# Causal Effect Estimation with Context and Confounders (2) 

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Gatsby Computational Neuroscience Unit
Deepmind
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## Questions we will solve



## Outline

Previous slides: Causal effect estimation, observed covariates:
■ Average treatment effect (ATE), conditional average treatment effect (CATE)

These slides: 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 $\gamma$ )

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:

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

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

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

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$$

Neural net solution at $x$ :

$$
\begin{aligned}
\hat{\gamma}(x) & =C_{Y X}\left(C_{X X}+\lambda\right)^{-1} \varphi(x) \\
C_{Y X} & =\frac{1}{n} \sum_{i=1}^{n}\left[y_{i} \varphi\left(x_{i}\right)^{\top}\right] \\
C_{X X} & =\frac{1}{n} \sum_{i=1}^{n}\left[\varphi\left(x_{i}\right) \varphi\left(x_{i}\right)^{\top}\right]
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$$

Kernel solution at $x$ (as weighted sum of $y$ )

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



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


Simplification of example from Hartford, Lewis, Leyton-Brown, Taddy (2017): Deep IV: A Flexible7/39 Approach for Counterfactual Prediction.

## Illustration: ticket prices for air travel

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


■ Desire for travel:

$$
\begin{aligned}
& \varepsilon \sim \mathcal{N}(\mu, 0.1) \\
& \mu \sim \mathcal{U}\left\{-\frac{1}{2}, 0, \frac{1}{2}\right\}
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■ Price:

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& A=\varepsilon+Z \\
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$A=\varepsilon+Z$,

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- Seats sold:

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Average treatment effect:

$$
\operatorname{ATE}(a)=\mathbb{E}\left[Y^{(a)}\right]=\int(10-a+2 \varepsilon) d p(\varepsilon)=10-a
$$

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

$$
\mathbb{E}[Y \mid Z]=10-\mathbb{E}[A \mid Z]+2 \underbrace{\mathbb{E}[\varepsilon \mid Z]}_{=0}
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Regressing from $\mathbb{E}[A \mid Z]$ to $\mathbb{E}[Y \mid Z]$ recovers ATE!

## IV: the linear case

Output $y \in \mathbb{R}$, noise $\varepsilon \in \mathbb{R}$, input $a$ with NN features $\phi_{\theta}(a)$.
Crucially, $\varepsilon \not \Perp a$ and

$$
C_{a \varepsilon}:=\mathbb{E}\left[\phi_{\theta}(A) \varepsilon\right] \neq 0
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Average treatment effect:

$$
\begin{aligned}
& y=\gamma_{0}^{\top} \phi_{\theta}(a)+\varepsilon \quad \mathbb{E}(\varepsilon)=0 \\
& A T E:=\mathbb{E}\left(Y^{(a)}\right)=\int\left(\gamma_{0}^{\top} \phi_{\theta}(a)+\varepsilon\right) d P(\varepsilon)=\gamma_{0}^{\top} \phi_{\theta}(a) .
\end{aligned}
$$

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Least-squares loss for $\gamma, \theta$ :

$$
\mathcal{L}(\gamma, \theta)=\mathbb{E}\left\|Y-\gamma^{\top} \phi_{\theta}(A)-\varepsilon\right\|^{2}
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\mathcal{L}(\gamma, \theta)=\mathbb{E}\left\|Y-\gamma^{\top} \phi_{\theta}(A)-\varepsilon\right\|^{2}
$$

Minimizing for $\gamma$,

$$
\begin{aligned}
\gamma_{0}=C_{a a}^{-1}\left(C_{a y}-C_{a \varepsilon}\right) & C_{a a}
\end{aligned}=\mathbb{E}\left[\phi_{\theta}(A) \phi_{\theta}(A)^{\top}\right] \quad C_{a y}=\mathbb{E}\left[\phi_{\theta}(A) Y\right]
$$

...but we don't have $C_{a \varepsilon}$.

## Instrumental variable regression

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


© Nobel Prize Outreach. Photo Paul Kennedy David Card

Prize share: $1 / 2$

© Nobel Prize Outreach. Photo: Risdon Photography Joshua D. Angrist

Prize share: 1/4

© Nobel Prize Outreach. Photo: 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:
■ $\varepsilon$ : unobserved confounder.

- A: treatment

■ $Y$ : outcome
■ $Z$ : instrument
Assumptions


$$
\begin{aligned}
& \mathbb{E}[\varepsilon]=0 \quad \mathbb{E}[\varepsilon \mid Z]=0 \\
& Z \not \Perp A \\
& (Y \Perp Z \mid A)_{G_{\bar{A}}} \\
& Y=\gamma^{\top} \phi_{\theta}(A)+\varepsilon
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Average treatment effect:
$\operatorname{ATE}(a)=\int \mathbb{E}(Y \mid \varepsilon, a) d p(\varepsilon)=\gamma^{\top} \phi_{\theta}(a)$

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Y=\gamma^{\top} \phi_{\theta}(A)+\varepsilon &
\end{array}
$$

IV regression: Condition both sides on $Z$,

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

## Two-stage least squares for IV regression

## Kernel features (NeurIPS 2019):

| arXiv.org > cs > arXiv: 1906.00232 | Search... <br> Help IAc |
| :--- | :--- |
| Computer Science > Marhine Learning |  |

Computer Science > Machine Learning
[ Submitted on 1 Jun 2019 (v1), last revised 15 Jul 2020 (thls version, v6)]

## Kernel Instrumental Variable Regression

Rahul Singh, Maneesh Sahani, Arthur Gretton


## NN features (ICLR 2021):

## 

## Computer Science > Machine Learning

[Submitted on 140 Ot 2020 (v1), last revised 1 Nov 2020 (this version, v3)]
Learning Deep Features in Instrumental Variable Regression
Liyuan Xu, Yutian Chen, Siddarth Srinivasan, Nando de Freitas, Arnaud Doucet, Arthur Gretton


## Code for NN and kernel IV methods:

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

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| Computer Science > Marhine |  |

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[SSubmitted on 1 Jun 2019 (vI), last revised 15 Jut 2020 (thls version, ven]

## Kernel Instrumental Variable Regression

Rahul Singh, Maneesh Sahani, Arthur Gretton


## NN features (ICLR 2021):

## ar〈iv>cs a axiv2010.07154

Computer Science > Machine Learning
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Learning Deep Features in Instrumental Variable Regression
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## IV using neural net features

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

$$
\mathbb{E}_{Y Z}\left[\left(Y-\gamma^{\top} \mathbb{E}\left[\phi_{\theta}(A) \mid Z\right]\right)^{2}\right]+\lambda_{2}\|\gamma\|^{2}
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Stage 1 regression: learn NN features $\phi_{\zeta}(Z)$ and linear layer $F$ :

$$
\mathbb{E}\left[\phi_{\theta}(A) \mid Z\right] \approx F \boldsymbol{\phi}_{\zeta}(Z)
$$

with RR loss

$$
\mathbb{E}\left\|\phi_{\theta}(A)-F \phi_{\zeta}(Z)\right\|^{2}+\lambda_{1}\|F\|_{H S}^{2}
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Challenge: how to learn $\theta$ ?

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From Stage 2 regression?

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From Stage 2 regression?
...which requires $\mathbb{E}\left[\phi_{\theta}(A) \mid Z\right]$ from Stage 1 regression

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Challenge: how to learn $\theta$ ?
From Stage 2 regression?
...which requires $\mathbb{E}\left[\phi_{\theta}(A) \mid Z\right]$ from Stage 1 regression
...which requires $\phi_{\theta}(A) \ldots$ which requires $\theta \ldots$

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From Stage 2 regression?
...which requires $\mathbb{E}\left[\phi_{\theta}(A) \mid Z\right]$ from Stage 1 regression
...which requires $\phi_{\theta}(A) \ldots$ which requires $\theta \ldots$

## Use the linear final layers! (i.e. $\gamma$ and $F$ )

Xu, Chen, Srinivasan, De Freitas, Doucet, G. (2021) Learning Deep Features in Instrumental Variable

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\mathbb{E}\left[\left\|\phi_{\theta}(A)-F \boldsymbol{\phi}_{\zeta}(Z)\right\|^{2}\right]+\lambda_{1}\|F\|_{H S}^{2}
$$

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

$$
\begin{array}{ll}
\hat{F}_{\theta, \zeta}=C_{A Z}\left(C_{Z Z}+\lambda_{1} I\right)^{-1} & C_{A Z}
\end{array}=\mathbb{E}\left[\phi_{\theta}(A) \phi_{\zeta}^{\top}(Z)\right] .
$$

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& C_{Z Z}=\mathbb{E}\left[\phi_{\zeta}(Z) \phi_{\zeta}^{\top}(Z)\right]
\end{array}
$$

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

## Stage 2: IV regression

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

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

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

$$
\begin{aligned}
& \hat{\gamma}_{\theta}:=\widetilde{C}_{Y Z}\left(\widetilde{C}_{Z Z}+\lambda_{2} I\right)^{-1} \widetilde{C}_{Y Z} \\
&=\mathbb{E}\left[Y\left[\hat{F}_{\theta, \zeta} \boldsymbol{\phi}_{\zeta}(Z)\right]^{\top}\right] \\
& \widetilde{C}_{Z Z}=\mathbb{E}\left[\left[\hat{F}_{\theta, \zeta} \boldsymbol{\phi}_{\zeta}(Z)\right]\left[\hat{F}_{\theta, \zeta} \boldsymbol{\phi}_{\zeta}(Z)\right]^{\top}\right]
\end{aligned}
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\begin{aligned}
& \hat{\gamma}_{\theta}:=\widetilde{C}_{Y Z}\left(\widetilde{C}_{Z Z}+\lambda_{2} I\right)^{-1} \widetilde{C}_{Y Z} \\
&=\mathbb{E}\left[Y\left[\hat{F}_{\theta, \zeta} \boldsymbol{\phi}_{\zeta}(Z)\right]^{\top}\right] \\
& \widetilde{C}_{Z Z}=\mathbb{E}\left[\left[\hat{F}_{\theta, \zeta} \boldsymbol{\phi}_{\zeta}(Z)\right]\left[\hat{F}_{\theta, \zeta} \boldsymbol{\phi}_{\zeta}(Z)\right]^{\top}\right]
\end{aligned}
$$

From linear final layers in Stages 1,2:
Learn $\phi_{\theta}(A)$ by plugging $\hat{\gamma}_{\theta}$ into $S 2$ loss, taking gradient steps for $\theta$

## Stage 2: IV regression

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

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

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

$$
\begin{aligned}
& \hat{\gamma}_{\theta}:=\widetilde{C}_{Y Z}\left(\widetilde{C}_{Z Z}+\lambda_{2} I\right)^{-1} \widetilde{C}_{Y Z} \\
&=\mathbb{E}\left[Y\left[\hat{F}_{\theta, \zeta} \boldsymbol{\phi}_{\zeta}(Z)\right]^{\top}\right] \\
& \widetilde{C}_{Z Z}=\mathbb{E}\left[\left[\hat{F}_{\theta, \zeta} \boldsymbol{\phi}_{\zeta}(Z)\right]\left[\hat{F}_{\theta, \zeta} \boldsymbol{\phi}_{\zeta}(Z)\right]^{\top}\right]
\end{aligned}
$$

From linear final layers in Stages 1,2:
Learn $\phi_{\theta}(A)$ by plugging $\hat{\gamma}_{\theta}$ into $S 2$ loss, taking gradient steps for $\theta$
....but $\zeta$ changes with $\theta$
...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:

$$
Q^{\pi}(s, a)=\mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^{t} R_{t} \mid S_{0}=s, A_{0}=a\right]
$$

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

## Application of IV: reinforcement learning

Q value is a minimizer of Bellman loss

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

Corresponds to "IV-like" problem

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

with

$$
\begin{aligned}
Y & =R \\
X & =\left(S^{\prime}, A^{\prime}, S, A\right) \\
Z & =(S, A) \\
f_{0}(X) & =Q^{\pi}(s, a)-\gamma Q^{\pi}\left(s^{\prime}, a^{\prime}\right)
\end{aligned}
$$

## 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 $8 申 89$ 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 Regressior 9939 Deep Offline Policy Evaluation.
...but seriously, what if there are hidden confounders?

## The proxy correction

Unobserved $\varepsilon$ with (possibly) complex nonlinear effects on $A, Y$ The definitions are:
$■ \varepsilon$ : unobserved confounder.

- A: treatment

■ $Y$ : outcome

If $\varepsilon$ were observed (which it isn't),


$$
\mathbb{E}\left[Y^{(a)}\right]=\int \mathbb{E}[Y \mid \varepsilon, a] d p(\varepsilon)
$$

## The proxy correction

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

■ $\varepsilon$ : 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.

## Unobserved confounders: proxy methods

## Kernel features (ICML 2021):

| axXiv.org > cs > axivi. 1105.04544 |  |
| :---: | :---: |
| Computer Science > Machine Learning |  |
| Proximal Causal Learning Estimation and Moment Re |  |

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 Sermen
Computer Science > Machine Learning
[Submitted on 7 Jun 2021 (vI), 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/ 22/39

## The proxy correction

Unobserved $\varepsilon$ with (possibly) complex nonlinear effects on $A, Y$ The definitions are:
$■ \varepsilon$ : unobserved confounder.

- A: treatment

■ $Y$ : outcome
■ Z: treatment proxy
■ $W$ outcome proxy


Structural assumption:

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

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

## Main theorem

If $\varepsilon$ were observed, we would write (average treatment effect)

$$
p(y \mid d o(a))=\int_{u} p(y \mid a, \varepsilon) p(\varepsilon) d \varepsilon
$$

....but we do not observe $\varepsilon$.

## Main theorem

If $\varepsilon$ were observed, we would write (average treatment effect)

$$
p(y \mid d o(a))=\int_{u} p(y \mid a, \varepsilon) p(\varepsilon) d \varepsilon
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....but we do not observe $\varepsilon$.
Main theorem: Assume we solved:

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

(Fredholm integral equation of the first kind)

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If $\varepsilon$ were observed, we would write (average treatment effect)

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Main theorem: Assume we solved:

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

(Fredholm integral equation of the first kind)
Average treatment effect with $p(w)$ :

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

Both $p(y \mid a, z)$ and $p(w \mid a, z)$ are in terms of observed quantities, and can be learned from data.

## Proof (1)

Because $W \Perp(Z, A) \mid \varepsilon$, we have

$$
p(w \mid a, z)=\int p(w \mid \varepsilon) p(\varepsilon \mid a, z) d \varepsilon
$$



## Proof (1)

Because $W \Perp(Z, A) \mid \varepsilon$, we have

$$
p(w \mid a, z)=\int p(w \mid \varepsilon) p(\varepsilon \mid a, z) d \varepsilon
$$

Because $Y \Perp Z \mid(A, \varepsilon)$ we have


$$
p(y \mid a, z)=\int p(y \mid a, \varepsilon) p(\varepsilon \mid a, z) d \varepsilon
$$

## Proof (3)

Given the solution $h_{y}$ to:

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

(well defined under identifiability conditions for Fredholm equation of first kind)

## Proof (3)

Given the solution $h_{y}$ to:

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

(well defined under identifiability conditions for Fredholm equation of first kind)

## From last slide

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

## Proof (3)

Given the solution $h_{y}$ to:

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

(well defined under identifiability conditions for Fredholm equation of first kind)
From last slide

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

This implies:

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

under identifiability condition
$\mathbb{E}[f(\varepsilon) \mid A=a, Z=z]=0, \mathbb{P}_{Z \mid A=a}$ a.s. $\Longleftrightarrow f(\varepsilon)=0, \mathbb{P}_{\varepsilon \mid A=a}$ a.s.

## Proof (4)

From last slide,

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

Thus

$$
p(y \mid d o(a))=\int_{u} p(y \mid a, \varepsilon) p(\varepsilon) d u
$$

## Proof (4)

From last slide,

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

Thus

$$
\begin{aligned}
p(y \mid d o(a)) & =\int_{u} p(y \mid a, \varepsilon) p(\varepsilon) d u \\
& =\int_{u}\left[\int h_{y}(w, a) p(w \mid \varepsilon) d w\right] p(\varepsilon) d \varepsilon
\end{aligned}
$$

## Proof (4)

From last slide,

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

Thus

$$
\begin{aligned}
p(y \mid d o(a)) & =\int_{u} p(y \mid a, \varepsilon) p(\varepsilon) d u \\
& =\int_{u}\left[\int h_{y}(w, a) p(w \mid \varepsilon) d w\right] p(\varepsilon) d \varepsilon \\
& =\int h_{y}(w, a) p(w) d w
\end{aligned}
$$

## Feature implementation

Stage 2: minimize

$$
h_{\lambda_{2}}=\arg \min _{h \in \mathcal{H}} \mathbb{E}_{y, a, z}\left(y-\left\langle h, \mu_{W \mid a, z} \otimes \phi(a)\right\rangle\right)^{2}+\lambda_{2}\|h\|_{\mathcal{H}}^{2}
$$

which is conditional feature mean implementation of

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

```
Deaner (2021).
Mastouri, Zhu, Gultchin, Korba, Silva, Kusner, G., Muandet (2021).
Xu, Kanagawa, G. (2021).
```


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

Stage 1: ridge regression

$$
F_{\lambda_{1}}=\arg \min _{F \in H S} \mathbb{E}_{w, a, z}\|\phi(w)-F[\phi(a) \otimes \phi(z)]\|_{\mathcal{H}_{\mathcal{W}}}^{2}+\lambda_{1}\|F\|_{H S}^{2}
$$

which gives us

$$
\mu_{W \mid a, z}=F_{\lambda_{1}}[\phi(a) \otimes \phi(z)]
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\section*{Feature implementation}

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\]
which gives us
\[
\mu_{W \mid a, z}=F_{\lambda_{1}}[\phi(a) \otimes \phi(z)]
\]

Average treatment effect estimate:
\[
\mathbb{E}_{y}(y \mid d o(a))=\left\langle h_{\lambda_{2}}, \phi(a) \otimes \mu_{W}\right\rangle
\]
where \(\mu_{W}=\mathbb{E}_{W} \phi(W)\)
Deaner (2021).
Mastouri, Zhu, Gultchin, Korba, Silva, Kusner, G., Muandet (2021).
Xu, Kanagawa, G. (2021).

\section*{Failures of identifiability assumptions (1)}

Recall (one of the) identifiability assumptions:
\(\mathbb{E}[f(\varepsilon) \mid A=a, Z=z]=0, \mathbb{P}_{Z \mid A=a}\) a.s. \(\Longleftrightarrow f(\varepsilon)=0, \mathbb{P}_{\varepsilon \mid A=a}\) a.s. \(\quad(\triangle)\)
For conciseness, assume conditioning on some \(a\).
Failure 1: \(Z \Perp \varepsilon\) (no information about \(\varepsilon\) in proxy)
\[
\begin{aligned}
g(\varepsilon) & =\tilde{g}(\varepsilon)-\mathbb{E}_{\varepsilon} \tilde{g}(\varepsilon) \\
\mathbb{E}(g(\varepsilon) \mid Z) & =\mathbb{E} g(\varepsilon)=0 .
\end{aligned}
\]

\section*{Failures of identifiability assumptions (2)}

Failure 2: "exploitable invariance" of \(p(\varepsilon \mid z)\)
\[
\begin{aligned}
\varepsilon & \sim \mathcal{N}(0,1) \\
Z & =|\varepsilon|+\mathcal{N}(0,1)
\end{aligned}
\]
where \(p(\varepsilon \mid z) \propto p(z \mid \varepsilon) p(\varepsilon)\) symmetric in \(\varepsilon\). Consider square integrable antisymmetric function \(g(\varepsilon)=-g(-\varepsilon)\). Then
\[
\begin{aligned}
& \int_{-\infty}^{\infty} g(\varepsilon) p(\varepsilon \mid z) d \varepsilon \\
& =\int_{-\infty}^{0} g(\varepsilon) p(\varepsilon \mid z) d \varepsilon+\int_{0}^{\infty} g(\varepsilon) p(\varepsilon \mid z) d \varepsilon \\
& =0
\end{aligned}
\]

If distribution of \(\varepsilon \mid Z\) retains the same "symmetry class" over a set of \(Z\) with nonzero measure, then the assumption is violated by \(g(\varepsilon)\) with zero mean on this class.

\section*{How not to do it}

Stage 2: minimize
\[
h_{\lambda_{2}}=\arg \min _{h \in \mathcal{H}} \mathbb{E}_{y, a, z}\left(y-\left\langle h, \mu_{W, A \mid a, z}\right\rangle\right)^{2}+\lambda_{2}\|h\|_{\mathcal{H}}^{2}
\]
which is conditional feature mean implementation of
\[
p(y \mid a, z)=\int h_{y}(w, a) p(w \mid a, z) d w
\]

Stage 1: ridge regression
\[
F_{\lambda_{1}}=\arg \min _{F \in \mathcal{G}} \mathbb{E}_{w, a, z}\|\phi(w) \otimes \phi(a)-F[\phi(a) \otimes \phi(z)]\|_{\mathcal{H} \mathcal{W}}^{2}+\lambda_{1}\|F\|_{H S}^{2}
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which gives us
\[
\mu_{W, A \mid a, z}=F_{\lambda_{1}}[\phi(a) \otimes \phi(z)]
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\]
which gives us
\[
\mu_{W, A \mid a, z}=F_{\lambda_{1}}[\phi(a) \otimes \phi(z)]
\]

Problem: ridge regressing from \(\phi(a)\) to \(\phi(a)\). Theoretical issue: \(\mathcal{I}_{\mathcal{H}_{\mathcal{A}}}\) is not Hilbert-Schmidt so consistency of \(F\) not established.

\section*{Demo: bias introduced by stage 1 RR}

Implementation issue: this can introduce unnecessary bias.


Stage 1:
\(a \sim \mathcal{N}\left(0, \sigma^{2}\right)\).
Stage 2:
\(a \sim \mathcal{U}[-3,3]\).

\section*{Demo: bias introduced by stage 1 RR}

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Stage 2:
\(a \sim \mathcal{U}[-3,3]\).

\section*{Synthetic experiment, adaptive neural net features}
dSprite example:
- \(X=\{\) scale, rotation, posX, posY \(\}\)
- Treatment \(A\) is the image generated (with Gaussian noise)
- Outcome \(Y\) is quadratic function of \(A\) with multiplicative confounding by posY.
- \(Z=\{\) scale, rotation, posX \(\}\), \(W=\) noisy image sharing posY



\section*{Confounded offline policy evaluation}

Synthetic dataset, demand prediction for flight purchase.
- Treatment \(A\) is ticket price.
\(■\) Policy \(A \sim \pi(Z)\) depends on fuel price.


\section*{Conclusions}

Neural net and kernel solutions:
■ ...for instrumental variable regression
- ...for proxy methods

■ ...with treatment \(A\), covariates \(X, V\), proxies \((W, Z)\) multivariate, "complicated"
■ Convergence guarantees for kernels and NN

\section*{Code available for all methods}

\section*{Research support}

Work supported by:

The Gatsby Charitable Foundation


Deepmind
(9) DeepMind

\section*{Questions?}


\section*{Proxy proof (discrete variables)}

If \(X\) were observed,
\[
P(Y \mid d o(a)):=\sum_{i=1}^{D} P\left(y \mid x_{i}, a\right) P\left(x_{i}\right)
\]


\section*{Proxy proof (discrete variables)}

If \(X\) were observed,
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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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\[
\begin{aligned}
& P(W \mid Z, a)=P(W \mid X) P(X \mid Z, a) \\
& \quad \Longrightarrow P(X \mid Z, a)=P^{-1}(W \mid X) P(W \mid Z, a)
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& \Longrightarrow p(y \mid X, a)=p(y \mid Z, a) P^{-1}(W \mid Z, a) P(W \mid X)
\end{aligned}
\]

\section*{Proof (discrete variables)}

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


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


Average causal effect using only observed data!```

