An individual  $x$  is either treated or not
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**Figure:** For each  $x$ , only one potential outcome is observed. One can use similar samples to estimate the other.

# Learning ITE: Problems

- ▶ In observational datasets  $x$  and  $t$  may not be independent

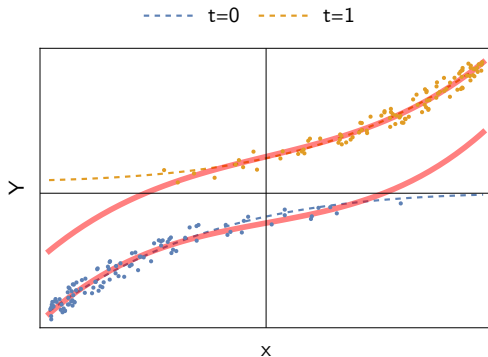
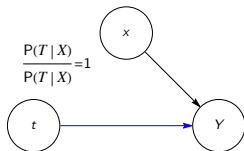
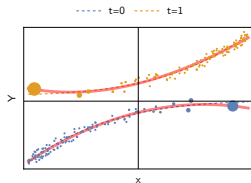
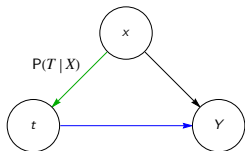
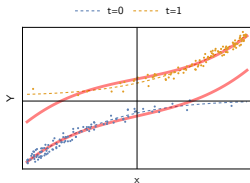


Figure: Induced selection bias from dependence between  $x$  and  $t$

# Inverse Propensity Score Weighting

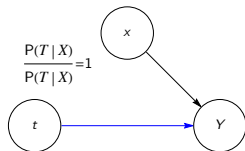
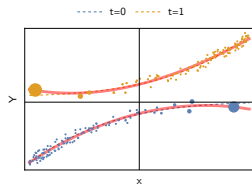
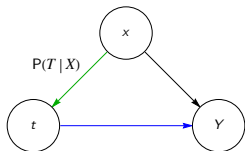
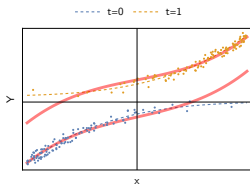
Turn observational data into pseudo-randomized trial data by re-weighting samples<sup>1</sup>



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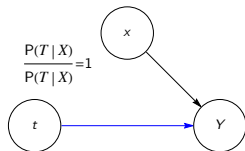
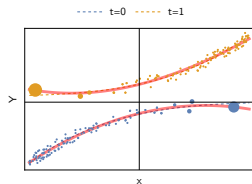
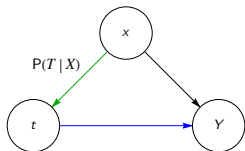
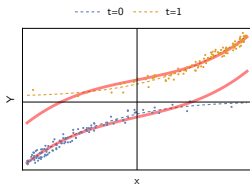


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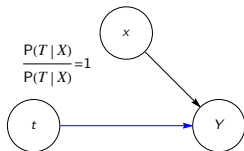
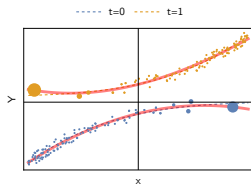
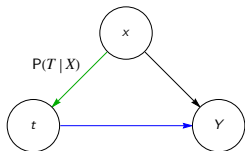
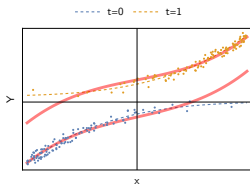


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- ▶ Small  $P(T|X)$  creates large variance

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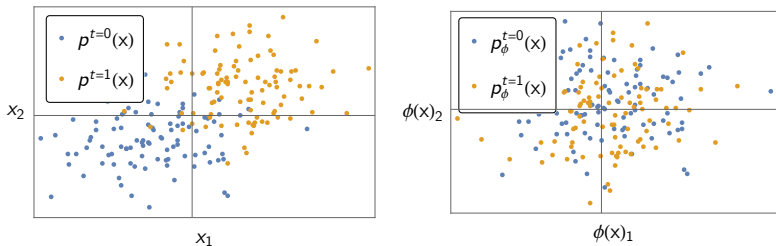
- ▶ Need to estimate  $P(T|X)$ , which is difficult for high-dim  $X$
- ▶ Small  $P(T|X)$  creates large variance
- ▶ Works primarily for ATE

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# Unbiased Representation Learning

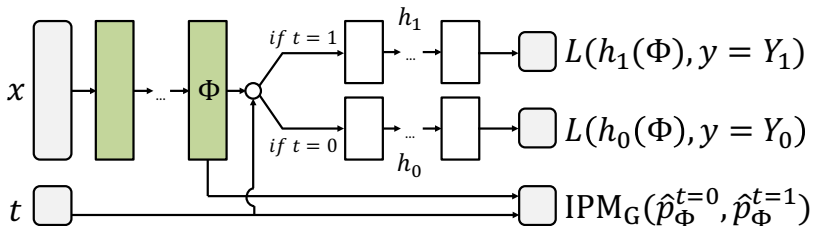
Learning a representation of data that removes the treatment bias<sup>2</sup>



**Figure:** A 2D example of unbiased representation learning. Different colored dots represent treatment groups. (Left) shows sample locations in original feature space (Right) shows a possible unbiased representation encoded by some function  $\phi$

<sup>2</sup>Johansson, Shalit, and Sontag, 2016.

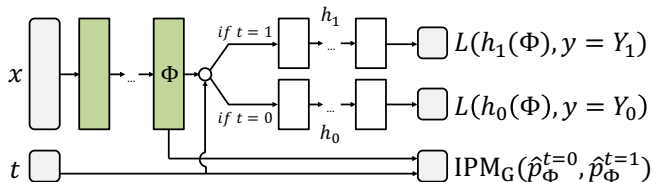
## Neural network architecture for ITE estimation



**Figure:** Neural network architecture for ITE estimation.  $L$  is a loss function,  $\text{IPM}$  is an integral probability metric. Note that only one of  $h_0$  and  $h_1$  is updated for each sample during training<sup>3</sup>.

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# Integral Probability Metric (IPM) Regularizer

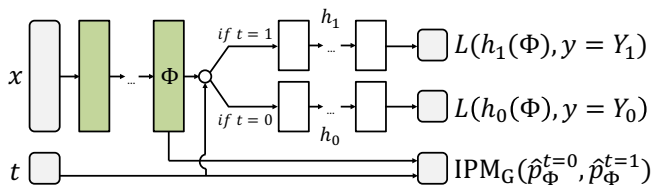


An IPM is a distance function between distributions<sup>a</sup>

- ▶ Minimizing the IPM between treatment groups encourages an unbiased representation

<sup>a</sup>Sriperumbudur et al., 2012.

# Integral Probability Metric (IPM) Regularizer



**Definition:**  $\text{IPM}_G$

$$\text{IPM}_G(p_1, p_2) = \sup_{g \in G} \left| \int_s g(s) (p_1(s) - p_2(s)) ds \right|$$

$G$  is some family of functions which defines the metric.

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Authors experiment with both Wasserstein and MMD as candidate metrics

## Error Bounds

Error in ITE Estimation:

$$\epsilon_{ITE} = \mathbb{E}_{p(x)} \left[ (\hat{ITE}(x) - ITE(x))^2 \right]$$

**Problem:** The true ITE is not known in real-world datasets

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But not counterfactual errors

$$\epsilon_{CF}^t = \mathbb{E}_{p(x)} [(Y_{1-t}(x) - \hat{Y}_{1-t}(x))^2]$$

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Factual Error Bound (Shalit et al.)

$$\underbrace{\epsilon_{\text{ITE}}}_{\text{Effect error}} \leq \epsilon_F + \epsilon_{CF} \leq \underbrace{2(\epsilon_F^{t=0} + \epsilon_F^{t=1})}_{\text{Prediction error}} + \underbrace{\alpha \text{IPM}_G(p^{t=1}, p^{t=0})}_{\text{Treatment/control distance}} \text{Loss}$$

# ITE Evaluation

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- ▶ No ground truth:  $Y_0$  and  $Y_1$  are never observed for the same  $x$
- ▶ Use synthetic data, where structural equations are known
- ▶ Real-world data + randomized controlled trial
  - Still no ground truth
  - Evaluate the risk of induced policy  $\pi_f(x) = \mathbb{I}(f(x, 1) - f(x, 0) > \lambda)$



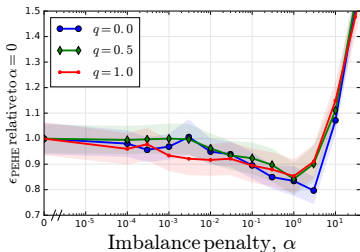
## ITE Evaluation: IHDP

- ▶ Dataset: Semi-synthetic IHDP<sup>4</sup>
- ▶ Real-world features and treatment
- ▶ Synthetic outcome

### Out-of-sample

	IHDP	
	$\epsilon_{ITE}$	$\epsilon_{ATE}$
OLS/LR-1	5.8 ± .3	.94 ± .06
OLS/LR-2	2.5 ± .1	.31 ± .02
BLR	5.8 ± .3	.93 ± .05
<i>k</i> -NN	4.1 ± .2	.79 ± .05
BART	2.3 ± .1	.34 ± .02
RAND.FOR.	6.6 ± .3	.96 ± .06
CAUS.FOR.	3.8 ± .2	.40 ± .03
BNN	2.1 ± .1	.42 ± .03
TARNET	<b>.95 ± .0</b>	.28 ± .01
CFR MMD	<b>.78 ± .0</b>	.31 ± .01
CFR WASS	<b>.76 ± .0</b>	.27 ± .01

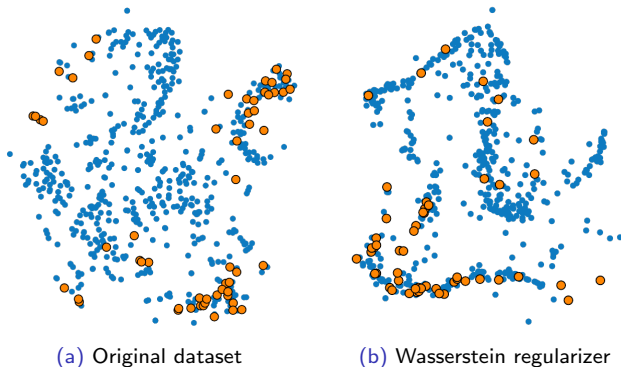
**Table:** Results on IHDP. Lower is better.



**Figure:** Out-of-sample ITE error versus IPM regularization for CFR Wass, with high ( $q = 1$ ), medium and low (artificial) imbalance between control and treated.

<sup>4</sup>Hill, 2011.

# ITE Evaluation: Balanced Representation



**Figure:** t-SNE visualizations of the balanced representations of IHDP learned by the algorithm. Blue (orange) points represent control (treatment) group.

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- + state of the art method for estimating ITE from observational data; can use general functions to estimate  $Y_0$  and  $Y_1$

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- Assumes no hidden confounding variables
- No results on tightness of bound
  - Does minimizing the bound always results in smaller error?
- Generalization to continuous treatments is not obvious



Austin, Peter (May 2011). “An Introduction to Propensity Score Methods for Reducing the Effects of Confounding in Observational Studies”. In: *Multivariate behavioral research* 46, pp. 399–424. DOI: 10.1080/00273171.2011.568786.



Johansson, Fredrik D., Uri Shalit, and David Sontag (May 2016). “Learning Representations for Counterfactual Inference”. In: *arXiv e-prints*, arXiv:1605.03661, arXiv:1605.03661. arXiv: 1605.03661 [stat.ML].



Shalit, Uri, Fredrik D. Johansson, and David Sontag (June 2016). “Estimating individual treatment effect: generalization bounds and algorithms”. In: *arXiv e-prints*, arXiv:1606.03976, arXiv:1606.03976. arXiv: 1606.03976 [stat.ML].



Sriperumbudur, Bharath K et al. (2012). “On the empirical estimation of integral probability metrics”. In: *Electronic Journal of Statistics* 6.none, pp. 1550–1599. DOI: 10.1214/12-EJS722. URL: <https://doi.org/10.1214/12-EJS722>.



Hill, Jennifer L (2011). “Bayesian nonparametric modeling for causal inference”. In: *Journal of Computational and Graphical Statistics* 20.1, pp. 217–240.