

Learning to act in noisy contexts using deep proxy learning

Arthur Gretton

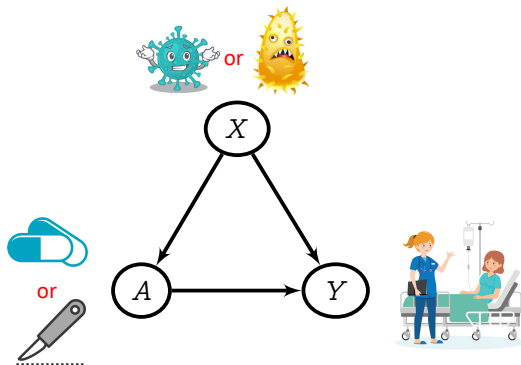
Gatsby Computational Neuroscience Unit

Google Deepmind

Stuttgart ELLIS Unit, 2024

Observation vs intervention

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



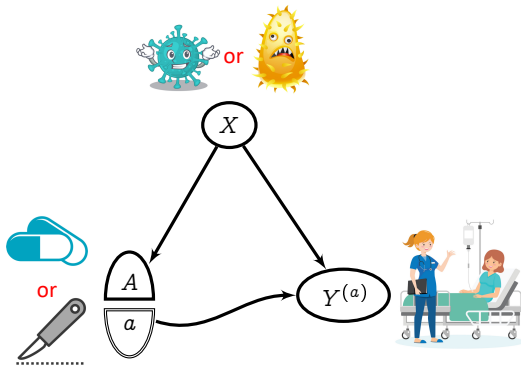
From our *observations* of historical hospital data:

- $P(Y = \text{cured} | A = \text{pills}) = 0.85$
- $P(Y = \text{cured} | A = \text{surgery}) = 0.72$

Observation vs intervention

Average causal effect/dose response curve (**intervention**):

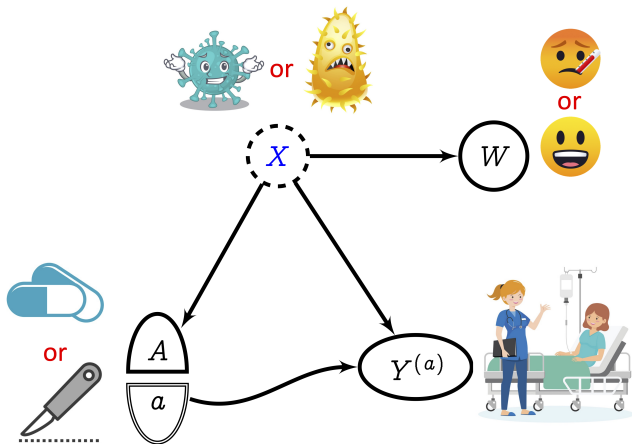
$$\mathbb{E}[Y^{(a)}] = \sum_x \mathbb{E}[Y|a, x]p(x)$$



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

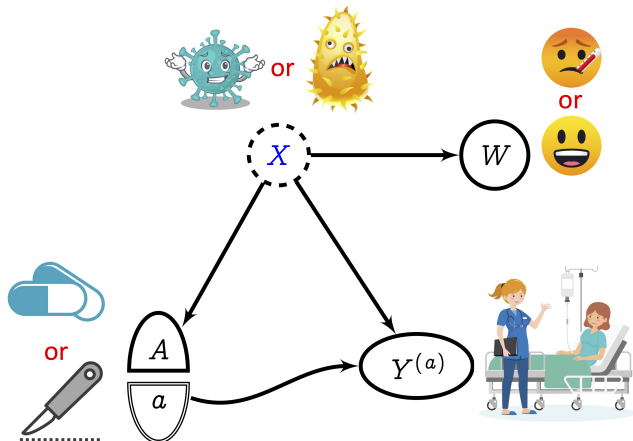
- $P(Y^{(\text{pills})} = \text{cured}) = 0.64$
- $P(Y^{(\text{surgery})} = \text{cured}) = 0.75$

We record symptom W , not disease X



- $P(W = \text{fever} | X = \text{mild}) = 0.2$
- $P(W = \text{fever} | X = \text{severe}) = 0.8$

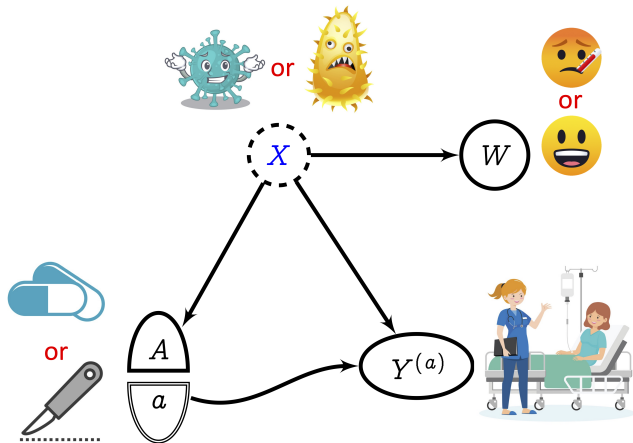
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- $P(W = \text{fever} | X = \text{mild}) = 0.2$
- $P(W = \text{fever} | X = \text{severe}) = 0.8$

Could we just write: $P(Y^{(a)}) \stackrel{?}{=} \sum_{w \in \{0,1\}} \mathbb{E}[Y | a, w] p(w)$

We record symptom W , not disease X

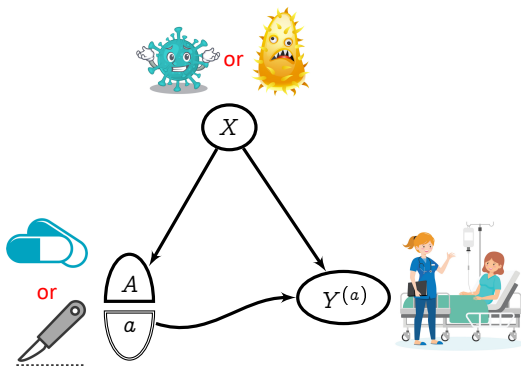


Wrong recommendation made:

- $\sum_{w \in \{0,1\}} \mathbb{E}[\text{cured} | \text{pills}, w] p(w) = 0.8 \quad (\neq 0.64)$
- $\sum_{w \in \{0,1\}} \mathbb{E}[\text{cured} | \text{surgery}, w] p(w) = 0.73 \quad (\neq 0.75)$

Correct answer **impossible** without observing X

Some core assumptions



Assume:

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

Outline

Causal effect estimation, with hidden covariates X :

- Use proxy variables (negative controls)

Applications: effect of actions under

- privacy constraints (email, ads, DMA)
- data gathering constraints (edge computing)
- fundamental limitations (preferences, state of mind)

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What's new and why?

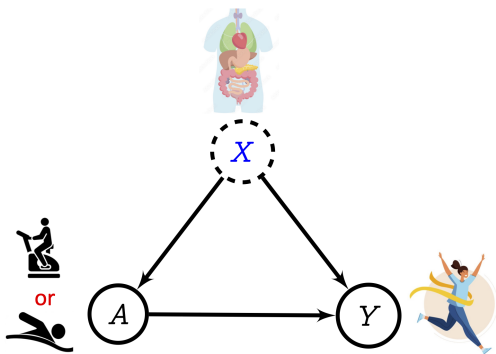
- Treatment A , proxy variables, etc can be multivariate, complicated...
- ...by using adaptive neural net feature representations
- Don't meet your heroes model your hidden variables!

What are proxies, and when are they useful?

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

In this example:

- X : true physical status
- A : exercise regimes
- Y : fitness goal

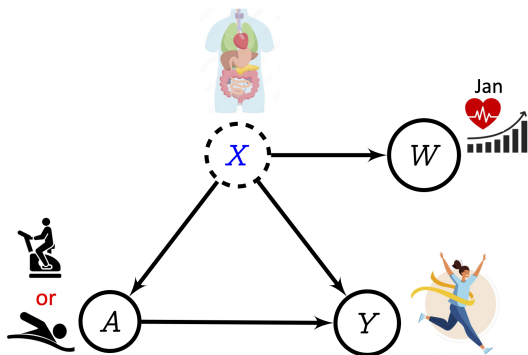


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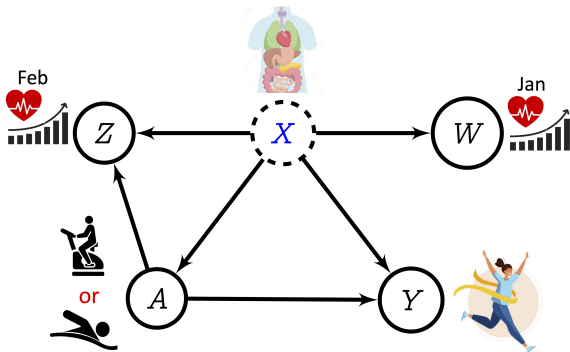


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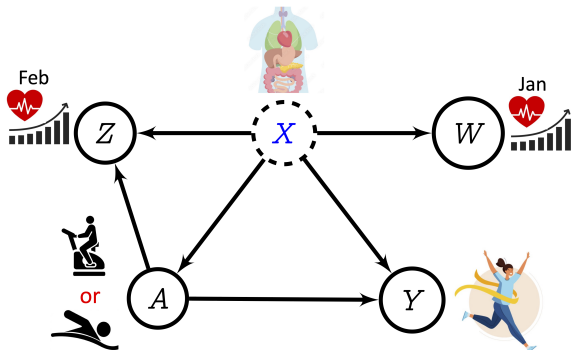


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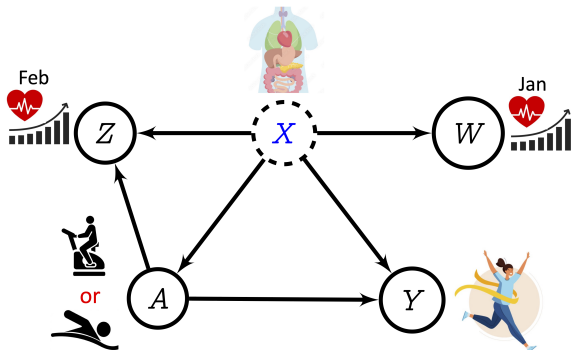
\Rightarrow Can recover $\mathbb{E}(Y^{(a)})$ from observational data

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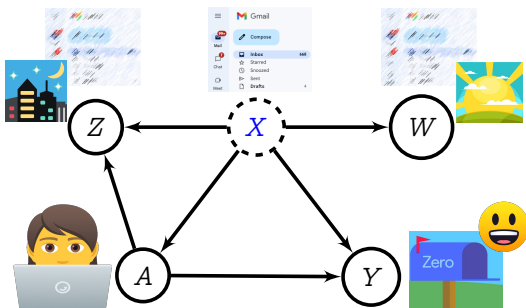
\Rightarrow More usefully: evaluate novel policy.

What are proxies, and when are they useful (2)?

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

In this example:

- X : email inbox
- A : prioritize important
- Y : outcome (efficiency)
- W : anonymized inbox before action A
- Z : anonymized inbox after action A

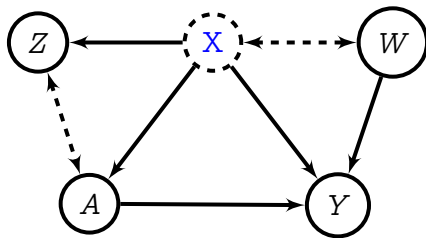


Proxy variables: general setting

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

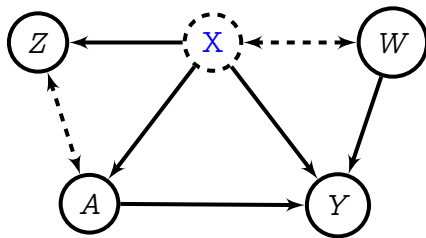


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Structural assumptions:

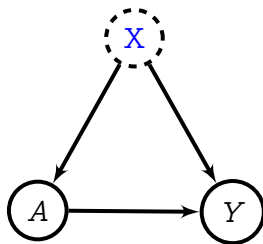
$$W \perp\!\!\!\perp (Z, A) | X$$

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

Why proxy variables? A simple proof

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- X : unobserved confounder.
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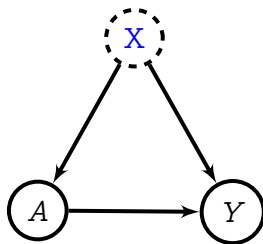
If X were observed,

$$\underbrace{P(Y^{(a)})}_{d_y \times 1} := \sum_{i=1}^{d_x} P(Y | x_i, a) P(x_i)$$

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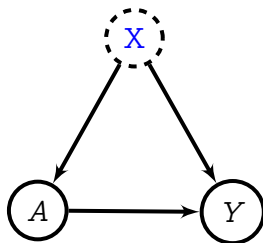
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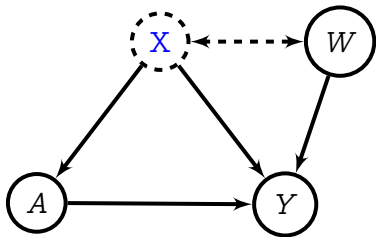
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Goal: “get rid of the blue” X

...add the outcome proxy W

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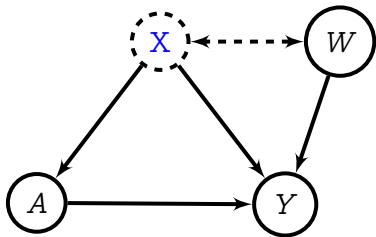
For each a , if we could solve:

$$\underbrace{P(Y|X, a)}_{d_y \times d_x} = \underbrace{H_{w,a}}_{d_y \times d_w} \underbrace{P(W|X)}_{d_w \times d_x}$$

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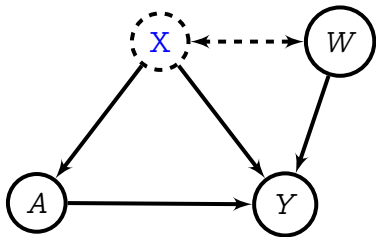
.....then

$$P(Y^{(a)}) = P(Y|X, a)P(X)$$

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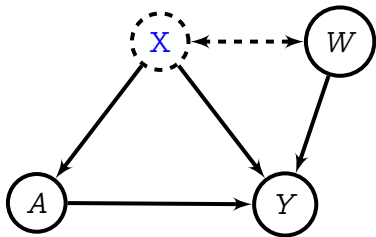
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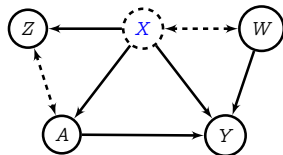
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$$\begin{aligned} P(Y^{(a)}) &= P(Y|X, a)P(X) \\ &= H_{w,a}P(W|X)P(X) \\ &= H_{w,a}P(W) \end{aligned}$$

...now project onto $p(X|Z, a)$

From last slide,

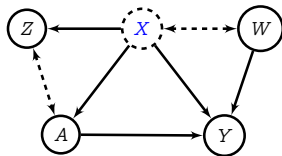
$$P(Y|X, a) = H_{w,a} P(W|X)$$



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$$P(Y|X, a) \underbrace{p(X|Z, a)}_{d_x \times d_z} = H_{w,a} P(W|X) \underbrace{p(X|Z, a)}_{d_x \times d_z}$$



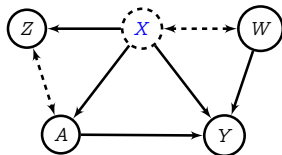
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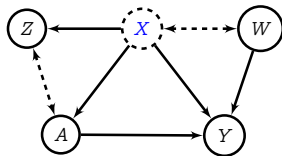
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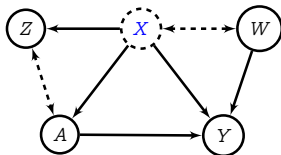
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Because $Y \perp\!\!\!\perp Z | (A, X)$,

$$P(Y|X, a)p(X|Z, a) = P(Y|Z, a)$$

Solve for $H_{w,a}$:

$$P(Y|Z, a) = H_{w,a} P(W|Z, a)$$

Everything observed!

Proxy/Negative Control Methods in the Real World

Unobserved confounders: proxy methods

Kernel features (ICML 2021):

arXiv.org > cs > arXiv:2105.04544

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

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

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



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arXiv.org > cs > arXiv:2106.03907

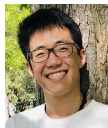
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One model: linear functions of features

All learned functions will take the form:

$$\gamma(x) = \gamma^\top \varphi_\theta(x)$$

NN approach: **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)

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

Model fitting: *neural* ridge regression

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

$$\hat{\gamma} = \arg \min_{\gamma \in \mathcal{H}} \left(\sum_{i=1}^n \left(y_i - \gamma^\top \varphi_\theta(x_i) \right)^2 + \lambda \|\gamma\|^2 \right) \quad (1)$$

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Solution for **linear final layer** γ :

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

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

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

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How to solve for θ :

Substitute $\hat{\gamma}$ into (1), backprop through Cholesky for θ .

Road map: NN proxy learning

We'll proceed as follows:

- Proxy relation for continuous variables
- Loss function for deep proxy learning
- Define **primary** (ridge) regression with this loss
- Define **secondary** (ridge) regression as input to primary

Proxy relation, general domains

If X were observed, we would write (dose-response curve)

$$\mathbb{E}(Y^{(a)}) = \int_x \mathbb{E}(Y|a, x)p(x)dx.$$

....but we do not observe X .

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Main theorem: Assume we solved for link function:

$$\mathbb{E}(Y|a, z) = \mathbb{E}_{W|a, z} h_y(W, a)$$

- “Primary” $\mathbb{E}(Y|a, z)$, “secondary” $\mathbb{E}_{W|a, z}$ linked by h_y
- All variables observed, X not seen *or modeled*.

Fredholm equation of first kind. Link existence requires \diamond , identification of ATE requires \triangle (and further technical assumptions) [XKG: Assumption 2, Prop. 1, Corr. 1; Deaner]

$$\begin{aligned}\mathbb{E}[f(X)|A = a, Z = z] = 0, \forall(z, a) &\iff f(X) = 0, \mathbb{P}_X \text{ a.s.} \quad \triangle \\ \mathbb{E}[f(X)|A = a, W = w] = 0, \forall(w, a) &\iff f(X) = 0, \mathbb{P}_X \text{ a.s.} \quad \diamond\end{aligned}$$

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Dose-response curve via $p(w)$:

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Dose-response curve via $p(w)$:

$$\mathbb{E}(Y^{(a)}) = \int_w h_y(a, w)p(w)dw$$

Challenge: need a loss function for h_y

Primary loss function for $h_y(w, a)$

Goal:

$$\mathbb{E}(Y|a, z) = \mathbb{E}_{W|a, z} h_y(W, a)$$

Primary loss function:

$$\hat{h}_y = \arg \min_{h_y} \mathbb{E}_{Y, A, Z} \left(Y - \mathbb{E}_{W|A, Z} h_y(W, A) \right)^2$$

Why?

Deaner (2021).

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

Xu, Kanagawa, G. (2021).

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Why?

$f^*(a, z) = \mathbb{E}(Y|a, z)$ solves

$$\arg \min_f \mathbb{E}_{Y, A, Z} (Y - f(A, Z))^2$$

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Why?

$f^*(a, z) = \mathbb{E}(Y|a, z)$ solves

$$\operatorname{argmin}_f \mathbb{E}_{Y, A, Z} (Y - f(A, Z))^2$$

...and by the proxy model above,

$$\mathbb{E}(Y|a, z) = \mathbb{E}_{W|a, z} h_y(W, a)$$

Deaner (2021).

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

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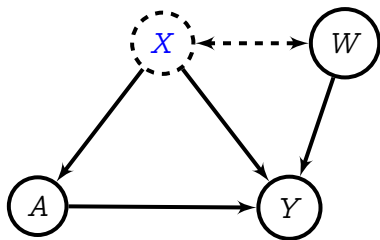
NN for link $h_y(a, w)$

The **link function** is a function of **two** arguments

$$h_y(a, w) = \gamma^\top [\varphi_\theta(w) \otimes \varphi_\xi(a)] = \gamma^\top \begin{bmatrix} \varphi_{\theta,1}(w)\varphi_{\xi,1}(a) \\ \varphi_{\theta,1}(w)\varphi_{\xi,2}(a) \\ \vdots \\ \varphi_{\theta,2}(w)\varphi_{\xi,1}(a) \\ \vdots \end{bmatrix}$$

Assume we have:

- output proxy NN features $\varphi_\theta(w)$
- treatment NN features $\varphi_\xi(a)$
- linear final layer γ
(argument of feature map indicates feature space)



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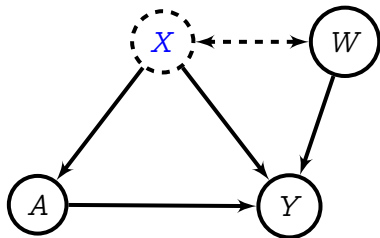
Assume we have:

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Questions:

- Why feature map $\varphi_\theta(w) \otimes \varphi_\xi(a)$?
- Why final linear layer γ ?

Both are necessary (next slide)!



NN ridge regression for $h_y(w, a)$

Goal:

$$\mathbb{E}(Y|a, z) = \mathbb{E}_{W|a, z} h_y(W, a)$$

Primary regression:

$$\hat{h}_y = \arg \min_{h_y} \mathbb{E}_{Y, A, Z} \left(Y - \mathbb{E}_{W|A, Z} h_y(W, A) \right)^2 + \lambda_2 \|\gamma\|^2$$

Deaner (2021).

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How to get **conditional expectation** $\mathbb{E}_{W|a, z} h_y(W, a)$?

Density estimation for $p(W|a, z)$? Sample from $p(W|a, z)$?

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Recall link function

$$h_y(W, a) = \left[\gamma^\top (\varphi_\theta(W) \otimes \varphi_\xi(a)) \right]$$

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(this is why linear γ and feature map $\varphi_\theta(w) \otimes \varphi_\xi(a)$)

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Ridge regression (again!)

$$\mathbb{E}_{W|a, z} \varphi_\theta(W) = \hat{F}_{\theta, \zeta} \varphi_\zeta(a, z)$$

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NN ridge regression for $\mathbb{E}_{W|a,z} \varphi_{\theta}(W)$

Secondary regression: learn NN features $\phi_{\zeta}(Z)$ and linear layer F :

$$\mathbb{E}_{W|a,z} \varphi_{\theta}(W) = \hat{F}_{\theta,\zeta} \varphi_{\zeta}(a, z)$$

with RR loss

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

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

NN ridge regression for $\mathbb{E}_{W|a,z} \varphi_\theta(W)$

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

Plug $\hat{F}_{\theta,\zeta}$ into S1 loss, backprop through Cholesky for ζ
(...not θ ...why not?)

Final algorithm

Solve for θ, ξ, ζ :

Repeat until convergence:

- **Secondary:** Solve for $\hat{F}_{\theta, \zeta}$, then gradient steps on ζ (backprop through Cholesky)

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Key point: features $\varphi_{\theta}(W)$ learned specially for:

$$\mathbb{E}(Y|a, z) = \mathbb{E}_{W|a, z} h_y(W, a)$$

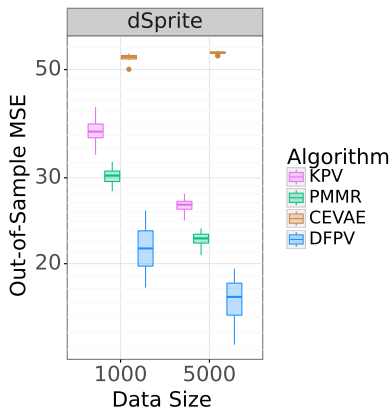
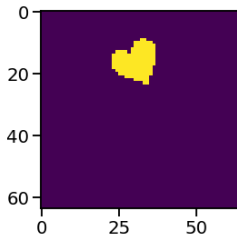
Contrast with autoencoders/sampling: must reconstruct/sample all of W .

Experiments

Synthetic experiment, adaptive neural net features

dSprite example:

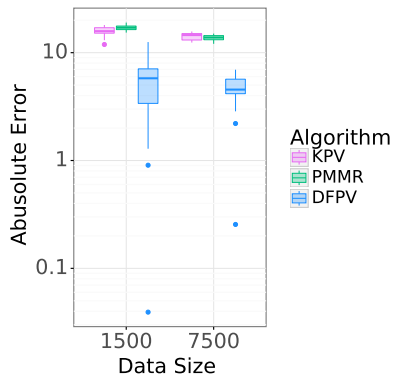
- $X = \{\text{scale, rotation, posX, posY}\}$
- Treatment A is the image generated (with Gaussian noise)
- Outcome Y is quadratic function of A with multiplicative confounding by posY .
- $Z = \{\text{scale, rotation, posX}\}$,
 $W = \text{noisy image sharing posY}$
- Comparison with **CEVAE** (Louzios et al. 2017)



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.

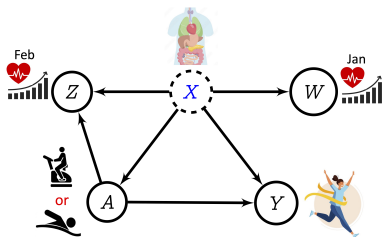


Conclusion

Causal effect estimation with unobserved X , (possibly) complex nonlinear effects on A , Y

We need to observe:

- Treatment proxy Z (interacts with A , but not directly with Y)
- Outcome proxy W (no direct interaction with A , can affect Y)

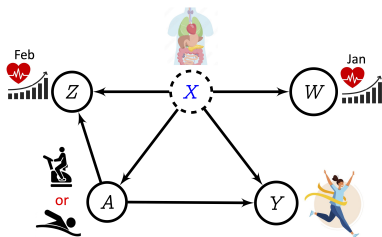


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Key messages:

- Don't meet-your-heroes model/sample latents X
- Don't model all of W , only relevant features for Y
- "Ridge regression is all you need"

Code available:

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

Research support

Work supported by:

The Gatsby Charitable Foundation



Google Deepmind



Questions?



Failures of completeness assumptions (1)

Recall (one of the) completeness assumptions:

$$\mathbb{E}[f(X)|A = a, Z = z] = 0, \forall(a, z) \iff f(X) = 0, \mathbb{P}_X \text{ a.s.} \quad (\triangle)$$

For conciseness, assume conditioning on some a .

Failure 1: $Z \perp\!\!\!\perp X$ (no information about X in proxy)

$$\begin{aligned} g(X|) &= \tilde{g}(X) - \mathbb{E}_X \tilde{g}(X) \\ \mathbb{E}(g(X)|Z, a) &= \mathbb{E}g(X) = 0. \end{aligned}$$

Failures of identifiability assumptions (2)

Failure 2: “exploitable invariance” of $p(\mathbf{X}|z)$

$$\mathbf{X} \sim \mathcal{N}(0, 1),$$

$$Z = |\mathbf{X}| + \mathcal{N}(0, 1),$$

where $p(\mathbf{X}|z) \propto p(z|\mathbf{X})p(\mathbf{X})$ symmetric in \mathbf{X} . Consider square integrable *antisymmetric* function $g(\mathbf{X}) = -g(-\mathbf{X}) \neq 0$. Then

$$\begin{aligned}\mathbb{E}[g(\mathbf{X})|Z = z] &= \int_{-\infty}^{\infty} g(\mathbf{X})p(\mathbf{X}|z)d\mathbf{X} \\ &= \int_{-\infty}^0 g(\mathbf{X})p(\mathbf{X}|z)d\mathbf{X} + \int_0^{\infty} g(\mathbf{X})p(\mathbf{X}|z)d\mathbf{X} \\ &= 0.\end{aligned}$$

If distribution of $\mathbf{X}|Z$ retains the same “symmetry class” over a set of Z with nonzero measure, then the assumption is violated by $g(\mathbf{X})$ with zero mean on this class.