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

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## A medical treatment scenario



From our observations of historical hospital data:

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

Just recommend pills? Cheaper and more effective!

## A medical treatment scenario



From our intervention (making all patients take a treatment):
■ $P(Y=\operatorname{cured} \mid d o($ pills $))=0.64$
■ $P(Y=$ cured $\mid d o($ surgery $))=0.75$
What went wrong?

## Observational vs interventional

Conditioning from observation:

$$
\mathrm{E}(Y \mid A=a)=\sum_{x} E(y \mid a, x) p(x \mid a)
$$



## Observational vs interventional

Average causal effect (intervention):

$$
\mathrm{E}\left(Y^{(a)}\right)=\sum_{x} E(y \mid a, x) p(x)
$$



## Questions we will solve



## Outline

Talk structure:

- Average treatment effect (ATE)
- ...via kernel/NN mean embedding (marginalization)
$■$ Conditional average treatment effect (CATE)
- via conditional mean embedding
- Average treatment on treated

■ Mediation effect, dynamic treatment effect
■ Proxy methods

- ...when covariates are hidden

Properties and advantages of approach:

- Treatment $A$, covariates $X$, etc are by default multivariate, complicated...
■ Simple, robust implementation;
■ Strong statistical guarantees under general smoothness assumptions


## Key requirement: linear functions of features

All learned functions will take the form:

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

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:

$$
\left\langle\varphi\left(x_{i}\right), \varphi(x)\right\rangle_{\mathcal{H}}=k\left(x_{i}, x\right)
$$

Kernel is feature dot product.
Primary focus of this talk.

## Building block: kernel ridge regression

Learn $\gamma_{0}(x):=\mathrm{E}[Y \mid X=x]$ from features $\varphi\left(x_{i}\right)$ with outcomes $y_{i}$ :

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

Kernel as feature dot product:

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$$

Kernel as feature dot product:

$$
\left\langle\varphi\left(x_{i}\right), \varphi(x)\right\rangle_{\mathcal{H}}=k\left(x_{i}, x\right)
$$

Solution at $x$ :

$$
\begin{aligned}
\hat{\gamma}(x) & =\sum_{i=1}^{n} \alpha_{i} k\left(x_{i}, x\right) \\
\alpha & =(K+\lambda I)^{-1} Y \\
\left(K_{X X}\right)_{i j} & =k\left(x_{i}, x_{j}\right),
\end{aligned}
$$



## Building block: kernel ridge regression

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$$

Kernel as feature dot product:

$$
\left\langle\varphi\left(x_{i}\right), \varphi(x)\right\rangle_{\mathcal{H}}=k\left(x_{i}, x\right)
$$

Solution at $x$ (as weighted sum of $y$ )

$$
\begin{aligned}
\hat{\gamma}(x) & =\sum_{i=1}^{n} y_{i} \beta_{i}(x) \\
\beta(x) & =(K+\lambda I)^{-1} k_{X x} \\
\left(K_{X X}\right)_{i j} & =k\left(x_{i}, x_{j}\right) \\
\left(k_{X x}\right)_{i} & =k\left(x_{i}, x\right)
\end{aligned}
$$



8/41

## KRR: consistency in RKHS norm

## Assume problem well specified

■ Denote: $\gamma_{0} \in \mathcal{H}^{c}$ where $\mathcal{H}^{c} \subset \mathcal{H}, \quad c \in(1,2]$
■ Larger $c \Longrightarrow$ smoother $\gamma_{0} \Longrightarrow$ easier problem.
[A] Singh, Xu, G (2021a), Generalized Kernel Ridge Regression for Nonparametric Structural Functions and Semiparametric Treatment Effects.

Results from:
Smale and Ding-Xuan Zhou (2007). Learning theory estimates via integral operators and their approximations; Caponnetto, De Vito (2007), Optimal rates for the regularized least-squares algorithm.

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■ Larger $c \Longrightarrow$ smoother $\gamma_{0} \Longrightarrow$ easier problem.
Consistency [A, Prop. F.1]

$$
\left\|\hat{\gamma}-\gamma_{0}\right\|_{\mathcal{H}}=O_{P}\left(n^{-\frac{1}{2} \frac{c-1}{c+1}}\right)
$$

best rate is $O_{P}\left(n^{-1 / 6}\right)$.
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# (Conditional) average treatment effect, average treatment on treated 



## Average treatment effect

Average causal effect (intervention):

$$
\mathrm{E}\left(Y^{(a)}\right)=\int E(y \mid a, x) d p(x)
$$

(the average structural function; in epidemiology, for continuous $a$, the dose-response curve).
Assume: (1) no interference/spillover, (2) conditional exchangeability $Y^{(a)} \Perp A \mid X$. (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

$$
\gamma_{0}(a, x):=\mathrm{E}[Y \mid a, x]
$$

Assume we have:

- covariate features $\varphi(x)$ with kernel $k\left(x, x^{\prime}\right)$
- treatment features $\varphi(a)$ with kernel $k\left(a, a^{\prime}\right)$

(argument of kernel/feature map indicates feature space)


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- treatment features $\varphi(a)$ with kernel $k\left(a, a^{\prime}\right)$

(argument of kernel/feature map indicates feature space)
We use outer product of features ( $\Longrightarrow$ product of kernels):

$$
\phi(x, a)=\varphi(a) \otimes \varphi(x) \quad \mathfrak{K}\left([a, x],\left[a^{\prime}, x^{\prime}\right]\right)=k\left(a, a^{\prime}\right) k\left(x, x^{\prime}\right)
$$

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$$

Ridge regression solution:

$$
\hat{\gamma}(x, a)=\sum_{i=1}^{n} y_{i} \beta_{i}(a, x), \quad \beta(a, x)=\left[K_{A A} \odot K_{X X}+\lambda I\right]^{-1} K_{A a} \odot K_{2 \chi \nmid x_{1}}
$$

## ATE (dose-response curve)

Well specified setting:

$$
\gamma_{0}(a, x)=\mathrm{E}[Y \mid a, x] \in \mathcal{H}
$$

ATE as feature space dot product:

$$
\begin{aligned}
\theta_{0}^{\mathrm{ATE}}(a) & =\mathrm{E}_{P}\left[\gamma_{0}(a, X)\right] \\
& =\mathrm{E}_{P}\left\langle\gamma_{0}, \varphi(a) \otimes \varphi(X)\right\rangle
\end{aligned}
$$



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& =\langle\gamma_{0}, \underbrace{\mu_{P}}_{\mathrm{E}_{P} \varphi(X)} \otimes \varphi(a)\rangle
\end{aligned}
$$



Feature map of probability $P$,

$$
\mu_{P}=\left[\ldots \mathrm{E}_{P}\left[\varphi_{i}(X)\right] \ldots\right]
$$

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& =\langle\gamma_{0}, \underbrace{\mu_{P}}_{\mathrm{E}_{P} \varphi(X)} \otimes \varphi(a)\rangle
\end{aligned}
$$



For characteristic kernels, $\mu_{P}$ is injective.
Consistency: $\left\|\hat{\mu}_{P}-\mu_{P}\right\|_{\mathcal{H}}=O_{P}\left(n^{-1 / 2}\right)$

## ATE: empirical estimate and consistency

Empirical estimate of ATE:

$$
\hat{\theta}^{\mathrm{ATE}}(a)=\frac{1}{n} \sum_{i=1}^{n} Y^{\top}\left(K_{A A} \odot K_{X X}+n \lambda I\right)^{-1}\left(K_{A a} \odot K_{X x_{i}}\right)
$$

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$$

Consistency:

$$
\left\|\hat{\theta}^{\mathrm{ATE}}-\theta_{o}^{\mathrm{ATE}}\right\|_{\infty}=O_{P}\left(n^{-\frac{1}{2} \frac{c-1}{c+1}}\right)
$$

Follows from consistency of $\hat{\mu}_{P}$, and of $\hat{\gamma}$ under smoothness assumption $\gamma_{0} \in \mathcal{H}^{c}$.

## 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 (2021a).

## ATE: results



■ First 12.5 weeks of classes confer employment gain: from $35 \%$ to $47 \%$.

- [RKHS] is our $\hat{\theta}^{\mathrm{ATE}}(a)$

■ [DML2] Colangelo, Lee (2020), Double debiased machine learning nonparametric inference with continuous treatments.

Singh, Xu, G (2021a)

## Confidence intervals for discretized treatment



■ Doubly robust estimator: semiparametric efficiency, asymptotic normality, confidence intervals

- Automated debiasing (via kernel regression)
- Requires discretized treatment (here, equiprobable bins)

Singh, Xu, G (2021a)
Chernozhukov, Newey, Singh (2018). Automatic debiased machine learning of causal and structural $17 / 41$
effects.

## Conditional ATE: example

US job corps: training for disadvantaged youths:

■ $X$ : confounder/context (education, marital status, ...)

- A: treatment (training hours)

■ $Y$ : outcome (percent
 employed)
■ $V$ : age

Singh, Xu, G (2021a)

## Conditional average treatment effect

Learned conditional mean:

$$
\begin{aligned}
& \mathrm{E}[Y \mid a, x, v] \approx \gamma_{0}(a, x, v) \\
& =\left\langle\gamma_{0}, \varphi(a) \otimes \varphi(x) \otimes \varphi(v)\right\rangle .
\end{aligned}
$$

Conditional ATE

$$
\begin{aligned}
& \theta_{o}^{\mathrm{CATE}}(a, v) \\
& =\mathrm{E}\left(Y^{(a)} \mid V=v\right)
\end{aligned}
$$



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$\theta_{o}^{\mathrm{CATE}}(a, v)$


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& =\mathrm{E}_{P}\left(\left\langle\gamma_{0}, \varphi(a) \otimes \varphi(X) \otimes \varphi(V)\right\rangle \mid V=v\right) \\
& =\ldots ?
\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

Learned conditional mean:

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& =\mathrm{E}_{P}\left(\left\langle\gamma_{0}, \varphi(a) \otimes \varphi(X) \otimes \varphi(V)\right\rangle \mid V=v\right) \\
& =\langle\gamma_{0}, \varphi(a) \otimes \underbrace{\mathrm{E}_{P}[\varphi(X) \mid V=v]}_{\mu_{X \mid V=v}} \otimes \varphi(v)\rangle
\end{aligned}
$$

Learn conditional mean embedding: $\mu_{X \mid V=v}:=\mathrm{E}_{P}(\varphi(X) \mid V=v)$

## Regressing from feature space to feature space

Our goal: an operator $E_{0}: \mathcal{H}_{\nu} \rightarrow \mathcal{H}_{\mathcal{X}}$ such that

$$
E_{0} \varphi(v)=\mu_{X \mid V=v}
$$

[^0]
## Regressing from feature space to feature space

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$$

Assume

$$
E_{0} \in \overline{\operatorname{span}\{\varphi(x) \otimes \varphi(v)\}} \Longleftrightarrow E_{0} \in \operatorname{HS}\left(\mathcal{H}_{\nu}, \mathcal{H}_{\mathcal{X}}\right)
$$

Smoothness assumption:

$$
\mathrm{E}_{P}[h(X) \mid V=v] \in \mathcal{H} \nu \quad \forall h \in \mathcal{H}_{\mathcal{X}}
$$

[^1]
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$$



[^2]
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$$

Smoothness assumption:

$$
\mathrm{E}_{P}[h(X) \mid V=v] \in \mathcal{H}_{\nu} \quad \forall h \in \mathcal{H}_{\mathcal{X}}
$$

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

$$
\widehat{E}=\underset{E \in H S}{\operatorname{argmin}} \sum_{\ell=1}^{n}\left\|\varphi\left(x_{\ell}\right)-E \varphi\left(v_{\ell}\right)\right\|_{\mathcal{H}_{X}}^{2}+\lambda_{2}\|E\|_{H S}^{2}
$$

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

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Our goal: an operator $E_{0}: \mathcal{H}_{\nu} \rightarrow \mathcal{H}_{\mathcal{X}}$ such that

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$$

Ridge regression solution:

$$
\begin{aligned}
\mu_{X \mid V=v}:=\mathrm{E}_{P}[\varphi(X) \mid V=v] & \approx \widehat{E} \varphi(v)=\sum_{\ell=1}^{n} \varphi\left(x_{\ell}\right) \beta_{\ell}(v) \\
\beta(v) & =\left[K_{V V}+\lambda_{2} I\right]^{-1} k_{V v}
\end{aligned}
$$

## Consistency of conditional mean embedding

Assume problem well specified [A, Hypothesis 5]

$E_{0} \in \operatorname{HS}\left(\mathcal{H}_{\nu}^{c_{1}}, \mathcal{H}_{X}\right)$

$■$ Larger $c_{1} \Longrightarrow$ smoother $E_{0} \Longrightarrow$ easier problem.
[A] Singh, Sahani, G (2019)
Earlier consistency proof for finite dimensional $\varphi(x)$ :
Grunewalder, Lever, Baldassarre, Patterson, G, Pontil (2012).
Caponnetto, De Vito (2007).

## Consistency of conditional mean embedding

Assume problem well specified [A, Hypothesis 5]

$$
E_{0} \in \operatorname{HS}\left(\mathcal{H}_{V}^{c_{1}}, \mathcal{H}_{X}\right)
$$

■ Larger $c_{1} \Longrightarrow$ smoother $E_{0} \Longrightarrow$ easier problem.
Consistency [A, Theorem 2]

$$
\left\|\widehat{E}-E_{0}\right\|_{\mathrm{HS}}=O_{P}\left(n^{-\frac{1}{2} \frac{c_{1}-1}{c_{1}+1}}\right),
$$

best rate is $O_{P}\left(n^{-1 / 6}\right)$.
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## Consistency of CATE

Empirical CATE:
$\hat{\theta}^{\mathrm{CATE}}(a, v)=\left\langle\hat{\gamma}, \varphi(a) \otimes \hat{\mu}_{X \mid V=v} \otimes \varphi(v)\right\rangle$

## Consistency of CATE

## Empirical CATE:

$\hat{\theta}^{\mathrm{CATE}}(a, v)=\left\langle\hat{\gamma}, \varphi(a) \otimes \hat{\mu}_{X \mid V=v} \otimes \varphi(v)\right\rangle$
$=Y^{\top}\left(K_{A A} \odot K_{X X} \odot K_{V V}+n \lambda I\right)^{-1}(K_{A a} \odot \underbrace{K_{X X}\left(K_{V V}+n \lambda_{1} I\right)^{-1} K_{V v}}_{\text {from } \hat{\mu}_{X \mid V=v}} \odot K_{V v})$

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Consistency:

$$
\left\|\hat{\theta}^{\mathrm{CATE}}-\theta_{0}^{\mathrm{CATE}}\right\|_{\infty}=O_{P}\left(n^{-\frac{1}{2} \frac{c-1}{c+1}}+n^{-\frac{1}{2} \frac{c_{1}-1}{c_{1}+1}}\right)
$$

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

Singh, Xu, G (2021a)

## Conditional ATE: example

US job corps: training for disadvantaged youths:

■ $X$ : confounder/context (education, marital status, ...)

- A: treatment (training hours)

■ $Y$ : outcome (percent
 employed)
■ $V$ : age

Singh, Xu, G (2021a)

## Conditional ATE: results



Average percentage employment $Y^{(a)}$ for class hours $a$, conditioned on age $v$. Given around 12-14 weeks of classes:
■ $16 \mathrm{y} / \mathrm{o}$ : percent employment increases from $28 \%$ to at most $36 \%$.
■ $22 \mathrm{y} / \mathrm{o}$ : percent employment increases from $40 \%$ to $56 \%$.
Singh, Xu, G (2021a)

## Counterfactual: average treatment on treated

Conditional mean:
$\mathrm{E}[Y \mid a, x]=\gamma_{0}(a, x)$
Average treatment on treated:

$$
\begin{aligned}
& \theta^{A T T}\left(a, a^{\prime}\right) \\
& =\mathrm{E}\left(Y^{\left(a^{\prime}\right)} \mid A=a\right)
\end{aligned}
$$



Empirical ATT:

$$
\hat{\theta}^{\mathrm{ATT}}\left(a, a^{\prime}\right)
$$

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& =\mathrm{E}\left(Y^{\left(a^{\prime}\right)} \mid A=a\right) \\
& =\mathrm{E}_{P}\left(\left\langle\gamma_{0}, \varphi\left(a^{\prime}\right) \otimes \varphi(X)\right\rangle \mid A=a\right) \\
& =\langle\gamma_{0}, \varphi\left(a^{\prime}\right) \otimes \underbrace{\left.\mathrm{E}_{P}[\varphi(X) \mid A=a]\right]}_{\mu_{X \mid A=a}}\rangle
\end{aligned}
$$



Empirical ATT:

$$
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& =\mathrm{E}\left(Y^{\left(a^{\prime}\right)} \mid A=a\right) \\
& =\mathrm{E}_{P}\left(\left\langle\gamma_{0}, \varphi\left(a^{\prime}\right) \otimes \varphi(X)\right\rangle \mid A=a\right) \\
& =\langle\gamma_{0}, \varphi\left(a^{\prime}\right) \otimes \underbrace{\mathrm{E}_{P}[\varphi(X) \mid A=a]}_{\mu_{X \mid A=a}}\rangle
\end{aligned}
$$



Empirical ATT:

$$
\begin{aligned}
& \hat{\theta}^{\operatorname{ATT}}\left(a, a^{\prime}\right) \\
& =Y^{\top}\left(K_{A A} \odot K_{X X}+n \lambda I\right)^{-1}(K_{A a^{\prime}} \odot \underbrace{K_{X X}\left(K_{A A}+n \lambda_{1} I\right)^{-1} K_{A a}}_{\text {from } \hat{\mu}_{X \mid A=a}})
\end{aligned}
$$

## 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) $\gamma_{0}(a, m, x) \approx \mathrm{E}[Y \mid A=a, M=m, X=x]$


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$\gamma_{0}(a, m, x) \approx \mathrm{E}[Y \mid A=a, M=m, X=x]$
A quantity of interest, the mediated effect:

$$
Y^{\left\{a^{\prime}, M^{(a)}\right\}}=\int \gamma_{0}\left(a^{\prime}, M, X\right) \operatorname{dP}(M \mid A=a, X) d \mathbb{P}(X)
$$

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

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& =\left\langle\gamma_{0}, \varphi\left(a^{\prime}\right) \otimes \mathrm{E}_{P}\left\{\mu_{M \mid A=a, X} \otimes \varphi(X)\right\}\right\rangle
\end{aligned}
$$

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

## Mediation analysis: results

Total effect:

$$
\theta_{0}^{T E}\left(a, a^{\prime}\right)
$$

$$
:=\mathbb{E}\left[Y^{\left\{a^{\prime}, M^{\left(a^{\prime}\right)}\right\}}-Y^{\left\{a, M^{(a)}\right\}}\right]
$$



- $a^{\prime}=1600$ hours vs $a=480$ means 0.1 reduction in arrests


## Mediation analysis: results

Total effect:
Direct effect:

$$
\begin{aligned}
& \theta_{0}^{T E}\left(a, a^{\prime}\right) \\
& :=\mathbb{E}\left[Y^{\left\{a^{\prime}, M^{\left(a^{\prime}\right)}\right\}}-Y^{\left\{a, M^{(a)}\right\}}\right]
\end{aligned}
$$

$$
\begin{aligned}
& \theta_{0}^{D E}\left(a, a^{\prime}\right) \\
& :=\mathbb{E}\left[Y^{\left\{a^{\prime}, M^{(a)}\right\}}-Y^{\left\{a, M^{(a)}\right\}}\right]
\end{aligned}
$$



- $a^{\prime}=1600$ hours vs $a=480$ means 0.1 reduction in arrests
- Indirect effect mediated via employment effectively zero
...dynamic treatment effect...
Dynamic treatment effect: sequence $A_{1}, A_{2}$ of treatments.


■ Causal effects $Y^{\left(a_{1}\right)}, Y^{\left(a_{2}\right)}, Y^{\left(a_{1}, a_{2}\right)}$,

- counterfactuals $\mathrm{E}\left(y^{\left(a_{1}^{\prime}, a_{2}^{\prime}\right)} \mid A_{1}=a_{1}, A_{2}=a_{2}\right) \ldots$
(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),


$$
E\left(Y^{(a)}\right)=\int E(y \mid x, a) d p(x)
$$

## 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:

$$
\begin{aligned}
& W \Perp(Z, A) \mid X \\
& Y \Perp Z \mid(A, X)
\end{aligned}
$$

$\Longrightarrow$ Can recover $E\left(Y^{(a)}\right)$ from observational data!
Miao, Geng, Tchetgen Tchetgen (2018): Identifying causal effects with proxy variables of an unmeasured confounder.

## Proof (discrete variables)

If $X$ were observed,

$$
P(Y \mid d o(a)):=\sum_{i=1}^{D} P\left(y \mid x_{i}, a\right) P\left(x_{i}\right)
$$



## Proof (discrete variables)

If $X$ were observed,

$$
P(Y \mid d o(a)):=\sum_{i=1}^{D} P\left(y \mid x_{i}, a\right) P\left(x_{i}\right)=P(y \mid X, a) P(X)
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P(W \mid Z, a)=P(W \mid X) P(X \mid Z, a)
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& \Longrightarrow p(y \mid X, a)=p(y \mid Z, a) P^{-1}(W \mid Z, a) P(W \mid X)
\end{aligned}
$$

## Proof (discrete variables)

From previous slide:
$p(y \mid X, a)=p(y \mid Z, a) P^{-1}(W \mid Z, a) P(W \mid X)$


## Proof (discrete variables)

From previous slide:
$p(y \mid X, a)=p(y \mid Z, a) P^{-1}(W \mid Z, a) P(W \mid X)$

Multiply LHS and RHS by $P(X)$ :

$$
\begin{aligned}
& P\left(Y^{(a)}\right):=P(y \mid X, a) P(X) \\
& =p(y \mid Z, a) P^{-1}(W \mid Z, a) \underbrace{P(W \mid X) P(X)}_{P(W)}
\end{aligned}
$$



## The proxy correction (continuous)

If $X$ were observed,

$$
\mathrm{E}\left(Y^{(a)}\right)=\int E(y \mid a, x) p(x) d x
$$

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

Miao, Geng, Tchetgen Tchetgen (2018)

## The proxy correction (continuous)

If $X$ were observed,

$$
\mathrm{E}\left(Y^{(a)}\right)=\int E(y \mid a, x) p(x) d x
$$

....but we do not see $p(x)$.
Main theorem: Assume we have solved...

$$
E(y \mid z, a)=\int h_{y}(w, a) p(w \mid z, a) d w
$$

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

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If $X$ were observed,

$$
\mathrm{E}\left(Y^{(a)}\right)=\int E(y \mid a, x) p(x) d x
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Main theorem: Assume we have solved...

$$
E(y \mid z, a)=\int h_{y}(w, a) p(w \mid z, a) d w
$$

(Fredholm integral of the first kind; subject to conditions for existence of solution)
...then causal effect via $p(w)$ :

$$
E\left(y^{(a)}\right)=\int h_{y}(a, w) p(w) d w
$$

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

Miao, Geng, Tchetgen Tchetgen (2018)

## Our solution

- Stage 1: ridge regression from $\phi(a) \otimes \phi(z)$ to $\phi(w)$
- yields conditional mean embedding $\mu_{W \mid a, z}$
$■$ Stage 2: ridge regression from $\mu_{W \mid a, z}$ 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

## 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

- Z: cognitive test scores in
 elementary school

■ $W$ : cognitive test scores from kindergarten
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 causal effect distributions over $Y$ (not just $E\left(Y^{(a)} \mid \ldots\right)$ )
■ Instrumental variable regression
■ Same algorithms but with adaptive NN features

## Selected papers

## Unobserved confounders:

ICML 2021:

## Observed confounders:

```
arXiv.org > econ > arXiv:2010.04855
    search
                            Help I Ad
Economics > Econometrics
[Submitted on 10 Oct 2020(v1), last revised 14 Dec 2021 (this version, v4)]
Generalized Kernel Ridge Regression for Nonparametric
Structural Functions and Semiparametric Treatment Effects
Rahul Singh, Liyuan Xu , Arthur Gretton
```



```
Statistics > Methodology
[Submitted on 6 Nov 2021]
Kernel Methods for Multistage Causal Inference: Mediation Analysis and Dynamic Treatment Effects
```

Rahul Singh, Liyuan Xu , Arthur Gretton

```
arXiv.org > cs > arxiv:2105.04544 Search.
MalplAdaan
```

Computer Science > Machine Learning
[Submitted on 10 May 2021 (v1), last revised 90 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

## NeurIPS 2021:

```
arXiv.org > cs > arXiv:2106.03907 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

## NeurIPS 2019:

```
arXiv.org > cs > arXiv:1906.00232 (arch..._
    Computer Science > Machine Learning
    [Submitted on 1 Jun 2019(vI), last revised 15 /J/2020 (this version, v6)]
    Kernel Instrumental Variable Regression
```

    Rahul Singh, Maneesh Sahani, Arthur Gretton
    
## Questions?



## Instrumental variable setting (1)

■ Unobserved confounder $e \Longrightarrow$ 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 $h$


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

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■ Unobserved confounder $e \Longrightarrow$ prediction $\neq$ counterfactual prediction

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

## Instrumental variable setting (2)



■ Ridge regression of $\psi(X)$ on $\phi(Z)$

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

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


[^0]:    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.
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