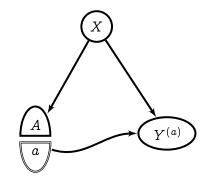
Causal Effect Estimation with Context and Confounders (2)

Arthur Gretton

Gatsby Computational Neuroscience Unit Deepmind

Columbia, 2023

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:

$$oldsymbol{\gamma}(x) = oldsymbol{\gamma}^ op arphi(x) = raket{\gamma, arphi(x)}_{\mathcal{H}}$$

Model assumption: linear functions of features

All learned functions will take the form:

$$oldsymbol{\gamma}(x) = oldsymbol{\gamma}^ op arphi(x) = raket{\gamma, arphi(x)}_{\mathcal{H}}$$

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:

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

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)

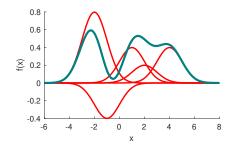
Model fitting: ridge regression

 $\begin{array}{lll} \text{Learn } \gamma_0(x) := \mathbb{E}[\,Y|X\,=x] \,\, \text{from features } \varphi(x_i) \,\, \text{with outcomes } y_i \colon \\ \hat{\gamma} &=& \arg\min_{\gamma\in\mathcal{H}} \left(\sum_{i=1}^n \left(y_i - \langle\gamma,\varphi(x_i)\rangle_{\mathcal{H}}\right)^2 + \lambda \|\gamma\|_{\mathcal{H}}^2\right). \end{array}$

Model fitting: ridge regression

Neural net solution at x:

$$egin{aligned} \hat{\gamma}(x) &= C_{YX}(C_{XX}+\lambda)^{-1}arphi(x) \ C_{YX} &= rac{1}{n}\sum_{i=1}^n [y_i \ arphi(x_i)^ op] \ C_{XX} &= rac{1}{n}\sum_{i=1}^n [arphi(x_i) \ arphi(x_i)^ op] \end{aligned}$$



Model fitting: ridge regression

 $\begin{array}{lll} \text{Learn } \gamma_0(x) := \mathbb{E}[\,Y|X\,=x] \,\, \text{from features } \varphi(x_i) \,\, \text{with outcomes } y_i \colon \\ \hat{\gamma} &=& \arg\min_{\gamma\in\mathcal{H}} \left(\sum_{i=1}^n \left(y_i - \langle\gamma,\varphi(x_i)\rangle_{\mathcal{H}}\right)^2 + \lambda \|\gamma\|_{\mathcal{H}}^2\right). \end{array}$

Kernel solution at
$$x$$

(as weighted sum of y)
 $\hat{\gamma}(x) = \sum_{i=1}^{n} y_i \beta_i(x)$
 $\beta(x) = (K_{XX} + \lambda I)^{-1} k_{Xx}$
 $(K_{XX})_{ij} = k(x_i, x_j) = \langle \varphi(x_i), \varphi(x_j) \rangle_{\mathcal{H}}$
 $\overset{0.8}{\underset{0.6}{0.4}}$
 $\overset{0.8}{\underset{0.4}{0.2}}$
 $\overset{0.8}{\underset{0.4}{0.4}}$
 $\overset{0.8}{\underset{0.4}{0.2}}$
 $\overset{0.8}{\underset{0.4}{0.4}}$
 $\overset{0.8}{\underset{0.4}{0$

What if there are hidden confounders?

Ticket price A, seats sold Y.



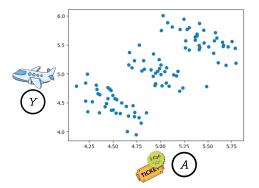
What is the effect on seats sold $Y^{(a)}$ of intervening on price a?

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

Ticket price A, seats sold Y.

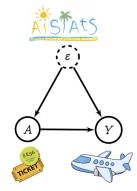


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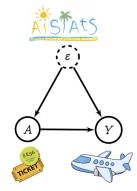
Unobserved variable ε =desire for travel, affects <u>both</u> price (via airline algorithms) and seats sold.



Desire for travel:

$$egin{split} arepsilon & \sim \mathcal{N}(\mu, 0.1) \ \mu & \sim \mathcal{U}\left\{-rac{1}{2}, 0, rac{1}{2}
ight\} \end{split}$$

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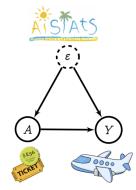
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Price:

$$egin{aligned} A &= arepsilon + Z, \ Z &\sim \mathcal{N}(5, 0.04) \end{aligned}$$

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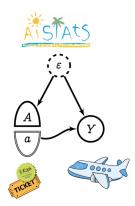
Price:

$$egin{array}{lll} A = oldsymbol{arepsilon} + Z, \ Z \sim \mathcal{N}(5, 0.04) \end{array}$$

Seats sold:

 $Y = 10 - A + 2\varepsilon$

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



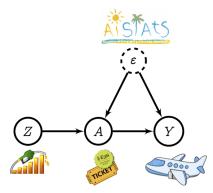
- Desire for travel:
 - $egin{split} arepsilon & \sim \mathcal{N}(\mu, 0.1) \ \mu & \sim \mathcal{U}\left\{-rac{1}{2}, 0, rac{1}{2}
 ight\} \end{split}$
- Price:
 - $A = \varepsilon + Z,$ $Z \approx N(5, 0.04)$
 - $Z \sim \mathcal{N}(5, 0.04)$
- Seats sold: $Y = 10 - A + 2\varepsilon$

8/39

Average treatment effect:

$$\operatorname{ATE}(a) = \mathbb{E}[\,Y^{(a)}] = \int \left(10 - a + 2arepsilon
ight) dp(arepsilon) = 10 - a$$

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



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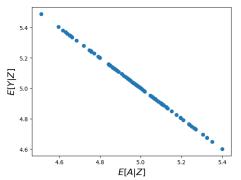
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Seats sold:

 $Y = 10 - A + 2\varepsilon$

Z is an instrument (cost of fuel). Condition on Z, $\mathbb{E}[Y|Z] = 10 - \mathbb{E}[A|Z] + 2\underbrace{\mathbb{E}[\varepsilon|Z]}_{=0}$

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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!

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

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

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

$$C_{aarepsilon}:=\mathbb{E}[\phi_{ heta}(A)arepsilon]
eq 0$$

Average treatment effect:

$$egin{aligned} &y = {\pmb{\gamma}_0}^{ op} {\pmb{\phi}_ heta}(a) + arepsilon & \mathbb{E}(arepsilon) = 0 \ ATE := \mathbb{E}(\,Y^{(a)}) = \int ({\pmb{\gamma}_0}^{ op} {\pmb{\phi}_ heta}(a) + arepsilon) dP(arepsilon) = {\pmb{\gamma}_0}^{ op} {\pmb{\phi}_ heta}(a). \end{aligned}$$

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Least-squares loss for γ, θ :

$$\mathcal{L}(\gamma, heta) = \mathbb{E} \left\| Y - \gamma^ op \phi_ heta(A) - arepsilon
ight\|^2$$

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Least-squares loss for γ, θ :

$$\mathcal{L}(\gamma, heta) = \mathbb{E} \left\| Y - \gamma^ op \phi_ heta(A) - arepsilon
ight\|^2$$

Minimizing for γ ,

$$egin{aligned} &\gamma_0 = C_{aa}^{-1}(C_{ay} - C_{aarepsilon}) & C_{aa} = \mathbb{E}[\phi_ heta(A)\phi_ heta(A)^ op] \ & C_{ay} = \mathbb{E}[\phi_ heta(A)Y] \end{aligned}$$

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

Instrumental variable regression

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



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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"

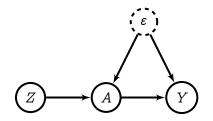
Instrumental variable regression with NN features

Definitions:

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

Assumptions

$$egin{aligned} \mathbb{E}[arepsilon] &= 0 & \mathbb{E}[arepsilon|Z] &= 0 \ Z
ot \hspace{-0.5ex} \not \perp A \ (Y \ \hspace{-0.5ex} \perp Z|A)_{G_{ar{A}}} \ Y &= \gamma^ op \phi_ heta(A) + arepsilon \end{aligned}$$



Instrumental variable regression with NN features

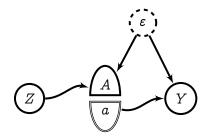
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- A: treatment
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- \blacksquare Z: instrument

Assumptions

$$\mathbb{E}[\varepsilon] = 0 \qquad \mathbb{E}[\varepsilon|Z] = Z \not\perp A$$
$$(Y \perp Z|A)_{G_{\bar{A}}}$$
$$Y = \gamma^{\top} \phi_{\theta}(A) + \varepsilon$$

0



Average treatment effect:

$$\operatorname{ATE}(a) = \int \mathbb{E}(\left.Y|arepsilon, a
ight) dp(arepsilon) = \gamma^{ op} \phi_{ heta}(a)$$

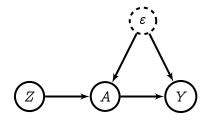
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Average treatment effect:

$$ext{ATE}(a) = \int \mathbb{E}(\left.Y|arepsilon,a
ight) dp(arepsilon) = oldsymbol{\gamma}^{ op} \phi_{ heta}(a)$$

IV regression: Condition both sides on Z,

$$\mathbb{E}[\left.Y|Z
ight] = \gamma^{ op}\mathbb{E}[\phi_ heta(A)|Z] + \underbrace{\mathbb{E}[arepsilon|Z]}_{=0}$$

Two-stage least squares for IV regression

Kernel features (NeurIPS 2019):

arXiv.org > cs > arXiv:1906.00232 Computer Science > Machine Learning

[Submitted on 1 Jun 2019 (v1), last revised 15 Jul 2020 (this version, v6)]

Kernel Instrumental Variable Regression

Rahul Singh, Maneesh Sahani, Arthur Gretton





NN features (ICLR 2021):

arXiv > cs > arXiv:2010.07154

Computer Science > Machine Learning

[Submitted on 14 Oct 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/

Two-stage least squares for IV regression

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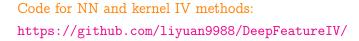












Stage 2 regression (IV): learn NN features $\phi_{\theta}(A)$ and linear layer γ to obtain Y with RR loss:

$$\mathbb{E}_{YZ}\left[(|Y-\gamma^{ op}\mathbb{E}[\pmb{\phi}_{ heta}(A)|Z])^2
ight]+\lambda_2\|\pmb{\gamma}\|^2$$

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

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

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

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

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Challenge: how to learn θ ?

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Challenge: how to learn θ ?

From Stage 2 regression?

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

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

Challenge: how to learn θ ?

From Stage 2 regression?

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

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

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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 ...

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

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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)

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

$$\mathbb{E}\left[\| oldsymbol{\phi}_{ heta}(A) - oldsymbol{F} oldsymbol{\phi}_{\zeta}(Z) \|^2
ight] + \lambda_1 \| oldsymbol{F} \|_{HS}^2$$

Stage 1 regression: learn NN features $\phi_{\zeta}(Z)$ and linear layer F: $\mathbb{E}[\phi_{\theta}(A)|Z] \approx F\phi_{\zeta}(Z)$

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

$$egin{aligned} \hat{F}_{ heta,\zeta} &= C_{AZ}(C_{ZZ}+\lambda_1I)^{-1} & C_{AZ} &= \mathbb{E}[\phi_ heta(A)\phi_\zeta^ op(Z)] \ & C_{ZZ} &= \mathbb{E}[\phi_\zeta(Z)\phi_\zeta^ op(Z)] \end{aligned}$$

Stage 1 regression: learn NN features $\phi_{\zeta}(Z)$ and linear layer F: $\mathbb{E}[\phi_{\theta}(A)|Z] \approx F\phi_{\zeta}(Z)$

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

Xu, Chen, Srinivasan, De Freitas, Doucet, G. (2021) Learning Deep Features in Instrumental Variable Regression 15/39

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

$$\mathcal{L}_2(\gamma, heta) = \mathbb{E}_{YZ}\left[(|Y-\gamma^ op\mathbb{E}[\phi_ heta(A)|Z])^2
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Stage 2 regression (IV): learn NN features $\phi_{\theta}(A)$ and linear layer γ to obtain Y with RR loss:

$$egin{aligned} \mathcal{L}_2(m{\gamma}, m{ heta}) &= \mathbb{E}_{YZ} \left[(|Y - m{\gamma}^ op \mathbb{E}[m{\phi}_{m{ heta}}(A)|Z])^2
ight] + \lambda_2 \|m{\gamma}\|^2 \ &= \mathbb{E}_{YZ}[(|Y - m{\gamma}^ op \underbrace{\hat{F}_{m{ heta},\zeta}m{\phi}_{\zeta}(Z)}_{ ext{Starmal}})^2] + \lambda_2 \|m{\gamma}\|^2 \end{aligned}$$

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

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ight] + \lambda_2 \|\gamma\|^2 \ &= \mathbb{E}_{YZ}[(\,Y-\gamma^ op\hat{F}_{ heta,\zeta}\phi_\zeta(Z))^2] + \lambda_2 \|\gamma\|^2 \end{aligned}$$

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

$$egin{aligned} \hat{\gamma}_{ heta} &:= \widetilde{C}_{YZ} (\widetilde{C}_{ZZ} + \lambda_2 I)^{-1} & ~~ \widetilde{C}_{YZ} = \mathbb{E} \left[Y \; [\hat{F}_{ heta, \zeta} \phi_{\zeta}(Z)]^{ op}
ight] \ &~~ \widetilde{C}_{ZZ} = \mathbb{E} \left[[\hat{F}_{ heta, \zeta} \phi_{\zeta}(Z)] \; [\hat{F}_{ heta, \zeta} \phi_{\zeta}(Z)]^{ op}
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ight] \ \widetilde{C}_{ZZ} &= \mathbb{E} \left[[\hat{F}_{ heta, \zeta} \phi_{\zeta}(Z)] \; [\hat{F}_{ heta, \zeta} \phi_{\zeta}(Z)]^{ op}
ight] \end{aligned}$$

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

$$egin{aligned} \mathcal{L}_2(m{\gamma}, heta) &= \mathbb{E}_{YZ}\left[(\,Y - m{\gamma}^ op \mathbb{E}[m{\phi}_ heta(A)|Z])^2
ight] + \lambda_2 \|m{\gamma}\|^2 \ &= \mathbb{E}_{YZ}[(\,Y - m{\gamma}^ op \hat{F}_{ heta,\zeta}m{\phi}_\zeta(Z))^2] + \lambda_2 \|m{\gamma}\|^2 \end{aligned}$$

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

$$egin{aligned} \hat{\gamma}_{ heta} &:= \widetilde{C}_{YZ} (\widetilde{C}_{ZZ} + \lambda_2 I)^{-1} \qquad \widetilde{C}_{YZ} = \mathbb{E} \left[Y \; [\hat{F}_{ heta, \zeta} \phi_{\zeta}(Z)]^{ op}
ight] \ \widetilde{C}_{ZZ} &= \mathbb{E} \left[[\hat{F}_{ heta, \zeta} \phi_{\zeta}(Z)] \; [\hat{F}_{ heta, \zeta} \phi_{\zeta}(Z)]^{ op}
ight] \end{aligned}$$

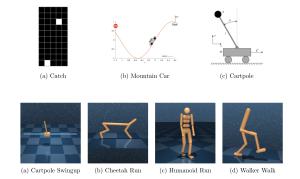
From linear final layers in Stages 1,2:

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.

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

Neural IV in reinforcement learning



Policy evaluation: want Q-value:

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

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

Osband et al (2019). Behaviour suite for reinforcement learning.https://github.com/deepmind/buite Tassa et al. (2020). dm_control:Software and tasks for continuous control. 17/39 https://github.com/deepmind/dm_control

Application of IV: reinforcement learning

Q value is a minimizer of Bellman loss

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

Corresponds to "IV-like" problem

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

with

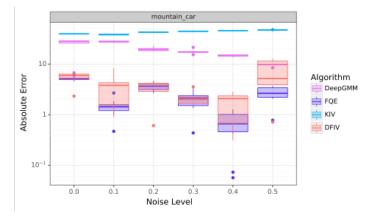
$$egin{aligned} Y &= R, \ X &= (S', A', S, A) \ Z &= (S, A), \ 0 &= Q^{\pi}(s, a) - \gamma Q^{\pi}(s', a') \end{aligned}$$

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**18**989 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 §739 Deep Offline Policy Evaluation.

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

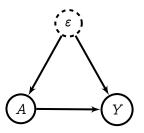
The proxy correction

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

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

If ε were observed (which it isn't),

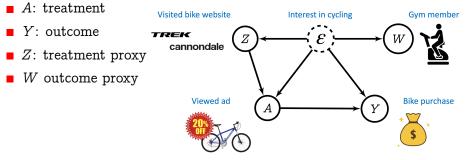
$$\mathbb{E}[\,Y^{(a)}] = \int \mathbb{E}[\,Y|oldsymbol{arepsilon},\,a]dp(oldsymbol{arepsilon})$$



The proxy correction

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

 ε : unobserved confounder.



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

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 I, Kusner, Arthur Gretton, Krikamol Muandet











NN features (NeurIPS 2021):

arXiv.org > cs > arXiv:2106.03907 Search. Help | Adv. 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



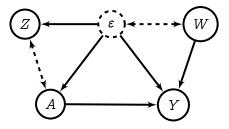


Code for NN and kernel proxy methods: https://github.com/liyuan9988/DeepFeatureProxyVariable/ 22/39

The proxy correction

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

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



Structural assumption:

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

Main theorem

If ε were observed, we would write (average treatment effect)

$$p(y|do(a)) = \int_u p(y|a, \varepsilon) p(\varepsilon) d\varepsilon.$$

....but we do not observe ε .

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

(Fredholm integral equation of the first kind)

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Main theorem: Assume we solved:

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

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

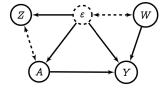
$$p(y|do(a)) = \int h_y(a,w)p(w)dw$$

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



Because $W \perp (Z, A) | \varepsilon$, we have

$$p(w|a,z) = \int p(w|oldsymbol{arepsilon}) p(oldsymbol{arepsilon}|a,z) darepsilon$$



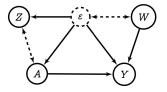


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$$p(y|a,z) = \int p(y|a, arepsilon) p(arepsilon|a, z) darepsilon$$





Given the solution h_y to:

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

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



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

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



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This implies:

$$p(y|a,arepsilon) = \int h_y(w,a) p(w|oldsymbol{arepsilon}) dw$$

under identifiability condition

$$\mathbb{E}[f(oldsymbol{arepsilon})|A=a,Z=z]=0,\ \mathbb{P}_{Z|A=a}\, ext{a.s.}\ \Longleftrightarrow\ f(oldsymbol{arepsilon})=0,\ \mathbb{P}_{oldsymbol{arepsilon}|A=a}\, ext{a.s.}\ (riangle)$$



From last slide,

$$p(y|a,oldsymbol{arepsilon}) = \int h_y(w,a) p(w|oldsymbol{arepsilon}) dw$$

Thus

$$p(y|do(a)) = \int_u p(y|a,arepsilon) p(arepsilon) du$$



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Thus

$$egin{aligned} p(y|do(a)) &= \int_u p(y|a,arepsilon) p(arepsilon) du \ &= \int_u \left[\int h_y(w,a) p(w|arepsilon) dw
ight] p(arepsilon) darepsilon \end{aligned}$$



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$$egin{aligned} p(y|do(a)) &= \int_u p(y|a,arepsilon) p(arepsilon) du \ &= \int_u \left[\int h_y(w,a) p(w|arepsilon) dw
ight] p(arepsilon) darepsilon \ &= \int h_y(w,a) p(w) dw \end{aligned}$$

Feature implementation

Stage 2: minimize

$$h_{\lambda_2} = rg\min_{h \in \mathcal{H}} \mathbb{E}_{y,a,z} \left(y - \left\langle h, \mu_{W|a,z} \otimes \phi(a)
ight
angle
ight)^2 + \lambda_2 \|h\|_{\mathcal{H}}^2$$

which is conditional feature mean implementation of

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

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

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Stage 1: ridge regression

$$F_{\lambda_1} = \arg\min_{F \in HS} \mathbb{E}_{w,a,z} \|\phi(w) - F[\phi(a) \otimes \phi(z)]\|_{\mathcal{H}_{\mathcal{W}}}^2 + \lambda_1 \|F\|_{HS}^2$$

which gives us

$$\mu_{W|a,z} = F_{\lambda_1}[\phi(a)\otimes\phi(z)]$$

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Average treatment effect estimate:

$$\mathbb{E}_y(y|\mathit{do}(a)) = \langle h_{\lambda_2}, \phi(a) \otimes \mu_W
angle,$$

where $\mu_W = \mathbb{E}_W \phi(W)$

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

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Failures of identifiability assumptions (1)

Recall (one of the) identifiability assumptions:

$$\mathbb{E}[f(oldsymbol{arepsilon})|A=a,Z=z]=0,\ \mathbb{P}_{Z|A=a}\, ext{a.s.}\ \Longleftrightarrow\ f(oldsymbol{arepsilon})=0,\ \mathbb{P}_{oldsymbol{arepsilon}|A=a}\, ext{a.s.}\ (riangle)$$

For conciseness, assume conditioning on some a. Failure 1: $Z \perp \epsilon$ (no information about ϵ in proxy)

$$egin{aligned} g(arepsilon) &= ilde{g}(arepsilon) - \mathbb{E}_arepsilon ilde{g}(arepsilon) \ \mathbb{E}(g(arepsilon)|Z) &= \mathbb{E}g(arepsilon) = 0. \end{aligned}$$

Failures of identifiability assumptions (2)

Failure 2: "exploitable invariance" of $p(\varepsilon|z)$

$$egin{aligned} oldsymbol{arepsilon} & oldsymbol{arepsilon} & \sim \mathcal{N}(0,1), \ & Z & = |oldsymbol{arepsilon}| + \mathcal{N}(0,1), \end{aligned}$$

where $p(\varepsilon|z) \propto p(z|\varepsilon)p(\varepsilon)$ symmetric in ε . Consider square integrable antisymmetric function $g(\varepsilon) = -g(-\varepsilon)$. Then

$$egin{aligned} &\int_{-\infty}^{\infty}g(arepsilon)p(arepsilon|z)darepsilon \ &=\int_{-\infty}^{0}g(arepsilon)p(arepsilon|z)darepsilon+\int_{0}^{\infty}g(arepsilon)p(arepsilon|z)darepsilon \ &=0. \end{aligned}$$

If distribution of $\varepsilon | Z$ 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.

How not to do it

Stage 2: minimize

$$h_{\lambda_2} = rg\min_{h \in \mathcal{H}} \mathbb{E}_{y,a,z} \left(y - \left\langle h, \mu_{W,A|a,z} \right\rangle \right)^2 + \lambda_2 \|h\|_{\mathcal{H}}^2$$

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

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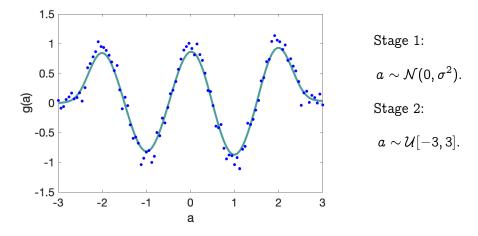
$$\mu_{W,A|a,z} = F_{\lambda_1}[\phi(a)\otimes\phi(z)]$$

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.

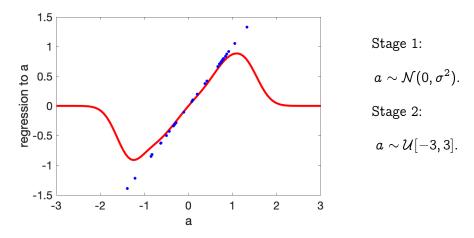
Demo: bias introduced by stage 1 RR

Implementation issue: this can introduce unnecessary bias.



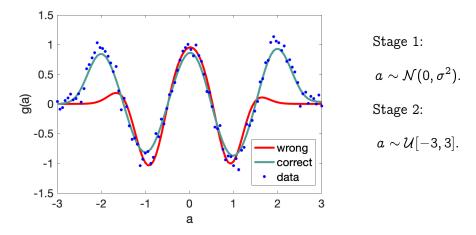
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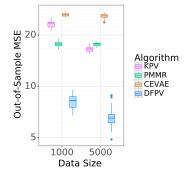


Synthetic experiment, adaptive neural net features

dSprite example:

- $\blacksquare X = \{\texttt{scale}, \texttt{rotation}, \texttt{posX}, \texttt{posY}\}$
- 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

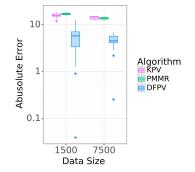




Confounded offline policy evaluation

Synthetic dataset, demand prediction for flight purchase.

- Treatment A is ticket price.
- Policy A ~ π(Z) depends on fuel price.



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

Code available for all methods

Research support

Work supported by:

The Gatsby Charitable Foundation



Deepmind

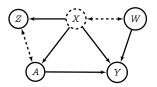


Questions?



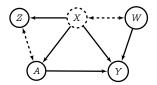
If X were observed,

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



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

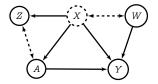


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Because $W \perp (Z, A) | X$,

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

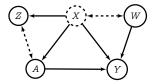


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$$egin{aligned} & P(W|Z,a) = P(W|X)P(X|Z,a) \ &\implies P(X|Z,a) = P^{-1}(W|X)P(W|Z,a) \end{aligned}$$



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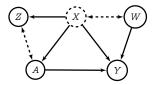
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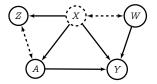


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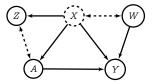
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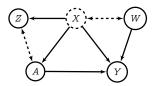
$$P(y|Z, a) = P(y|X, a) \underbrace{P^{-1}(W|X)P(W|Z, a)}_{P(X|Z, a)}$$

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

Proof (discrete variables)

From previous slide:

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



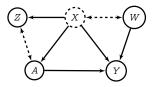
Proof (discrete variables)

From previous slide:

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

Multiply LHS and RHS by P(X):

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



Average causal effect using only observed data!