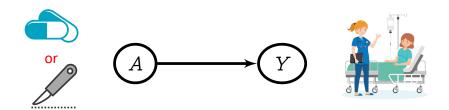
# Causal modelling with kernels: treatment effects, counterfactuals, mediation, and proxies

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DeepLearn 2022

#### A medical treatment scenario

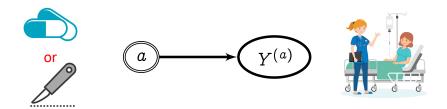


From our observations of historical hospital data:

- P(Y = cured|A = pills) = 0.80
- P(Y = cured|A = surgery) = 0.72

Just recommend pills? Cheaper and more effective!

#### A medical treatment scenario



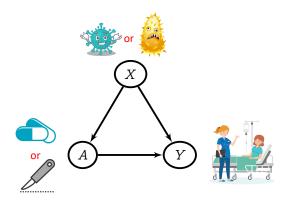
From our intervention (making all patients take a treatment):

- P(Y = cured | do(pills)) = 0.64
- P(Y = cured|do(surgery)) = 0.75

What went wrong?

#### Observation vs intervention

Conditioning from observation:  $E(Y|A=a) = \sum_x E(y|a,x)p(x|a)$ 

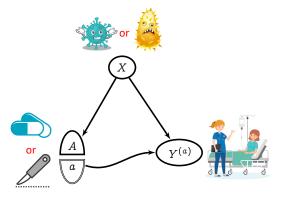


From our observations of historical hospital data:

- P(Y = cured|A = pills) = 0.80
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#### Observation vs intervention

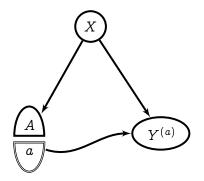
Average causal effect (intervention):  $E(Y^{(a)}) = \sum_x E(y|a,x)p(x)$ 



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

- P(Y = cured | do(pills)) = 0.64
- P(Y = cured|do(surgery)) = 0.75

## Questions we will solve



#### Outline

#### Talk structure:

- Average treatment effect (ATE)
  - ...via kernel mean embedding (marginalization)
- <u>Conditional</u> average treatment effect (CATE)
  - via kernel conditional mean embedding
- Average treatment on treated
- Mediation effect, dynamic treatment effect
- Proxy methods
  - ...when covariates are hidden

#### Advantages of the approach:

- Treatment A, covariates X, etc can be multivariate, complicated...
- Simple, robust implementation;
- Strong statistical guarantees under general smoothness assumptions

Methods also implemented for adaptive neural net features!

## Key requirement: linear functions of features

All learned functions will take the form:

$$\hat{oldsymbol{\gamma}}(x) = \hat{oldsymbol{\gamma}}^ op arphi(x) = \left<\hat{oldsymbol{\gamma}}, arphi(x)
ight>_{\mathcal{H}}$$

#### Option 1: Finite dictionaries of learned neural net features

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

Xu, Kanagawa, G. "Deep Proxy Causal Learning and its Application to Confounded Bandit Policy Evaluation". (NeurIPS 21)

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

$$\left\langle arphi(x_i),arphi(x)
ight
angle_{\mathcal{H}}=k(x_i,x)$$

Kernel is feature dot product.

Primary focus of this talk.

#### Building block: kernel ridge regression

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

$$\hat{\gamma} = rg \min_{\gamma \in \mathcal{H}} \left( \sum_{i=1}^n \left( y_i - \langle \gamma, arphi(x_i) 
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Kernel as feature dot product:

$$\langle arphi(x_i), arphi(x) 
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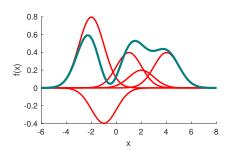
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Kernel as feature dot product:

$$\langle arphi(x_i), arphi(x) 
angle_{\mathcal{H}} = k(x_i, x)$$

Solution at x:

$$egin{aligned} \hat{\gamma}(x) &= \sum_{i=1}^n lpha_i rac{k(x_i,x)}{x} \ lpha &= (K_{XX} + \lambda I)^{-1} \, Y \ (K_{XX})_{ij} &= k(x_i,x_j), \end{aligned}$$



## Building block: kernel ridge regression

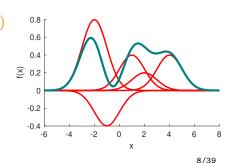
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angle_{\mathcal{H}} \right)^2 + \lambda \|\gamma\|_{\mathcal{H}}^2 \right).$$

Kernel as feature dot product:

$$\langle arphi(x_i), arphi(x) 
angle_{\mathcal{H}} = k(x_i, x)$$

Solution at x (as weighted sum of y) $\hat{\gamma}(x) = \sum_{i=1}^n y_i \beta_i(x) \ eta(x) = (K_{XX} + \lambda I)^{-1} k_{Xx} \ (K_{XX})_{ij} = k(x_i, x_j) \ (k_{Xx})_i = k(x_i, x)$ 



#### KRR: consistency in RKHS norm

#### Assume problem well specified

- Denote:  $\gamma_0 \in \mathcal{H}^c$  where  $\mathcal{H}^c \subset \mathcal{H}$ ,  $c \in (1,2]$ 
  - Larger  $c \implies$  smoother  $\gamma_0 \implies$  easier problem.
- Eigenspectrum decay of input feature covariance,  $\eta_i \sim j^{-b}$ ,  $b \geq 1$ 
  - Larger  $b \implies$  easier problem

[A] Fischer, Steinwart (2020). Sobolev norm learning rates for regularized least-squares algorithms.

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Consistency [A, Theorem 1.ii]

$$\left\|\hat{\gamma}-\gamma_0
ight\|_{\mathcal{H}}=O_P\left(n^{-rac{1}{2}rac{c-1}{c+1/b}}
ight),$$

Best rate is  $O_P(n^{-1/4})$  for  $c=2, b\to \infty$ .

[A] Fischer, Steinwart (2020). Sobolev norm learning rates for regularized least-squares algorithms.

# (Conditional) average treatment effect, average treatment on treated





## Average treatment effect

Potential outcome (intervention):

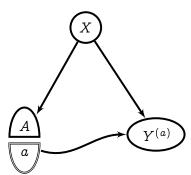
$$\mathrm{E}(\,Y^{(a)})=\int E(y|a,x)dp(x)$$

(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

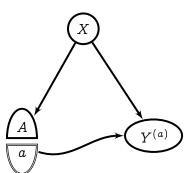
We may predict expected outcome from two inputs

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

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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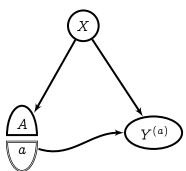
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We use outer product of features ( $\Longrightarrow$  product of kernels):

$$\phi(x,a)=arphi(a)\otimesarphi(x) \qquad \mathfrak{K}([a,x],[a',x'])=k(a,a')k(x,x')$$



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a

Ridge regression solution:

$$\hat{\gamma}(x,a) = \sum_{i=1}^{n} rac{y_i}{y_i} eta_i(a,x), \;\;\; eta(a,x) = \left[K_{AA} \odot K_{XX} + \lambda I
ight]^{-1} K_{Aa} \odot K_{XX}$$

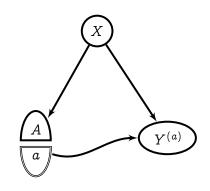
## ATE (dose-response curve)

Well specified setting:

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

ATE as feature space dot product:

$$egin{aligned} heta_0^{ ext{ATE}}(a) &= \operatorname{E}_P[\gamma_0(a,X)] \ &= \operatorname{E}_P\left\langle \gamma_0, arphi(a) \otimes arphi(X) 
ight
angle \end{aligned}$$



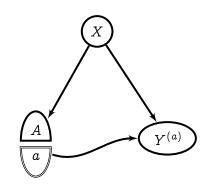
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ight
angle \ &= \left\langle \gamma_0, \underbrace{\mu_P}_{\operatorname{E}_P arphi(X)} \otimes arphi(a) 
ight
angle \end{aligned}$$



Feature map of probability P,

$$\mu_P = [\dots \operatorname{E}_P \left[ arphi_i(X) 
ight] \dots]$$

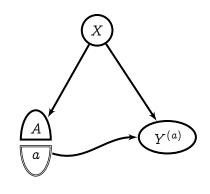
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ight
angle \end{aligned}$$



For characteristic kernels,  $\mu_P$  is injective.

Consistency: 
$$\|\hat{\mu}_P - \mu_P\|_{\mathcal{H}} = O_P(n^{-1/2})$$

## ATE: empirical estimate and consistency

Empirical estimate of ATE:

$$\hat{ heta}^{ ext{ATE}}(a) = rac{1}{n} \sum_{i=1}^n Y^ op (K_{AA} \odot K_{XX} + n\lambda I)^{-1} (K_{Aa} \odot K_{Xx_i})$$

Singh, Xu, G (2022a), Kernel Methods for Causal Functions: Dose-Response Curves and Heterogeneous Treatment Effects.

# ATE: empirical estimate and consistency

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Consistency:

$$\left\|\hat{ heta}^{ ext{ATE}} - heta_o^{ ext{ATE}}
ight\|_{\infty} = O_P\left(n^{-rac{1}{2}rac{c-1}{c+1/b}}
ight)$$

Follows from consistency of  $\hat{\mu}_P$  and  $\hat{\gamma}$ , under:

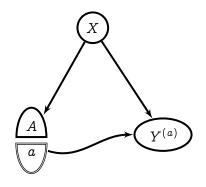
- smoothness assumption  $\gamma_0 \in \mathcal{H}^c$ ,  $c \in (1, 2]$
- eigenspectrum decay of input feature covariance,  $\eta_j \sim j^{-b}$ ,  $b \geq 1$ .

Singh, Xu, G (2022a), Kernel Methods for Causal Functions: Dose-Response Curves and Heterogeneous Treatment Effects.

#### ATE: example

US job corps: training for disadvantaged youths:

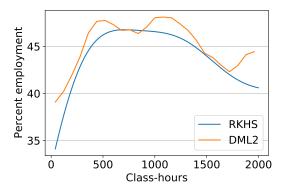
- X: covariate/context (age, education, marital status, ...)
- A: treatment (training hours)
- Y: outcome (percent employment)



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  $\hat{\theta}^{ATE}(a)$
- [DML2] Colangelo, Lee (2020), Double debiased machine learning nonparametric inference with continuous treatments.

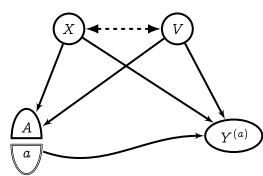
Singh, Xu, G (2022a)

#### Learned conditional mean:

$$egin{aligned} & \mathrm{E}[\,Y|\,a,x,v] pprox \gamma_0(\,a,x,v) \ & = \langle \gamma_0, arphi(\,a) \otimes arphi(x) \otimes arphi(v) 
angle \,. \end{aligned}$$

#### Conditional ATE

$$egin{aligned} heta_o^{ ext{CATE}}(a,v) \ &= ext{E}(Y^{(a)}|V=v) \end{aligned}$$

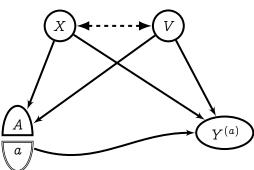


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angle |rac{oldsymbol{V}}{oldsymbol{V}} = oldsymbol{v}
ight) \end{aligned}$$



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angle \,. \end{aligned}$$

#### Conditional ATE

#### How to take conditional expectation?

Density estimation for p(X|V=v)? Sample from p(X|V=v)?

#### Learned conditional mean:

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#### Conditional ATE

Learn conditional mean embedding:  $\mu_{X|V=v} := \mathbb{E}_P\left(\varphi(X)|V=v\right)$ 

Our goal: an operator  $E_0: \mathcal{H}_{\mathcal{V}} \to \mathcal{H}_{\mathcal{X}}$  such that

$$E_0 \varphi(\mathbf{v}) = \mu_{X|\mathbf{V} = \mathbf{v}}$$

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.

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Singh, Sahani, G (2019), Kernel Instrumental Variable Regression.

Our goal: an operator  $E_0: \mathcal{H}_{\mathcal{V}} \to \mathcal{H}_{\mathcal{X}}$  such that

$$E_0 \varphi(v) = \mu_{X|V=v}$$

Assume

$$E_0 \in \overline{\operatorname{span}\left\{ \varphi(x) \otimes \varphi(v) \right\}} \iff E_0 \in \operatorname{HS}(\mathcal{H}_{\mathcal{V}}, \mathcal{H}_{\mathcal{X}})$$

Implied smoothness assumption:

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

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A Smooth Operator

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

$$\widehat{E} = \operatorname*{argmin}_{E \in HS} \sum_{\ell=1}^n \|arphi(x_\ell) - Earphi(v_\ell)\|_{\mathcal{H}_\mathcal{X}}^2 + \lambda_2 \|E\|_{HS}^2$$

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Ridge regression solution:

$$egin{align} \mu_{X|V=oldsymbol{v}} := \mathrm{E}_P[arphi(X)|oldsymbol{V}=oldsymbol{v}] &pprox \widehat{E}\,arphi(oldsymbol{v}) = \sum_{\ell=1}^n rac{arphi(x_\ell)eta_\ell(oldsymbol{v})}{eta(oldsymbol{v})} &= [K_{VV} + \lambda_2 I]^{-1}\,k_{Vv}. \end{align}$$

## Consistency of conditional mean embedding

Assume problem well specified [A, Assumption 6]

$$E_0 = G_1 \circ T_1^{rac{c_1-1}{2}}, \quad extbf{c}_1 \in (1,2], \quad \|G_1\|_{HS}^2 \leq \zeta_1,$$

 $T_1$  is covariance of features  $\varphi(v)$ :

■ Eigenspectrum decays as  $\eta_{1,j} \sim j^{-b_1}$ ,  $b_1 \geq 1$ .

Larger  $c_1 \implies$  smoother  $E_0 \implies$  easier problem.

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[A] Singh, Sahani, G (2022a)
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Earlier consistency proof for finite dimensional  $\varphi(x)$ :

Singh, Sahani, G (2019)

Grunewalder, Lever, Baldassarre, Patterson, G, Pontil (2012).

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Consistency [A, Proposition 3]

$$\|\widehat{E} - E_0\|_{\mathrm{HS}} = O_P\left(n^{-\frac{1}{2}\frac{c_1-1}{c_1+1/b_1}}\right),$$

best rate is  $O_P(n^{-1/4})$ .

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[A] Singh, Sahani, G (2022a)
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Caponnetto, De Vito (2007).

#### Consistency of CATE

#### Empirical CATE:

$$\hat{\theta}^{\text{CATE}}(a, \boldsymbol{v}) = Y^{\top} (K_{AA} \odot K_{XX} \odot K_{VV} + n\lambda I)^{-1} (K_{Aa} \odot \underbrace{K_{XX} (K_{VV} + n\lambda_1 I)^{-1} K_{V\boldsymbol{v}}}_{\text{from } \hat{\mu}_{X|V=\boldsymbol{v}}} \odot K_{V\boldsymbol{v}})$$

#### Consistency of CATE

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$$\hat{\theta}^{\text{CATE}}(a, \boldsymbol{v}) \\
= Y^{\top} (K_{AA} \odot K_{XX} \odot K_{VV} + n\lambda I)^{-1} (K_{Aa} \odot \underbrace{K_{XX} (K_{VV} + n\lambda_1 I)^{-1} K_{V\boldsymbol{v}}}_{\text{from } \hat{\mu}_{X|V=\boldsymbol{v}}} \odot K_{V\boldsymbol{v}})$$

#### Consistency: [A, Theorem 2]

$$\|\hat{ heta}^{ ext{CATE}} - heta_0^{ ext{CATE}}\|_{\infty} = O_P\left(n^{-rac{1}{2}rac{c-1}{c+1//b}} + n^{-rac{1}{2}rac{c_1-1}{c_1+1/b_1}}
ight).$$

Follows from consistency of  $\widehat{E}$  and  $\widehat{\gamma}$ , under the assumptions:

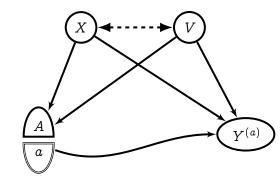
- $lacksquare E_0 = G_1 \circ T_1^{rac{c_1-1}{2}}, \|G_1\|_{HS}^2 \leq \zeta_1,$
- $\gamma_0 \in \mathcal{H}^c$ .

[A] Singh, Xu, G (2022a)

## Conditional ATE: example

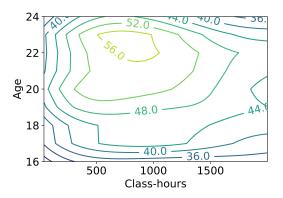
US job corps: training for disadvantaged youths:

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



Singh, Xu, G (2022a)

#### Conditional ATE: results



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

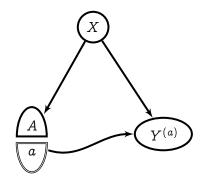
- 16 y/o: employment increases from 28% to at most 36%.
- 22 y/o: percent employment increases from 40% to 56%. Singh, Xu, G (2022a)

Conditional mean:

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

Average treatment on treated:

$$egin{aligned} heta^{ATT}(a, oldsymbol{a}') \ &= \mathbb{E}(y^{(oldsymbol{a}')}|A=a) \end{aligned}$$



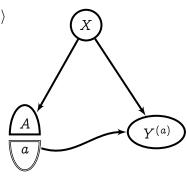
$$\hat{\theta}^{ATT}(a, a')$$

Conditional mean:

$$\operatorname{\mathbb{E}}[\,Y|\,a,x] = \gamma_0(\,a,x) = \langle \gamma_0, arphi(\,a) \otimes arphi(x) 
angle$$

Average treatment on treated:

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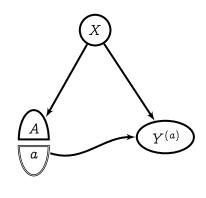
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Conditional mean:

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

Average treatment on treated:

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angle |A=a
ight) \ &= \langle \gamma_0, arphi(oldsymbol{a}') \otimes \underbrace{\mathrm{E}_P[arphi(X)|A=a]}_{\mu_{X|A=a}} 
angle \end{aligned}$$



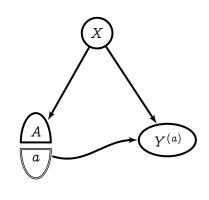
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angle \end{aligned}$$

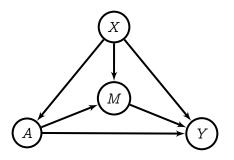


$$\hat{\theta}^{\text{ATT}}(a, \underline{a'}) = Y^{\top} (K_{AA} \odot K_{XX} + n\lambda I)^{-1} (K_{\underline{Aa'}} \odot \underbrace{K_{XX} (K_{AA} + n\lambda_1 I)^{-1} K_{\underline{Aa}}}_{\text{from } \hat{\mu}_{X|A=a}})$$

## Mediation analysis

- Direct path from treatment A to effect Y
- Indirect path  $A \rightarrow M \rightarrow Y$
- X: context

Is the effect Y mainly due to A? To M?

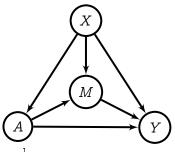


### Mediation analysis: example

US job corps: training for disadvantaged youths:

- X: confounder/context (age, education, marital status, ...)
- A: treatment (training hours)
- Y: outcome (arrests)
- *M*: mediator (employment)

$$\gamma_0(a, m, x) pprox \mathbb{E}[Y|A=a, M=m, X=x]$$



### Mediation analysis: example

US job corps: training for disadvantaged youths:

- X: confounder/context (age, education, marital status, ...)
- A: treatment (training hours)
- Y: outcome (arrests)
- *M*: mediator (employment)

 $\gamma_0(a, m, x) \approx \mathbb{E}[Y|A=a, M=m, X=x]$ 

A quantity of interest, the mediated effect:

$$Y^{\{oldsymbol{a}',oldsymbol{M}(a)\}} = \int \gamma_0(oldsymbol{a}',oldsymbol{M},X) \mathrm{d}\mathbb{P}(oldsymbol{M}|A=a,X) d\mathbb{P}(oldsymbol{X})$$

Effect of intervention a', with  $M^{(a)}$  as if intervention were a

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

#### Mediation analysis: example

US job corps: training for disadvantaged youths:

- X: confounder/context (age, education, marital status, ...)
- A: treatment (training hours)
- Y: outcome (arrests)
- M: mediator (employment)

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A quantity of interest, the mediated effect:

$$egin{aligned} Y^{\{oldsymbol{a}',oldsymbol{M}^{(a)}\}} &= \int \gamma_0(oldsymbol{a}',oldsymbol{M},X) \mathrm{d}\mathbb{P}(oldsymbol{M}|A=a,X) d\mathbb{P}(X) \ &= \langle \gamma_0, arphi(oldsymbol{a}') \otimes \mathrm{E}_P\{\mu_{oldsymbol{M}|A=a,X} \otimes arphi(X)\} 
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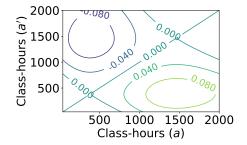
Effect of intervention a', with  $M^{(a)}$  as if intervention were a

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

#### Mediation analysis: results

#### Total effect:

$$egin{aligned} heta_0^{TE}(a, \mathbf{a}') \ &:= \mathbb{E}[\,Y^{\{\mathbf{a}', \mathbf{M}^{(\mathbf{a}')}\}} - \,Y^{\{a, \mathbf{M}^{(a)}\}}] \end{aligned}$$

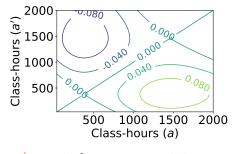


a' = 1600 hours vs a = 480 means 0.1 reduction in arrests

#### Mediation analysis: results

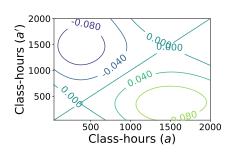
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#### Direct effect:

$$egin{aligned} heta_0^{DE}(a, oldsymbol{a}') \ &:= \mathbb{E}[\,Y^{\{oldsymbol{a}', oldsymbol{M}^{(a)}\}} - \,Y^{\{a, oldsymbol{M}^{(a)}\}}] \end{aligned}$$

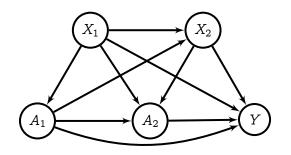


- a' = 1600 hours vs a = 480 means 0.1 reduction in arrests
- <u>Indirect</u> effect mediated via employment effectively zero

Singh, Xu, G (2022b)

#### ...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  $\mathrm{E}(y^{(a_1',a_2')}|A_1=a_1,A_2=a_2)...$  (c.f. the Robins G-formula)

# Unobserved confounders

















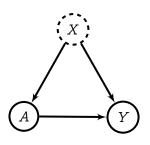
### The proxy correction

Unobserved X with (possibly) complex nonlinear effects on A, Y The definitions are:

- *X*: unobserved confounder.
- A: treatment
- *Y*: outcome

If X were observed (which it isn't),

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



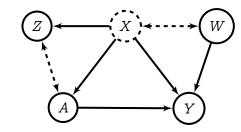
#### The proxy correction

Unobserved X with (possibly) complex nonlinear effects on A, Y The definitions are:

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

Bidirected arrow: possible confounding.

Structural assumption:



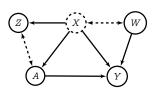
$$W \perp \!\!\! \perp (Z, A)|X$$
  
 $Y \perp \!\!\! \perp Z|(A, X)$ 

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

Miao, Geng, Tchetgen Tchetgen (2018): Identifying causal effects with proxy variables of an unmeasured confounder. 29/39

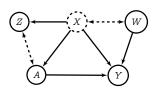
If X were observed,

$$P(Y|do(a)) := \sum_{i=1}^{D} P(y|\mathbf{x}_i, a) P(\mathbf{x}_i)$$



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$$P(Y|do(a)) := \sum_{i=1}^{D} P(y| extbf{ extit{x}}_i, a) P( extbf{ extit{x}}_i) = P(y| extbf{ extit{X}}, a) P( extbf{ extit{X}})$$

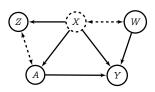


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Because  $W \perp \!\!\!\perp (Z, A)|X$ ,

$$P(W|Z,a) = P(W|X)P(X|Z,a)$$



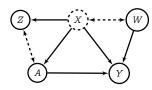
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,

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$$\implies P(X|Z, a) = P^{-1}(W|X)P(W|Z, a)$$



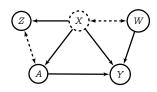
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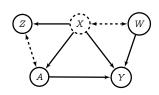
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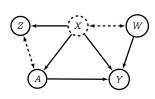
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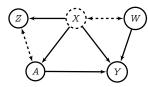
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$$\implies p(y|X, a) = p(y|Z, a)P^{-1}(W|Z, a)P(W|X)$$

From previous slide:

$$p(y|X, a) = p(y|Z, a)P^{-1}(W|Z, a)P(W|X)$$

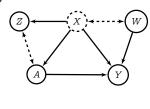


From previous slide:

$$p(y|X, a) = p(y|Z, a)P^{-1}(W|Z, a)P(W|X)$$

Multiply LHS and RHS by P(X):

$$egin{align} P(Y^{(a)}) &:= P(y|X,a)P(X) \ &= p(y|Z,a)P^{-1}(W|Z,a) \underbrace{P(W|X)P(X)}_{P(W)} \ \end{array}$$



Average causal effect using only observed data!

### The proxy correction (continuous)

If X were observed,

$$\mathrm{E}(\,Y^{(a)})=\int E(y|a,x)p(x)dx.$$

....but we do not see p(x).

## The proxy correction (continuous)

If X were observed,

$$\operatorname{E}(Y^{(a)}) = \int E(y|a,x) p(x) dx.$$

....but we do not see p(x).

Main theorem: Assume we have solved...

$$E(y|z,a) = \int h_y(w,a) p(w|z,a) dw$$

(Fredholm integral of the first kind; subject to conditions for existence of solution)

## The proxy correction (continuous)

If X were observed,

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Main theorem: Assume we have solved...

$$E(y|z,a) = \int h_y(w,a) p(w|z,a) dw$$

(Fredholm integral of the first kind; subject to conditions for existence of solution)

...then average causal effect via p(w):

$$E(y^{(a)}) = \int h_y(a,w) p(w) dw$$

Expressions in terms of observed quantities, can be learned from data.

#### Our solution

- Stage 1: ridge regression from  $\phi(a) \otimes \phi(z)$  to  $\phi(w)$ 
  - yields conditional mean embedding  $\mu_{W|a,z}$
- Stage 2: ridge regression from  $\mu_{W|a,z}$  and  $\phi(a)$  to y
  - yields  $h_y(w, a)$ .
- Solved using sieves [A], kernel [B], or learned NN [C] features

Code available for kernel and NN solutions

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

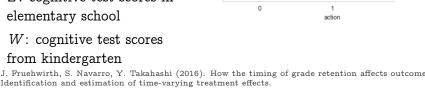
- [A] Deaner (2021) Proxy controls and panel data.
- $[B]\ Mastouri^*,\ Zhu^*,\ Gultchin,\ Korba,\ Silva,\ Kusner,\ G,^{\dagger}\ Muandet^{\dagger}\ (2021);\ Proximal\ Causal\ Learning$

with Kernels: Two-Stage Estimation and Moment Restriction
[C] Xu, Kanagawa, G. (2021) Deep Proxy Causal Learning and its Application to Confounded Bandit
Policy Evaluation

33/39

## Grade retention and cognitive outcome

- X: unobserved confounder ("ability")
- A: 0: no retention. 1: kindergarten retention. 2: early elementary retention.
- Y: math scores, age 11
- $\blacksquare$  Z: cognitive test scores in elementary school
- W: cognitive test scores



J. Fruehwirth, S. Navarro, Y. Takahashi (2016). How the timing of grade retention affects outcomes: Identification and estimation of time-varying treatment effects. Deaner (2021)

#### Conclusions

#### Kernel ridge regression:

- Solution for ATE, ATT, CATE, mediation analysis, dynamic treatment effects, proximal learning
- ....with treatment A, covariates X, V, mediator M, proxies (W, Z) multivariate, "complicated"
- Simple, robust implementation
- Strong statistical guarantees under general smoothness assumptions

#### In the papers, but not in this talk:

- Doubly robust estimates for discrete A, V with automatic debiasing
- Elasticities
- Regression to potential outcome distributions over Y (not just  $E(Y^{(a)}|...)$ )
- Instrumental variable regression
- Same algorithms but with adaptive NN features

#### Selected papers

#### Observed confounders:



#### Unobserved confounders:

#### ICML 2021:



#### NeurIPS 2019:

Rahul Singh, Maneesh Sahani, Arthur Gretton

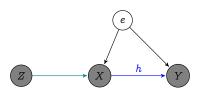


# Questions?



## Instrumental variable setting (1)

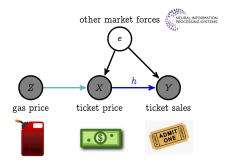
- Unobserved confounder  $e \implies$  prediction  $\neq$  counterfactual prediction
- goal: learn causal relationship h between input X and output Y
   if we intervened on X, what would be the effect on Y?
- Instrument Z only influences Y via X, identifying h



$$Y = \langle h, \psi(X) \rangle + e$$
  $\mathbb{E}(e|Z) = 0$ 

## Instrumental variable setting (1)

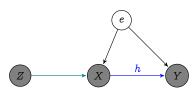
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$$Y = \langle h, \psi(X) \rangle + e$$
  $\mathbb{E}(e|Z) = 0$ 

$$\mathbb{E}(e|Z)=0$$

# Instrumental variable setting (2)



- Ridge regression of  $\psi(X)$  on  $\phi(Z)$ 
  - using *n* observations
  - construct conditional mean embedding  $\mu(z) := \mathbb{E}[\psi(X)|Z=z]$
- Ridge regression of Y on  $\mu(Z)$ 
  - using remaining *m* observations
  - this is the estimator for h
- Solved using kernel and learned NN features

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Singh, Sahani, G., (NeurIPS 2019)
Xu, Chen, Srinivasan, de Freitas, Doucet, G. (ICLR 2021)
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