

Causal Effect Estimation with Context and Confounders

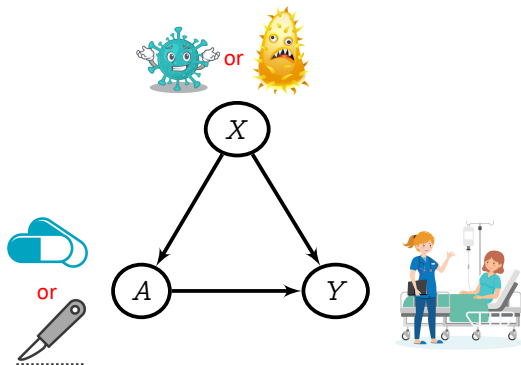
Arthur Gretton

Gatsby Computational Neuroscience Unit,
University College London

AISTATS, 2023

Observation vs intervention

Conditioning from observation: $\mathbb{E}[Y|A = a] = \sum_x \mathbb{E}[Y|a, x]p(x|a)$

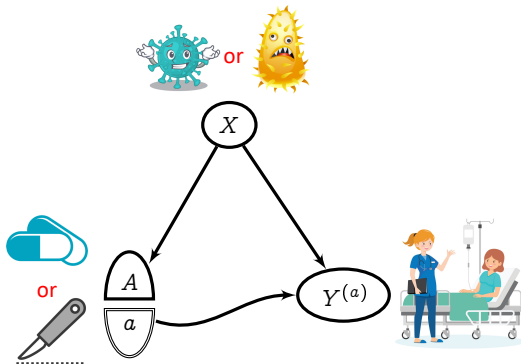


From our observations of historical hospital data:

- $P(Y = \text{cured} | A = \text{pills}) = 0.80$
- $P(Y = \text{cured} | A = \text{surgery}) = 0.72$

Observation vs intervention

Average causal effect (**intervention**): $\mathbb{E}[Y^{(a)}] = \sum_x \mathbb{E}[Y|a, x]p(x)$

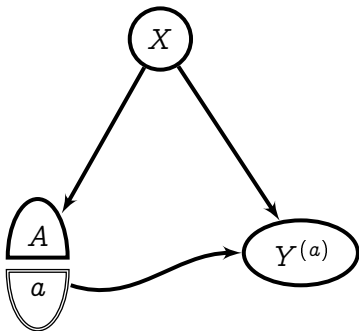


From our intervention (making all patients take a treatment):

- $P(Y^{(\text{pills})} = \text{cured}) = 0.64$
- $P(Y^{(\text{surgery})} = \text{cured}) = 0.75$

Richardson, Robins (2013), Single World Intervention Graphs (SWIGs): A Unification of the Counterfactual and Graphical Approaches to Causality

Questions we will solve



Outline

Causal effect estimation, **observed** covariates:

- Average treatment effect (**ATE**), conditional average treatment effect (**CATE**)

Causal effect estimation, **hidden** covariates:

- ... **instrumental** variables, **proxy** variables

What's new? What is it good for?

- Treatment A , covariates X , etc can be **multivariate, complicated...**
- ...by using **kernel** or **adaptive neural net** feature representations

Model assumption: linear functions of features

All learned functions will take the form:

$$\gamma(x) = \gamma^\top \varphi(x) = \langle \gamma, \varphi(x) \rangle_{\mathcal{H}}$$

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Option 1: Finite dictionaries of **learned** neural net features $\varphi_\theta(x)$
(linear final layer γ)

Xu, G., A Neural mean embedding approach for back-door and front-door adjustment. (ICLR 23)

Xu, Chen, Srinivasan, de Freitas, Doucet, G. Learning Deep Features in Instrumental Variable Regression. (ICLR 21)

Option 2: Infinite dictionaries of **fixed** kernel features:

$$\langle \varphi(x_i), \varphi(x) \rangle_{\mathcal{H}} = k(x_i, x)$$

Kernel is feature dot product.

Singh, Xu, G. Kernel Methods for Causal Functions: Dose, Heterogeneous, and Incremental Response Curves. (Biometrika, in revision)

Singh, Sahani, G. Kernel Instrumental Variable Regression. (NeurIPS 19)

Model fitting: ridge regression

Learn $\gamma_0(x) := \mathbb{E}[Y|X = x]$ from features $\varphi(x_i)$ with outcomes y_i :

$$\hat{\gamma} = \arg \min_{\gamma \in \mathcal{H}} \left(\sum_{i=1}^n (y_i - \langle \gamma, \varphi(x_i) \rangle_{\mathcal{H}})^2 + \lambda \|\gamma\|_{\mathcal{H}}^2 \right).$$

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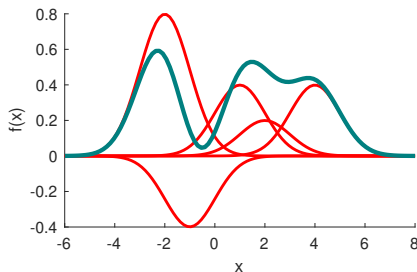
$$\hat{\gamma} = \arg \min_{\gamma \in \mathcal{H}} \left(\sum_{i=1}^n (y_i - \langle \gamma, \varphi(x_i) \rangle_{\mathcal{H}})^2 + \lambda \|\gamma\|_{\mathcal{H}}^2 \right).$$

Neural net solution at x :

$$\hat{\gamma}(x) = C_{YX} (C_{XX} + \lambda)^{-1} \varphi(x)$$

$$C_{YX} = \frac{1}{n} \sum_{i=1}^n [y_i \varphi(x_i)^{\top}]$$

$$C_{XX} = \frac{1}{n} \sum_{i=1}^n [\varphi(x_i) \varphi(x_i)^{\top}]$$



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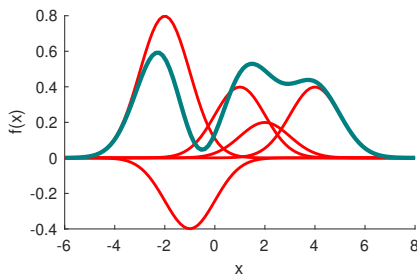
Kernel solution at x
(as weighted sum of y)

$$\hat{\gamma}(x) = \sum_{i=1}^n y_i \beta_i(x)$$

$$\beta(x) = (K_{XX} + \lambda I)^{-1} k_{Xx}$$

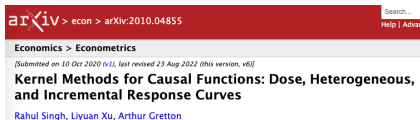
$$(K_{XX})_{ij} = k(x_i, x_j) = \langle \varphi(x_i), \varphi(x_j) \rangle_{\mathcal{H}}$$

$$(k_{Xx})_i = k(x_i, x)$$



Observed covariates: (conditional) ATE

Kernel features
(in revision, Biometrika):



NN features (ICLR 2023):



Code for NN and kernel causal estimation with observed covariates:
<https://github.com/liyuan9988/DeepFrontBackDoor/>

Observed covariates: (conditional) ATE

Kernel features (in revision, Biometrika):

arXiv > econ > arXiv:2010.04855

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Economics > Econometrics

[Submitted on 10 Oct 2020 (v1), last revised 23 Aug 2022 (this version, v6)]

Kernel Methods for Causal Functions: Dose, Heterogeneous, and Incremental Response Curves

Rahul Singh, Liyuan Xu, Arthur Gretton



NN features (ICLR 2023):

arXiv > cs > arXiv:2210.06610

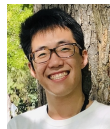
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Computer Science > Machine Learning

[Submitted on 12 Oct 2022]

A Neural Mean Embedding Approach for Back-door and Front-door Adjustment

Liyuan Xu, Arthur Gretton



Code for NN and kernel causal estimation with observed covariates:

<https://github.com/liyuan9988/DeepFrontBackDoor/>

Average treatment effect

Potential outcome (intervention):

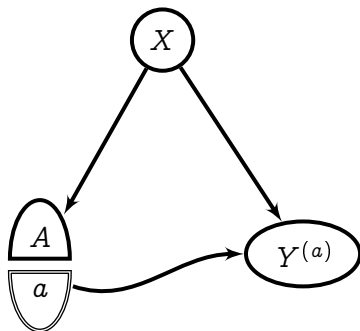
$$\mathbb{E}[Y^{(a)}] = \int \mathbb{E}[Y|a, x] dp(x)$$

(the average structural function; in epidemiology, for continuous a , the dose-response curve).

Assume: (1) Stable Unit Treatment Value Assumption (aka “no interference”), (2) Conditional exchangeability $Y^{(a)} \perp\!\!\!\perp A|X$. (3) Overlap.

Example: US job corps, training for disadvantaged youths:

- A : treatment (training hours)
- Y : outcome (percentage employment)
- X : covariates (age, education, marital status, ...)



Multiple inputs via products of kernels

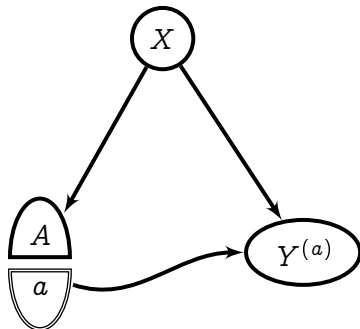
We may predict expected outcome
from two inputs

$$\gamma_0(a, x) := \mathbb{E}[Y | a, x]$$

Assume we have:

- covariate features $\varphi(x)$ with kernel $k(x, x')$
- treatment features $\varphi(a)$ with kernel $k(a, a')$

(argument of kernel/feature map indicates
feature space)



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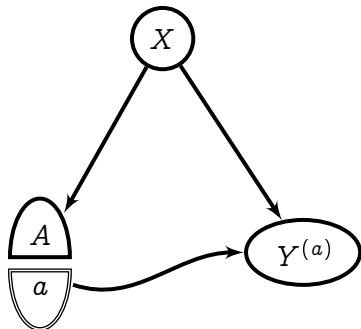
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We use outer product of features (\implies product of kernels):

$$\phi(x, a) = \varphi(a) \otimes \varphi(x) \quad \mathcal{K}([a, x], [a', x']) = k(a, a')k(x, x')$$



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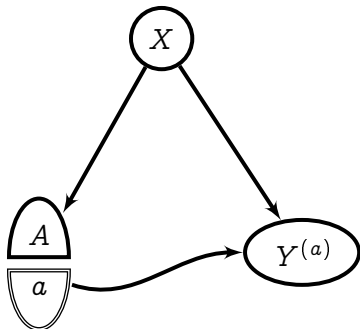
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Ridge regression solution:

$$\hat{\gamma}(x, a) = \sum_{i=1}^n \mathbf{y}_i \mathbf{\beta}_i(a, x), \quad \mathbf{\beta}(a, x) = [K_{AA} \odot K_{XX} + \lambda I]^{-1} K_{Aa} \odot K_{Xx}$$



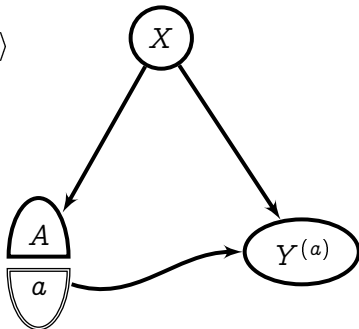
ATE (dose-response curve)

Well-specified setting:

$$\mathbb{E}[Y|a, x] =: \gamma_0(a, x) = \langle \gamma_0, \varphi(a) \otimes \varphi(x) \rangle$$

ATE as feature space dot product:

$$\begin{aligned}\text{ATE}(a) &= \mathbb{E}[\gamma_0(a, X)] \\ &= \mathbb{E}[\langle \gamma_0, \varphi(a) \otimes \varphi(X) \rangle]\end{aligned}$$



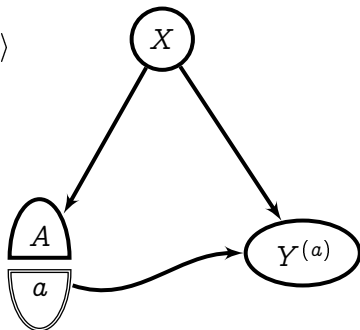
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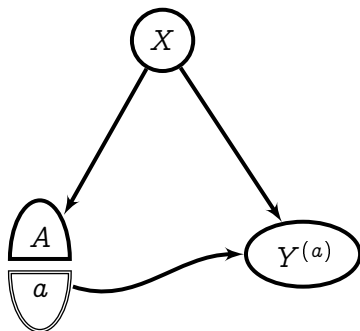
Feature map of probability $P(X)$,

$$\mu_X = [\dots \mathbb{E}[\varphi_i(X)] \dots]$$

ATE: example

US job corps: training for disadvantaged youths:

- X : covariate/context (age, education, marital status, ...)
- A : treatment (training hours)
- Y : outcome (percent employment)



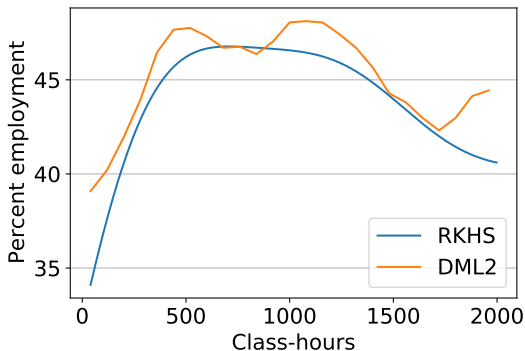
Empirical ATE:

$$\begin{aligned}\widehat{\text{ATE}}(a) &= \widehat{\mathbb{E}} [\langle \hat{\gamma}_0, \varphi(X) \otimes \varphi(a) \rangle] \\ &= \frac{1}{n} \sum_{i=1}^n Y^\top (K_{AA} \odot K_{XX} + n\lambda I)^{-1} (K_{Aa} \odot K_{Xx_i})\end{aligned}$$

Schochet, Burghardt, and McConnell (2008). Does Job Corps work? Impact findings from the national Job Corps study.

Singh, Xu, G (2022a).

ATE: results



- First 12.5 weeks of classes confer employment gain: from 35% to 47%.
- [RKHS] is our $\widehat{ATE}(a)$.
- [DML2] Colangelo, Lee (2020), Double debiased machine learning nonparametric inference with continuous treatments.

Singh, Xu, G (2022a)

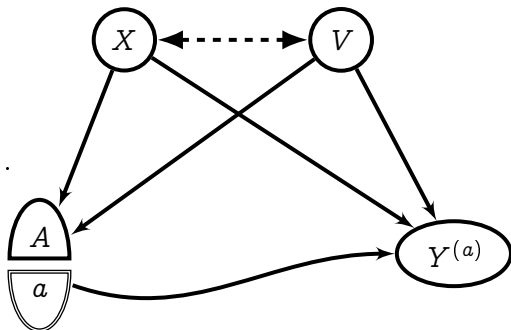
Conditional average treatment effect

Well-specified setting:

$$\begin{aligned}\mathbb{E}[Y|a, x, v] &=: \gamma_0(a, x, v) \\ &= \langle \gamma_0, \varphi(a) \otimes \varphi(x) \otimes \varphi(v) \rangle.\end{aligned}$$

Conditional ATE

$$\begin{aligned}\text{CATE}(a, v) \\ = \mathbb{E} \left[Y^{(a)} \mid V = v \right]\end{aligned}$$



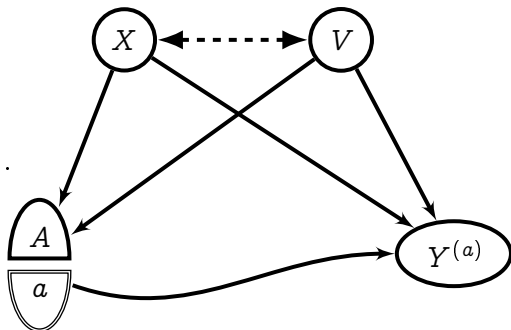
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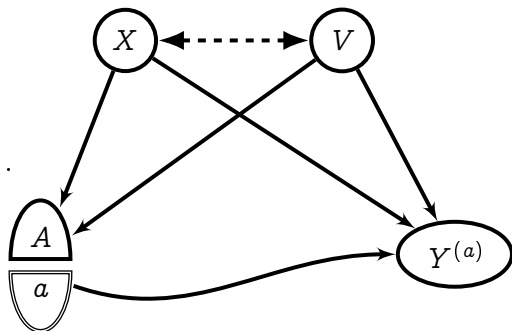
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Conditional ATE

CATE(a, v)

$$\begin{aligned}&= \mathbb{E} \left[Y^{(a)} \mid V = v \right] \\ &= \mathbb{E} \left[\langle \gamma_0, \varphi(a) \otimes \varphi(X) \otimes \varphi(V) \rangle \mid V = v \right] \\ &= \dots?\end{aligned}$$



How to take conditional expectation?

Density estimation for $p(X \mid V = v)$? Sample from $p(X \mid V = v)$?

Conditional average treatment effect

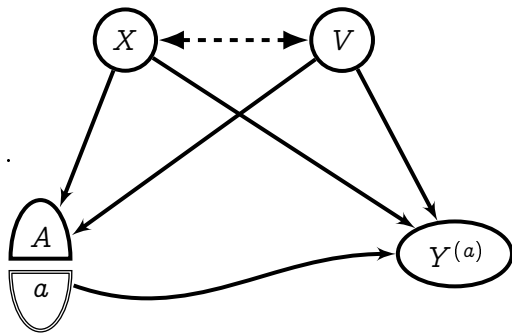
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Learn **conditional mean embedding**: $\mu_{X|V=v} := \mathbb{E}_X [\varphi(X) \mid V = v]$



Regressing from feature space to feature space

Our goal: an operator $F_0 : \mathcal{H}_\mathcal{V} \rightarrow \mathcal{H}_\mathcal{X}$ such that

$$F_0 \varphi(v) = \mu_{X|V=v}$$

Song, Huang, Smola, Fukumizu (2009). Hilbert space embeddings of conditional distributions with applications to dynamical systems.

Grunewalder, Lever, Baldassarre, Patterson, G, Pontil (2012). Conditional mean embeddings as regressors.

Grunewalder, G, Shawe-Taylor (2013) Smooth operators.

Li, Meunier, Mollenhauer, G (2022), Optimal Rates for Regularized Conditional Mean Embedding Learning

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Assume

$$F_0 \in \overline{\text{span}\{\varphi(x) \otimes \varphi(v)\}} \iff F_0 \in \text{HS}(\mathcal{H}_\mathcal{V}, \mathcal{H}_\mathcal{X})$$

Implied smoothness assumption:

$$\mathbb{E}[h(\mathbf{X})|\mathbf{V}=\mathbf{v}] \in \mathcal{H}_\mathcal{V} \quad \forall h \in \mathcal{H}_\mathcal{X}$$

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A Smooth Operator

Song, Huang, Smola, Fukumizu (2009). Hilbert space embeddings of conditional distributions with applications to dynamical systems.

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Implied smoothness assumption:

$$\mathbb{E}[h(\mathbf{X})|\mathbf{V}=\mathbf{v}] \in \mathcal{H}_\mathcal{X} \quad \forall h \in \mathcal{H}_\mathcal{V}$$

Kernel ridge regression from $\varphi(v)$ to infinite features $\varphi(x)$:

$$\hat{F} = \underset{F \in \text{HS}}{\text{argmin}} \sum_{\ell=1}^n \|\varphi(x_\ell) - F\varphi(v_\ell)\|_{\mathcal{H}_\mathcal{X}}^2 + \lambda_2 \|F\|_{\text{HS}}^2$$

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Grunewalder, Lever, Baldassarre, Patterson, G, Pontil (2012). Conditional mean embeddings as regressors.

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Li, Meunier, Mollenhauer, G (2022), Optimal Rates for Regularized Conditional Mean Embedding Learning

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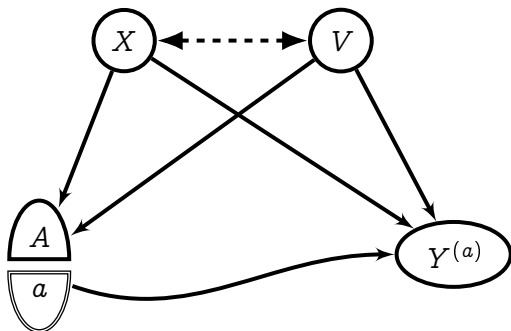
Ridge regression solution:

$$\mu_{X|V=v} := \mathbb{E}[\varphi(X)|V=v] \approx \hat{F} \varphi(v) = \sum_{\ell=1}^n \varphi(x_\ell) \beta_\ell(v)$$
$$\beta(v) = [K_{VV} + \lambda_2 I]^{-1} k_{Vv}$$

Conditional ATE: example

US job corps:

- X : confounder/context (education, marital status, ...)
- A : treatment (training hours)
- Y : outcome (percent employed)
- V : age

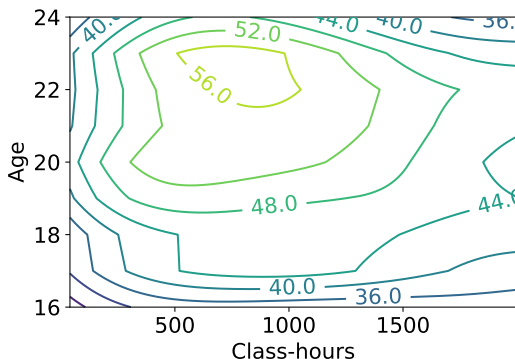


Empirical CATE:

$$\widehat{\text{CATE}}(a, \mathbf{v}) = \langle \hat{\gamma}_0, \varphi(a) \otimes \underbrace{\hat{F} \varphi(\mathbf{v})}_{\hat{\mathbb{E}}[\varphi(\mathbf{X}) | V=\mathbf{v}]} \otimes \varphi(\mathbf{v}) \rangle$$

(with consistency guarantees: see paper!)

Conditional ATE: results



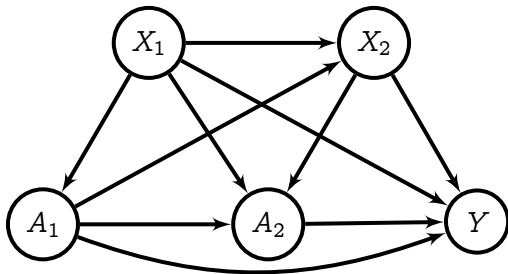
Average percentage employment $Y^{(a)}$ for class hours a , **conditioned on age v** . Given around 12-14 weeks of classes:

- 16 y/o: employment increases from 28% to at most 36%.
- 22 y/o: percent employment increases from 40% to 56%.

Singh, Xu, G (2022a)

...dynamic treatment effect...

Dynamic treatment effect: sequence A_1, A_2 of treatments.



- potential outcomes $Y^{(a_1)}, Y^{(a_2)}, Y^{(a_1, a_2)},$
- counterfactuals $\mathbb{E} \left[Y^{(a'_1, a'_2)} | A_1 = a_1, A_2 = a_2 \right] \dots$

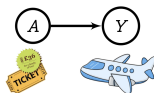
(c.f. the Robins G-formula)

Singh, Xu, G. (2022b) Kernel Methods for Multistage Causal Inference: Mediation Analysis and Dynamic Treatment Effects

What if there are hidden confounders?

Illustration: ticket prices for air travel

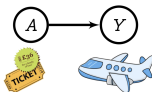
Ticket price A , seats sold Y .



What is the effect on seats sold $Y^{(a)}$ of intervening on price a ?

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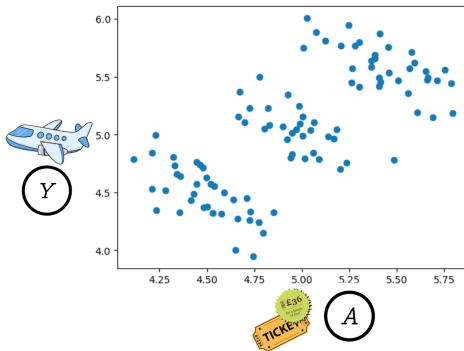
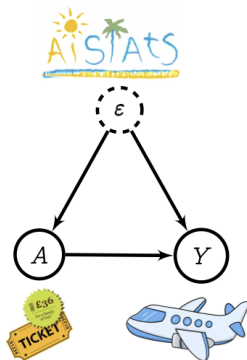


Illustration: ticket prices for air travel

Unobserved variable ε = desire for travel, affects both price (via airline algorithms) and seats sold.



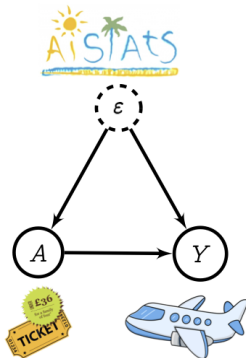
■ Desire for travel:

$$\varepsilon \sim \mathcal{N}(\mu, 0.1)$$

$$\mu \sim \mathcal{U}\left\{-\frac{1}{2}, 0, \frac{1}{2}\right\}$$

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■ Desire for travel:

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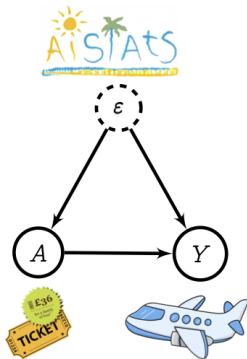
■ Price:

$$A = \varepsilon + Z,$$

$$Z \sim \mathcal{N}(5, 0.04)$$

Illustration: ticket prices for air travel

Unobserved variable ε = desire for travel, affects both price (via airline algorithms) and seats sold.



■ Desire for travel:

$$\varepsilon \sim \mathcal{N}(\mu, 0.1)$$

$$\mu \sim \mathcal{U}\left\{-\frac{1}{2}, 0, \frac{1}{2}\right\}$$

■ Price:

$$A = \varepsilon + Z,$$

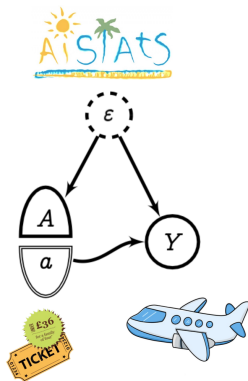
$$Z \sim \mathcal{N}(5, 0.04)$$

■ Seats sold:

$$Y = 10 - A + 2\varepsilon$$

Illustration: ticket prices for air travel

Unobserved variable ε = **desire for travel**, affects both price (via airline algorithms) and seats sold.



■ **Desire for travel:**

$$\varepsilon \sim \mathcal{N}(\mu, 0.1)$$

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■ **Price:**

$$A = \varepsilon + Z,$$

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■ **Seats sold:**

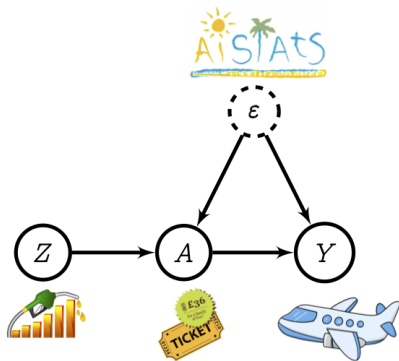
$$Y = 10 - A + 2\varepsilon$$

Average treatment effect:

$$\text{ATE}(a) = \mathbb{E}[Y^{(a)}] = \int (10 - a + 2\varepsilon) dp(\varepsilon) = 10 - a$$

Illustration: ticket prices for air travel

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$$\varepsilon \sim \mathcal{N}(\mu, 0.1)$$

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■ **Price:**

$$A = \varepsilon + Z,$$

$$Z \sim \mathcal{N}(5, 0.04)$$

■ **Seats sold:**

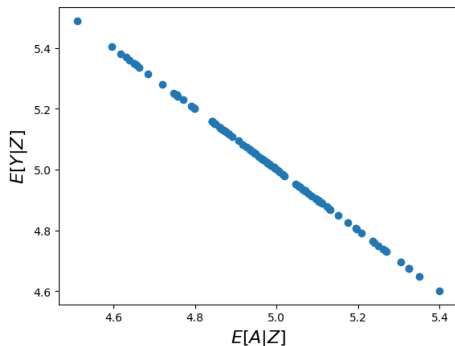
$$Y = 10 - A + 2\varepsilon$$

Z is an **instrument** (cost of fuel). Condition on Z ,

$$\mathbb{E}[Y|Z] = 10 - \mathbb{E}[A|Z] + \underbrace{2\mathbb{E}[\varepsilon|Z]}_{=0}$$

Illustration: ticket prices for air travel

Unobserved variable ε = **desire for travel**, affects both price (via airline algorithms) and seats sold.



- **Desire for travel:**

$$\varepsilon \sim \mathcal{N}(\mu, 0.1)$$
$$\mu \sim \mathcal{U}\left\{-\frac{1}{2}, 0, \frac{1}{2}\right\}$$

- **Price:**

$$A = \varepsilon + Z,$$
$$Z \sim \mathcal{N}(5, 0.04)$$

- **Seats sold:**

$$Y = 10 - A + 2\varepsilon$$

Z is an instrument (cost of fuel). Condition on Z ,

$$\mathbb{E}[Y|Z] = 10 - \mathbb{E}[A|Z] + 2\underbrace{\mathbb{E}[\varepsilon|Z]}_{=0}$$

Regressing from $\mathbb{E}[A|Z]$ to $\mathbb{E}[Y|Z]$ recovers ATE!

Instrumental variable regression

The Sveriges Riksbank Prize in Economic Sciences in Memory of Alfred Nobel 2021



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Paul Kennedy

David Card

Prize share: 1/2



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Risdon Photography

Joshua D. Angrist

Prize share: 1/4



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Paul Kennedy

Guido W. Imbens

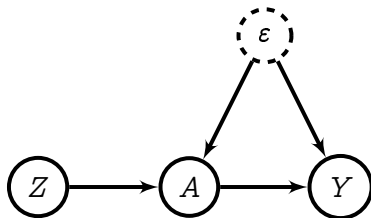
Prize share: 1/4

The Sveriges Riksbank Prize in Economic Sciences in Memory of Alfred Nobel 2021 was divided, one half awarded to David Card "for his empirical contributions to labour economics", the other half jointly to Joshua D. Angrist and Guido W. Imbens "for their methodological contributions to the analysis of causal relationships"

Instrumental variable regression with NN features

Definitions:

- ε : unobserved confounder.
- A : treatment
- Y : outcome
- Z : instrument



Assumptions

$$\mathbb{E}[\varepsilon] = 0 \quad \mathbb{E}[\varepsilon|Z] = 0$$

$$Z \not\perp\!\!\!\perp A$$

$$(Y \perp\!\!\!\perp Z|A)_{G_{\bar{A}}}$$

$$Y = \gamma^\top \phi_\theta(A) + \varepsilon$$

Instrumental variable regression with NN features

Definitions:

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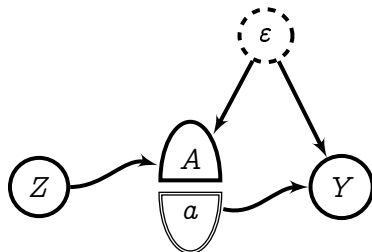
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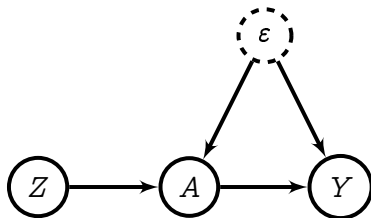
Average treatment effect:

$$\text{ATE}(a) = \int \mathbb{E}(Y|\varepsilon, a) dp(\varepsilon) = \gamma^\top \phi_\theta(a)$$

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- ε : unobserved confounder.
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Assumptions

$$\mathbb{E}[\varepsilon] = 0 \quad \mathbb{E}[\varepsilon|Z] = 0$$

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$$(Y \perp\!\!\!\perp Z|A)_{G_{\bar{A}}}$$

$$Y = \gamma^\top \phi_\theta(A) + \varepsilon$$

Average treatment effect:

$$\text{ATE}(a) = \int \mathbb{E}(Y|\varepsilon, a) dp(\varepsilon) = \gamma^\top \phi_\theta(a)$$

IV regression: Condition both sides on Z ,

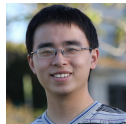
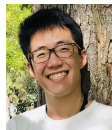
$$\mathbb{E}[Y|Z] = \gamma^\top \mathbb{E}[\phi_\theta(A)|Z] + \underbrace{\mathbb{E}[\varepsilon|Z]}_{=0}$$

Two-stage least squares for IV regression

Kernel features (NeurIPS 2019):



NN features (ICLR 2021):



Code for NN and kernel IV methods:

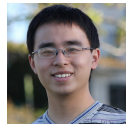
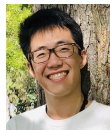
<https://github.com/liyuan9988/DeepFeatureIV/>

Two-stage least squares for IV regression

Kernel features (NeurIPS 2019):



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Code for NN and kernel IV methods:

<https://github.com/liyuan9988/DeepFeatureIV/>

IV using neural net features

Stage 2 regression (IV): learn NN features $\phi_\theta(A)$ and linear layer γ to obtain Y with RR loss:

$$\mathbb{E}_{YZ} \left[(Y - \gamma^\top \mathbb{E}[\phi_\theta(A)|Z])^2 \right] + \lambda_2 \|\gamma\|^2$$

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Stage 1 regression: learn NN features $\phi_\zeta(Z)$ and linear layer F :

$$\mathbb{E}[\phi_\theta(A)|Z] \approx F \phi_\zeta(Z)$$

with RR loss

$$\mathbb{E} \|\phi_\theta(A) - F \phi_\zeta(Z)\|^2 + \lambda_1 \|F\|_{HS}^2$$

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Challenge: how to learn θ ?

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From Stage 2 regression?

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From Stage 2 regression?

...which requires $\mathbb{E}[\phi_\theta(A)|Z]$ from Stage 1 regression

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Stage 2 regression (IV): learn NN features $\phi_\theta(A)$ and linear layer γ to obtain Y with RR loss:

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...which requires $\phi_\theta(A)$... which requires θ ...

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Challenge: how to learn θ ?

From Stage 2 regression?

...which requires $\mathbb{E}[\phi_\theta(A)|Z]$ from Stage 1 regression

...which requires $\phi_\theta(A)$... which requires θ ...

Use the linear final layers! (i.e. γ and F)

IV using neural net features

Stage 1 regression: learn NN features $\phi_\zeta(Z)$ and linear layer F :

$$\mathbb{E}[\phi_\theta(A)|Z] \approx F\phi_\zeta(Z)$$

with RR loss

$$\mathbb{E} \left[\|\phi_\theta(A) - F\phi_\zeta(Z)\|^2 \right] + \lambda_1 \|F\|_{HS}^2$$

IV using neural net features

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with RR loss

$$\mathbb{E}[\|\phi_\theta(A) - F\phi_\zeta(Z)\|^2] + \lambda_1 \|F\|_{HS}^2$$

$\hat{F}_{\theta,\zeta}$ in closed form wrt ϕ_θ, ϕ_ζ :

$$\begin{aligned}\hat{F}_{\theta,\zeta} &= C_{AZ}(C_{ZZ} + \lambda_1 I)^{-1} & C_{AZ} &= \mathbb{E}[\phi_\theta(A)\phi_\zeta^\top(Z)] \\ & & C_{ZZ} &= \mathbb{E}[\phi_\zeta(Z)\phi_\zeta^\top(Z)]\end{aligned}$$

IV using neural net features

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Plug $\hat{F}_{\theta,\zeta}$ into S1 loss, take gradient steps for ζ (...but not θ ...)

Stage 2: IV regression

Stage 2 regression (IV): learn NN features $\phi_{\theta}(A)$ and linear layer γ to obtain Y with RR loss:

$$\mathcal{L}_2(\gamma, \theta) = \mathbb{E}_{YZ} \left[(Y - \gamma^{\top} \mathbb{E}[\phi_{\theta}(A)|Z])^2 \right] + \lambda_2 \|\gamma\|^2$$

Stage 2: IV regression

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$\hat{\gamma}_\theta$ in closed form wrt ϕ_θ :

$$\begin{aligned}\hat{\gamma}_\theta &:= \widetilde{C}_{YZ} (\widetilde{C}_{ZZ} + \lambda_2 I)^{-1} & \widetilde{C}_{YZ} &= \mathbb{E} \left[Y [\hat{F}_{\theta, \zeta} \phi_\zeta(Z)]^\top \right] \\ & & \widetilde{C}_{ZZ} &= \mathbb{E} \left[[\hat{F}_{\theta, \zeta} \phi_\zeta(Z)] [\hat{F}_{\theta, \zeta} \phi_\zeta(Z)]^\top \right]\end{aligned}$$

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From linear final layers in Stages 1,2:

Learn $\phi_\theta(A)$ by plugging $\hat{\gamma}_\theta$ into S2 loss, taking gradient steps for θ

Stage 2: IV regression

Stage 2 regression (IV): learn NN features $\phi_\theta(A)$ and linear layer γ to obtain Y with RR loss:

$$\begin{aligned}\mathcal{L}_2(\gamma, \theta) &= \mathbb{E}_{YZ} \left[(Y - \gamma^\top \mathbb{E}[\phi_\theta(A)|Z])^2 \right] + \lambda_2 \|\gamma\|^2 \\ &= \mathbb{E}_{YZ} \left[(Y - \gamma^\top \hat{F}_{\theta, \zeta} \phi_\zeta(Z))^2 \right] + \lambda_2 \|\gamma\|^2\end{aligned}$$

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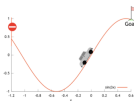
From linear final layers in Stages 1,2:

Learn $\phi_\theta(A)$ by plugging $\hat{\gamma}_\theta$ into S2 loss, taking gradient steps for θ
....but ζ changes with θ
...so alternate first and second stages until convergence.

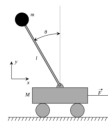
Neural IV in reinforcement learning



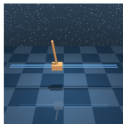
(a) Catch



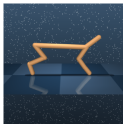
(b) Mountain Car



(c) Cartpole



(a) Cartpole Swingup



(b) Cheetah Run



(c) Humanoid Run



(d) Walker Walk

Policy evaluation: want Q-value:

$$Q^\pi(s, a) = \mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^t R_t \middle| S_0 = s, A_0 = a \right]$$

for policy $\pi(A|S=s)$.

Osband et al (2019). Behaviour suite for reinforcement learning. <https://github.com/deepmind/bsuite>

Tassa et al. (2020). dm_control: Software and tasks for continuous control.

https://github.com/deepmind/dm_control

Application of IV: reinforcement learning

Q value is a minimizer of Bellman loss

$$\mathcal{L}_{\text{Bellman}} = \mathbb{E}_{SAR} \left[(R + \gamma [\mathbb{E} [Q^\pi(S', A') | S, A] - Q^\pi(S, A))^2 \right].$$

Corresponds to “IV-like” problem

$$\mathcal{L}_{\text{Bellman}} = \mathbb{E}_{YZ} \left[(Y - \mathbb{E}[f(X) | Z])^2 \right]$$

with

$$Y = R,$$

$$X = (S', A', S, A)$$

$$Z = (S, A),$$

$$f_0(X) = Q^\pi(s, a) - \gamma Q^\pi(s', a')$$

RL experiments and data:

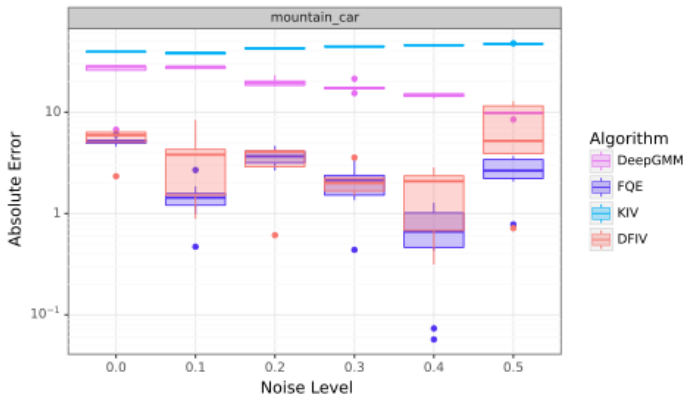
<https://github.com/liyuan9988/IVOPewithACME>

Bradtke and Barto (1996). Linear least-squares algorithms for temporal difference learning.

Xu, Chen, Srinivasan, De Freitas, Doucet, G. (2021)

Chen, Xu, Gulcehre, Le Paine, G, De Freitas, Doucet (2022). On Instrumental Variable Regression for Deep Offline Policy Evaluation.

Results on mountain car problem



Good performance compared with FQE.

Warning: IV assumption can fail when regression underfits. See papers for details.

Xu, Chen, Srinivasan, De Freitas, Doucet, G. (2021)

Chen, Xu, Gulcehre, Le Paine, G, De Freitas, Doucet (2022). On Instrumental Variable Regression for Deep Offline Policy Evaluation.

...but seriously, what if there are hidden confounders?

The proxy correction

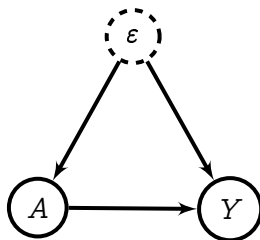
Unobserved ϵ with (possibly) complex nonlinear effects on A , Y

The definitions are:

- ϵ : unobserved confounder.
- A : treatment
- Y : outcome

If ϵ were observed (which it isn't),

$$\mathbb{E}[Y^{(a)}] = \int \mathbb{E}[Y | \epsilon, a] dp(\epsilon)$$

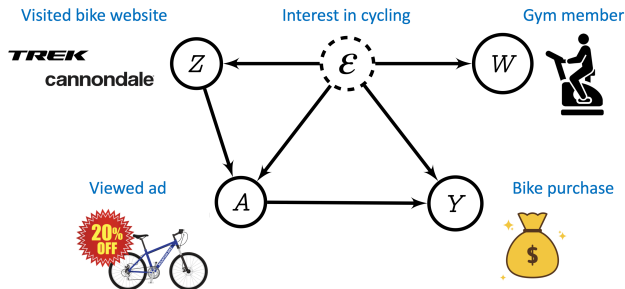


The proxy correction

Unobserved ε with (possibly) complex nonlinear effects on A , Y

The definitions are:

- ε : unobserved confounder.
- A : treatment
- Y : outcome
- Z : treatment proxy
- W outcome proxy



Miao, Geng, Tchetgen Tchetgen (2018): Identifying causal effects with proxy variables of an unmeasured confounder.

Tennenholtz, Mannor, Shalit (2020), OPE in Partially Observed Environments.

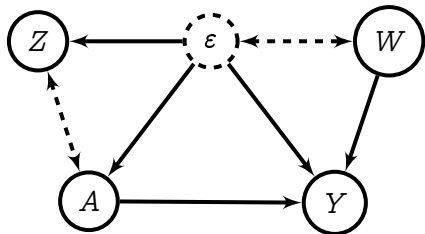
Uehara, Sekhari, Lee, Kallus, Sun (2022) Provably Efficient Reinforcement Learning in Partially Observable Dynamical Systems.

The proxy correction

Unobserved ϵ with (possibly) complex nonlinear effects on A , Y

The definitions are:

- ϵ : unobserved confounder.
- A : treatment
- Y : outcome
- Z : treatment proxy
- W outcome proxy



Structural assumption:

$$W \perp\!\!\!\perp (Z, A) | \epsilon$$

$$Y \perp\!\!\!\perp Z | (A, \epsilon)$$

\implies Can recover $E(Y^{(a)})$ from observational data!

Miao, Geng, Tchetgen Tchetgen (2018): Identifying causal effects with proxy variables of an unmeasured confounder.

Tennenholtz, Mannor, Shalit (2020), OPE in Partially Observed Environments.

Uehara, Sekhari, Lee, Kallus, Sun (2022) Provably Efficient Reinforcement Learning in Partially Observable Dynamical Systems.

Unobserved confounders: proxy methods

Kernel features (ICML 2021):

arXiv.org > cs > arXiv:2105.04544 [Help](#) | [Advanced Search](#)

Computer Science > Machine Learning

[Submitted on 10 May 2021 (v1), last revised 9 Oct 2021 (this version, v4)]

Proximal Causal Learning with Kernels: Two-Stage Estimation and Moment Restriction

Afsaneh Mastouri, Yuchen Zhu, Limor Gultchin, Anna Korba, Ricardo Silva, Matt J. Kusner, Arthur Gretton, Krikamol Muandet



NN features (NeurIPS 2021):

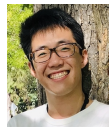
arXiv.org > cs > arXiv:2106.03907 [Help](#) | [Advanced Search](#)

Computer Science > Machine Learning

[Submitted on 7 Jun 2021 (v1), last revised 7 Dec 2021 (this version, v2)]

Deep Proxy Causal Learning and its Application to Confounded Bandit Policy Evaluation

Liyuan Xu, Heishiro Kanagawa, Arthur Gretton



Code for NN and kernel proxy methods:

<https://github.com/liyuan9988/DeepFeatureProxyVariable/>

Conclusions

Neural net and kernel solutions:

- ...for ATE, CATE, dynamic treatment effects
- ...even for unobserved covariates/confounders (IV and proxy methods)
- ...with treatment A , covariates X , V , proxies (W, Z) multivariate, “complicated”
- Convergence guarantees for kernels and NN

Not in this talk:

- Elasticities
- Regression to potential outcome distributions over Y (not just $E(Y^{(a)} | \dots)$)

Code available for all methods

Research support

Work supported by:

The Gatsby Charitable Foundation



Deepmind



Questions?



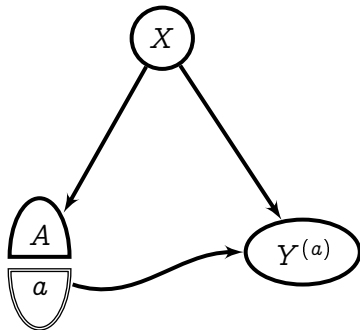
Counterfactual: average treatment on treated

Conditional mean:

$$\mathbb{E}[Y|a, x] = \gamma_0(a, x)$$

Average treatment on treated:

$$\begin{aligned}\theta^{ATT}(a, a') \\ = \mathbb{E}[y^{(a')} | A = a]\end{aligned}$$



Empirical ATT:

$$\hat{\theta}^{ATT}(a, a')$$

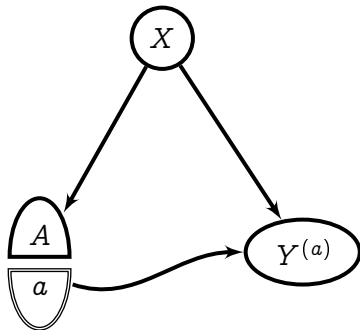
Counterfactual: average treatment on treated

Conditional mean:

$$\mathbb{E}[Y|a, x] = \gamma_0(a, x) = \langle \gamma_0, \varphi(a) \otimes \varphi(x) \rangle$$

Average treatment on treated:

$$\begin{aligned} \theta^{ATT}(a, a') \\ = \mathbb{E}[y^{(a')} | A = a] \end{aligned}$$



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$$\hat{\theta}^{ATT}(a, a')$$

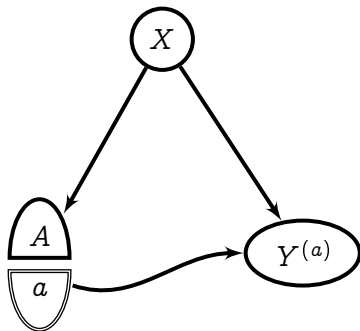
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Average treatment on treated:

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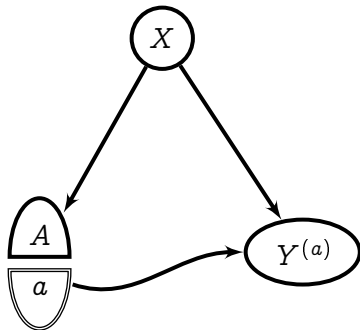
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Empirical ATT:

$$\begin{aligned}\hat{\theta}^{ATT}(a, a') &= Y^\top (K_{AA} \odot K_{XX} + n\lambda I)^{-1} (K_{Aa'} \odot \underbrace{K_{XX}(K_{AA} + n\lambda_1 I)^{-1} K_{Aa}}_{\text{from } \hat{\mu}_{X|A=a}})\end{aligned}$$