

Proxy Variables for Causal Effect Estimation with Hidden Confounding

Arthur Gretton

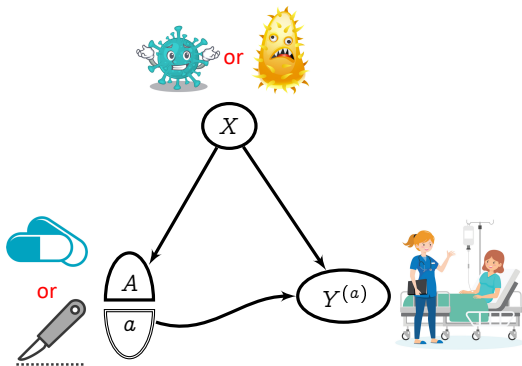
Gatsby Computational Neuroscience Unit
Google DeepMind

CLear 2026

Causal effects from observed data

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

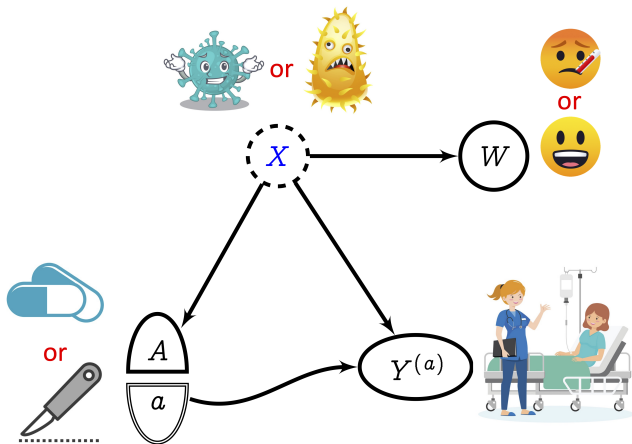
$$\mathbb{E}[Y^{(a)}] = \sum_x \mathbb{E}[Y|a, x]p(x)$$



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

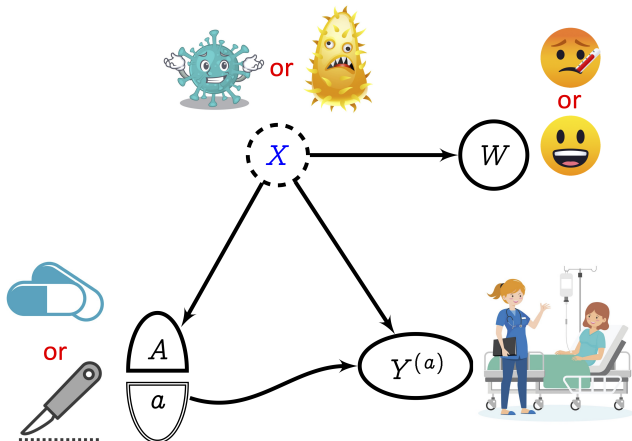
- $P(Y^{(\text{pills})} = \text{cured}) = 0.64$
- $P(Y^{(\text{surgery})} = \text{cured}) = 0.75$

We record symptom W , not disease X



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

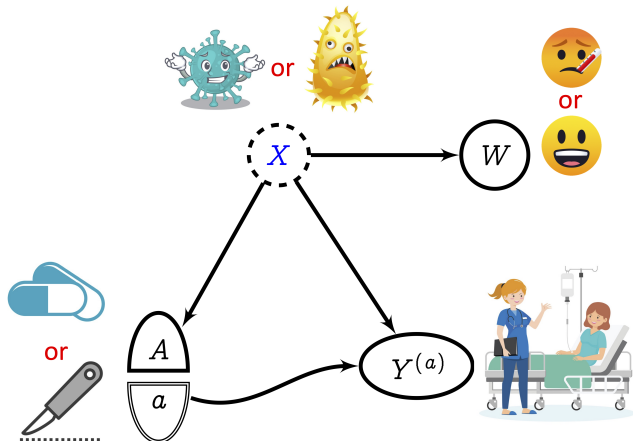
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- $P(W = \text{fever} | X = \text{mild}) = 0.2$
- $P(W = \text{fever} | X = \text{severe}) = 0.8$

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

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)

Outline

Causal effect estimation, with hidden covariates X :

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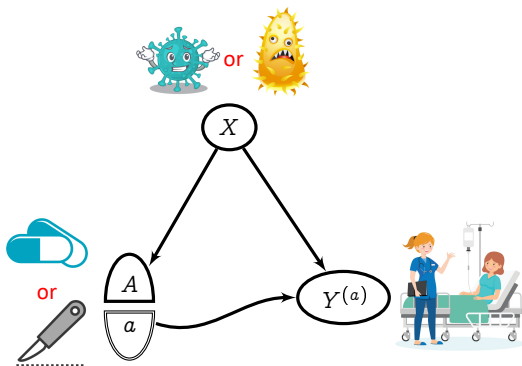
Applications: effect of actions under

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What's new and why?

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

Some core assumptions



Assume:

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

Identifying causal effects with proxy variables of an unmeasured confounder

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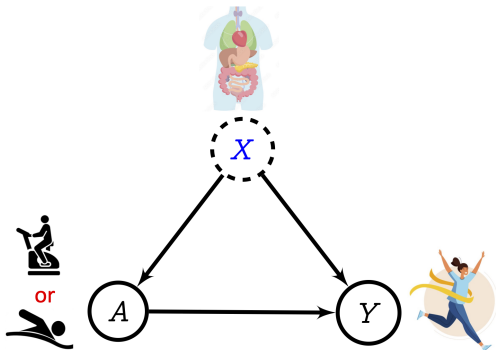
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etchetge@hsph.harvard.edu

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

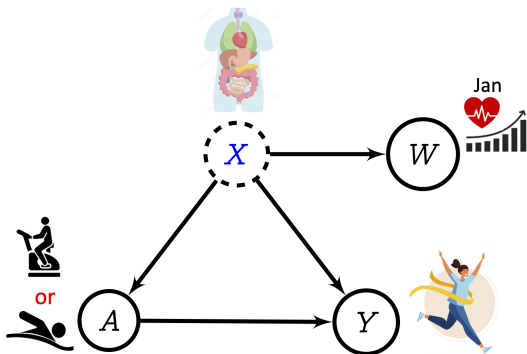


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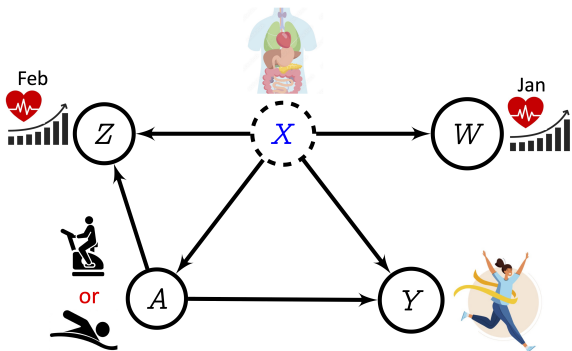


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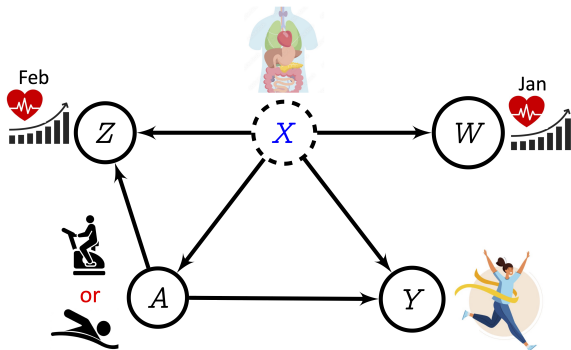


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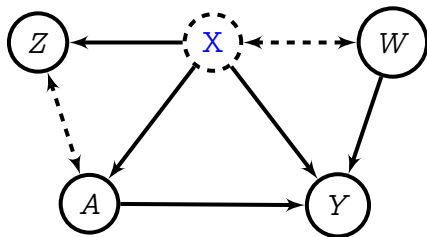
\Rightarrow Can recover $\mathbb{E}(Y^{(a)})$ from observational data

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

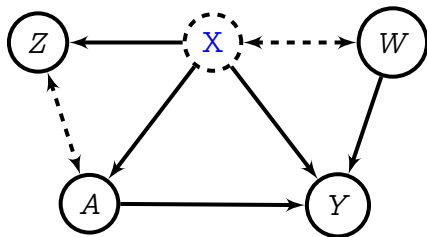


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Structural assumptions:

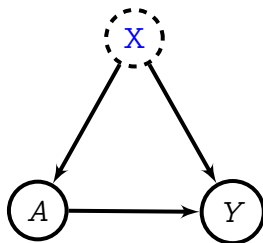
$$W \perp\!\!\!\perp (Z, A) | X$$

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

Why proxy variables? A simple proof

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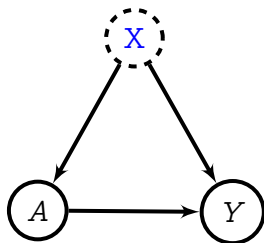
If X were observed,

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

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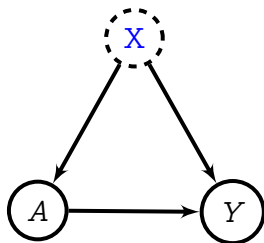
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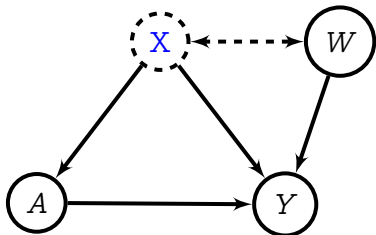
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Goal: “get rid of the blue” X

...add the outcome proxy W

The definitions are:

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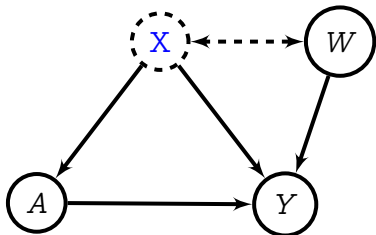
For each a , if we could solve:

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

...add the outcome proxy W

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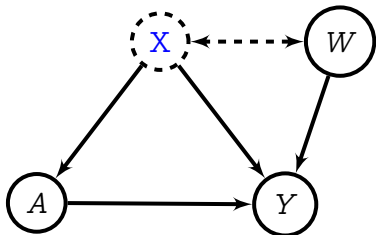
.....then

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

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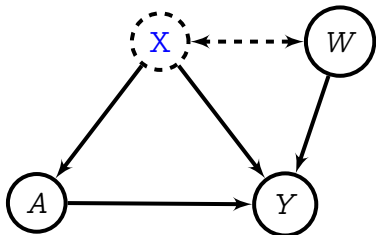
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$$\begin{aligned} P(Y^{(a)}) &= P(Y|X, a)P(X) \\ &= H_{w,a}P(W|X)P(X) \end{aligned}$$

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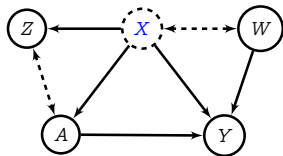
.....then

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

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

From last slide,

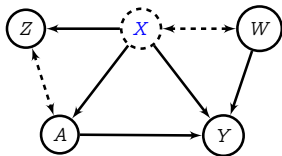
$$P(Y|X, a) = H_{w,a} P(W|X)$$



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

From last slide,

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



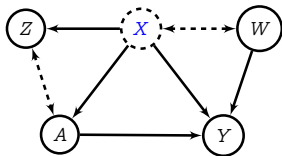
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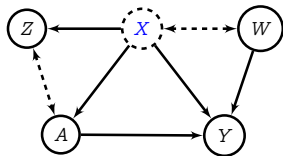
$$P(W|X)p(X|Z, a) = P(W|Z, a)$$



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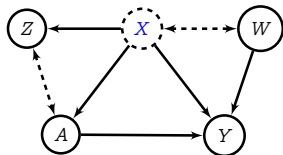
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Because $Y \perp\!\!\!\perp Z | (A, X)$,

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

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

Outcome bridge and proxy variables

Kernel features (ICML 2021):

arXiv.org > cs > arXiv:2105.04544

Search...
Help | Advan

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 J. Kusner, Arthur Gretton, Krikamol Muandet



NN features (NeurIPS 2021):

arXiv.org > cs > arXiv:2106.03907

Search...
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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/>

Proxy relation, outcome bridge

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 outcome bridge:

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

- “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. Bridge existence requires \diamond , identification of DR requires \triangle (and further technical assumptions) [XKG: Assumption 2, Prop. 1, Corr. 1; Deane]

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

$$\mathbb{E}[f(X)|A = a, W = w] = 0, \forall(w, a) \iff f(X) = 0, \mathbb{P}_X \text{ a.s. } \diamond$$

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

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

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

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

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:

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

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

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

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

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

...and by the proxy model above,

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

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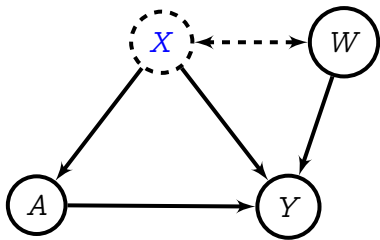
Feature parametrization of bridge $h_y(a, w)$

The **outcome bridge** function class \mathcal{H} defined as:

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

Assume we have:

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



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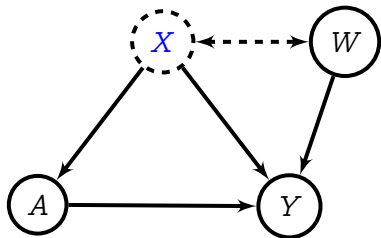
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Questions:

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

Both are necessary (next slide)!



Regression for $h_y(w, a)$

Goal:

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

Primary regression:

$$h_y^{(\lambda)} = \arg \min_{h \in \mathcal{H}} \mathbb{E}_{Y, A, Z} \left(Y - \mathbb{E}_{W|A, Z} h(W, A) \right)^2 + \lambda \Omega(\| \gamma \|^2)$$

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

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

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

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Recall bridge function

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

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$$h_y^{(\lambda)} = \arg \min_{h \in \mathcal{H}} \mathbb{E}_{Y, A, Z} \left(Y - \mathbb{E}_{W|A, Z} h(W, A) \right)^2 + \lambda \Omega(\|\gamma\|^2)$$

Recall bridge function

$$\begin{aligned} \mathbb{E}_{W|a, z} h(W, a) &= \mathbb{E}_{W|a, z} \left[\gamma^\top (\varphi_\theta(W) \otimes \varphi_\xi(a)) \right] \\ &= \gamma^\top \left(\underbrace{\mathbb{E}_{W|a, z} [\varphi_\theta(W)]}_{\text{cond. feat. mean}} \otimes \varphi_\xi(a) \right) \end{aligned}$$

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

Deaner (2021).

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

Xu, Kanagawa, G. (2021).

Regression for $h_y(w, a)$

Goal:

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

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$$h_y^{(\lambda)} = \arg \min_{h \in \mathcal{H}} \mathbb{E}_{Y, A, Z} \left(Y - \mathbb{E}_{W|A, Z} h(W, A) \right)^2 + \lambda \Omega(\|\gamma\|^2)$$

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Ridge regression (again!): 2SLS

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

Deaner (2021).

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

Xu, Kanagawa, G. (2021).

Domain shift: the blessings of multiple domains

Outcome bridge for domain shift

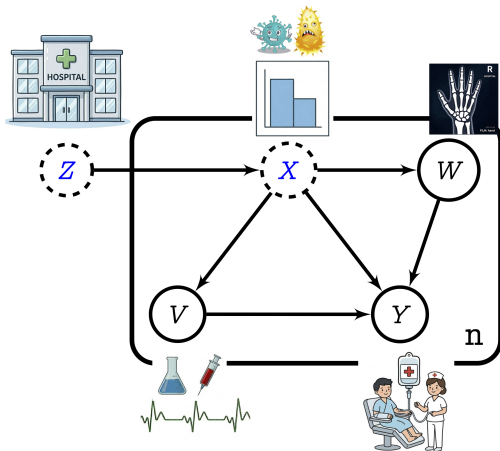
“The blessings of multiple domains”

Outcome bridge for domain shift

“The blessings of multiple domains”

In this example:

- X : which disease
- V : blood tests, ECG
- W : x-rays
- Y : diagnosis
- Z : domain (P_X param.)
- $n \in \{1 \dots D + 1\}$



arXiv > cs > arXiv:2403.07442

Computer Science > Machine Learning

Submitted on 12 Mar 2024

Proxy Methods for Domain Adaptation

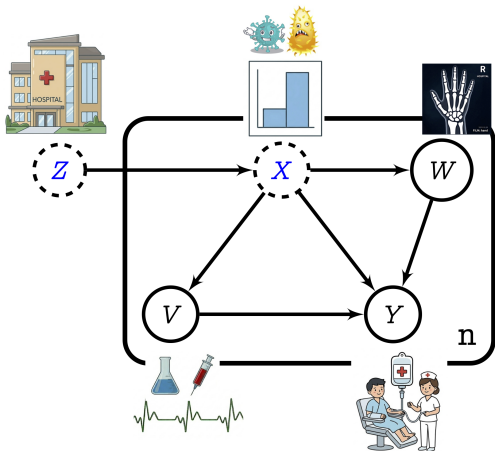
Katherine Tsai, Stephen R. Pfluh, Olawale Salaudeen, Nicole Chiou, Matt J. Kusner, Alexander D'Amour, Sanmi Koyejo, Arthur Gretton

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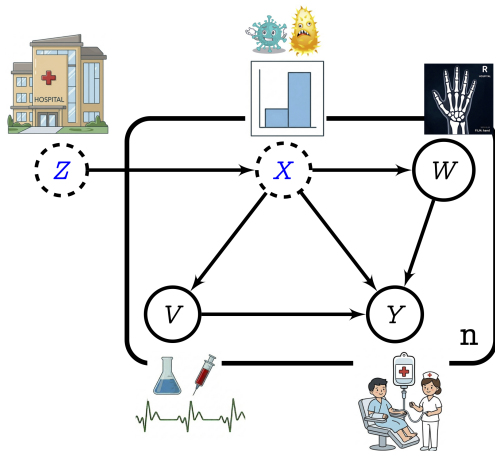
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Goal: prediction on new (*) domain $D+1$ via outcome bridge



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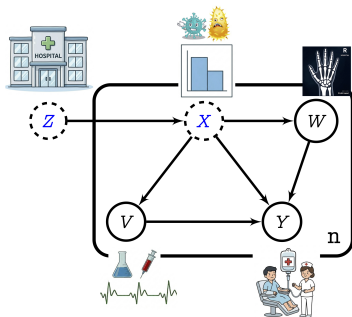
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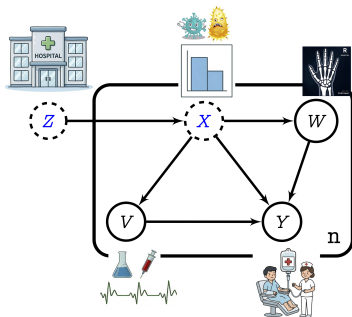
Proof (1)

- X : unobserved variable.
- V : “view 1”
- W : “view 2”
- Y : outcome
- n observations per domain



Proof (1)

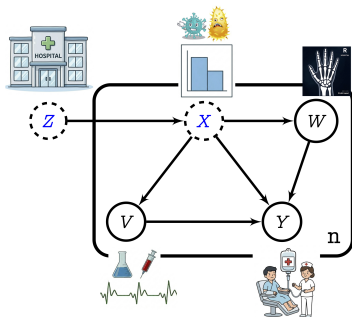
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Core assumption: only $P(X|Z)$ changes with Z , all $P(Q|X)$ invariant for $Q \subseteq \{V, Y, W\}$.

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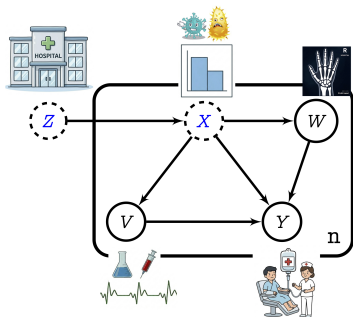
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For a new domain (*) given outcome bridge $M_{w,v}$ solving

$$P(Y|X, v) = M_{w,v} P(W|X)$$

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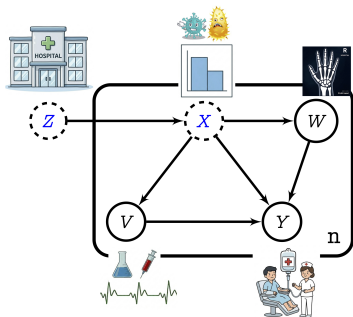
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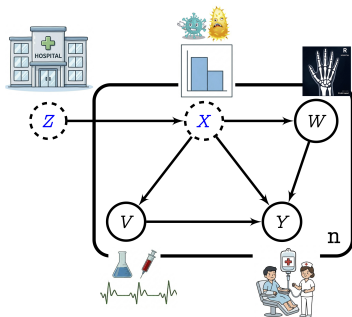
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Proof (2) - how to solve for outcome bridge?

Get rid of the blue!

For each v , define matrix of per-domain probabilities:

$$\underbrace{P^{(1..D)}(X|v)}_{d_x \times D} := \left[P^{(1)}(X|v) \quad \dots \quad P^{(D)}(X|v) \right]$$

Proof (2) - how to solve for outcome bridge?

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Similarly

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Then

$$P^{(1..D)}(Y|v) = M_{w,v} P^{(1..D)}(W|v)$$

Solve for $M_{w,v}$ when $\text{rank}(P^{(1..D)}(W|v)) \geq d_x$.

Treatment bridge and doubly robust proxy learning

AISTATS 2025

arXiv > cs > arXiv:2503.08371

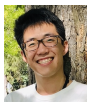
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[Submitted on 11 Mar 2025]

Density Ratio-based Proxy Causal Learning Without Density Ratios

Bariscan Bozkurt, Ben Deaner, Dimitri Meunier, Liyuan Xu, Arthur Gretton



NeurIPS 2025

arXiv > cs > arXiv:2505.19807

Computer Science > Machine Learning

[Submitted on 26 May 2025]

Density Ratio-Free Doubly Robust Proxy Causal Learning

Bariscan Bozkurt, Houssam Zenati, Dimitri Meunier, Liyuan Xu, Arthur Gretton



Code for treatment bridge and doubly robust:

<https://github.com/BariscanBozkurt/>

Doubly-Robust-Kernel-Proxy-Variable-Algorithm

Other DR approaches:

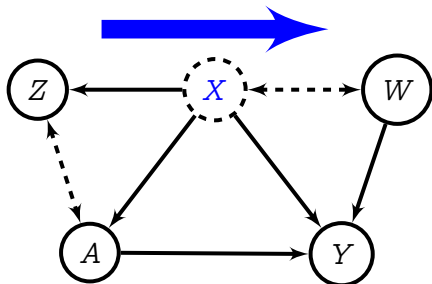
Cui, Pu, Shi, Miao, Tchetgen-Tchetgen. Semiparametric proximal causal inference. JASA (2024): binary treatment.

Wu, Fu, Wang, Sun. Doubly robust proximal causal learning for continuous treatments. ICLR (2024): density ratio + Parzen smoothed treatment

Treatment bridge: idea

Outcome bridge

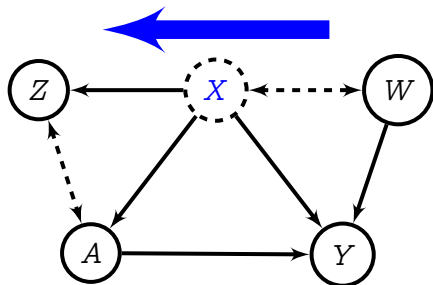
$$\mathbb{E}(Y | a, z) = \mathbb{E}_{W|a,z} h_y(W, a)$$



Treatment bridge: idea

Treatment bridge

$$?? = \mathbb{E}_{Z|a,w}[g_y(Z, a)]$$



Treatment bridge dose-response

Main theorem: Assume we solved for treatment bridge:

$$\frac{p(a)p(w)}{p(a, w)} = \mathbb{E}_{Z|a, w}[g_y(Z, a)]$$

Treatment bridge dose-response

Main theorem: Assume we solved for **treatment bridge**:

$$\frac{p(a)p(w)}{p(a, w)} = \mathbb{E}_{Z|a, w}[g_y(Z, a)]$$

Dose-response curve via $p(Z|A = a)$:

$$\mathbb{E}(Y^{(a)}) = DR^{(T)}(a; g_y) := \mathbb{E}_{Y, Z|a}[Y g_y(Z, a)]$$

Bridge existence requires \triangle , identification of DR requires \diamond
[BDMXG25: Assumptions 3.2, 3.3, 3.7].

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

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

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

$$\mathbb{E}[f(X)|A = a, W = w] = 0, \forall(w, a) \iff f(X) = 0, \mathbb{P}_X \text{ a.s. } \diamond$$

Orange assumption is slightly stronger than the one we used, and implies our actual
Assumption 3.2

Treatment bridge regression loss

Loss function

$$\mathcal{L}(g_y) = \mathbb{E}_{A, W} \left[\left(\frac{p(A)p(W)}{p(A, W)} - \mathbb{E}_{Z|A, W}[g_y(Z, A)] \right)^2 \right]$$

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Empirical estimates:

- 1 Squared mean
- 2 U-statistic

Feature parametrization of bridge $g_y(z, a)$

The **treatment bridge** is a function of **two** arguments

$$g_y(z, a) = \eta^\top [\varphi_\theta(z) \otimes \varphi_\xi(a)]$$

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Need a **third regression**

$$DR^{(T)}(a; g_y) = \mathbb{E}_{Y,Z|a} [Y g_y(Z, a)]$$

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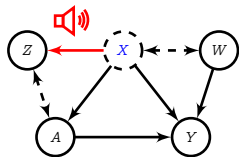
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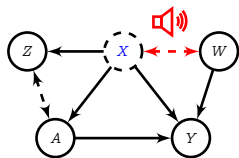
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Why treatment bridge? Synthetic demo



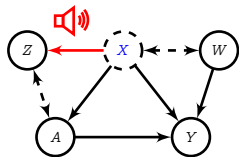
Setting	Outcome bridge	Treatment bridge
Set. 1	41.84 ± 26.61	5.53 ± 0.69

Why treatment bridge? Synthetic demo



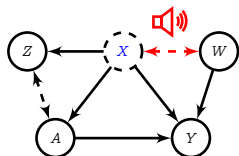
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Set. 2	5.41 ± 2.17	9.32 ± 5.29

Why treatment bridge? Synthetic demo



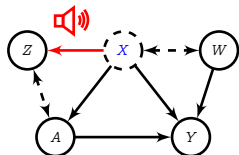
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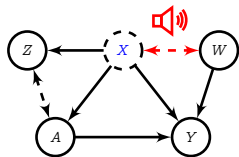
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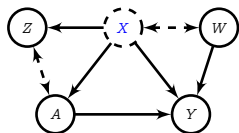
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Doubly robust proxy causal learning

$$\begin{aligned} DR^{(DR)}(a; h_y, g_y) \\ = \mathbb{E}_{Y,Z,W|a}[g_y(Z, a)(Y - h_y(W, a))] + \mathbb{E}_W[h_y(W, a)] \end{aligned}$$

Doubly robust proxy causal learning

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Guarantees?

Doubly robust proxy causal learning

$$\begin{aligned} DR^{(DR)}(a; h_y, g_y) &= \mathbb{E}_{Y,Z,W|a}[g_y(Z, a)(Y - h_y(W, a))] + \mathbb{E}_W[h_y(W, a)] \\ &= \underbrace{\mathbb{E}_{Y,Z|a}[Y g_y(Z, a)]}_{\text{3rd regression}} - \underbrace{\mathbb{E}_{Z,W|a}[g_y(Z, a)h_y(W, a)]}_{\text{4th regression}} + \mathbb{E}_W[h_y(W, a)] \end{aligned}$$

Guarantees?

- If either of h_y, g_y is correct then $DR^{(DR)}(a; h_y, g_y) = DR(a)$ (true dose-response)

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Guarantees?

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- Convergence:

$$\begin{aligned}&|DR(a) - \widehat{DR}^{(DR)}(a; \hat{h}_y, \hat{g}_y)| \\ &\lesssim \|g_y - \hat{g}_y\| \|h_y - \hat{h}_y\| + \|C_{YZ|A} - \widehat{C}_{YZ|A}\|_{HS} + \|C_{WZ|A} - \widehat{C}_{WZ|A}\|_{HS}\end{aligned}$$

where

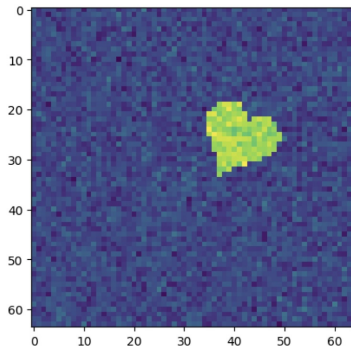
$$C_{YZ|A}\varphi(a) = \mathbb{E}_{Y,Z|a}[Y\varphi(Z)]$$

$$C_{WZ|A}\varphi(a) = \mathbb{E}_{W,Z|a}[\varphi(W) \otimes \varphi(Z)]$$

Synthetic experiment, kernel features

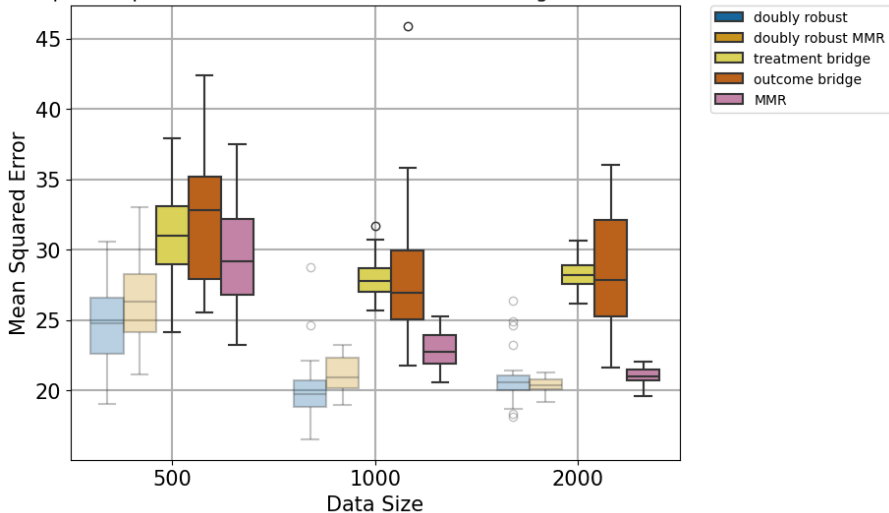
dSprite example:

- $X = \{\text{scale, rotation, posX, posY}\}$
- Treatment $A \in \mathbb{R}^{4096}$ is the image generated (with Gaussian noise)
- Outcome Y is linear function of A with multiplicative confounding by posY .
- $Z = \{\text{scale, rotation, posX}\}$,
 $W = \text{noisy image sharing posY}$

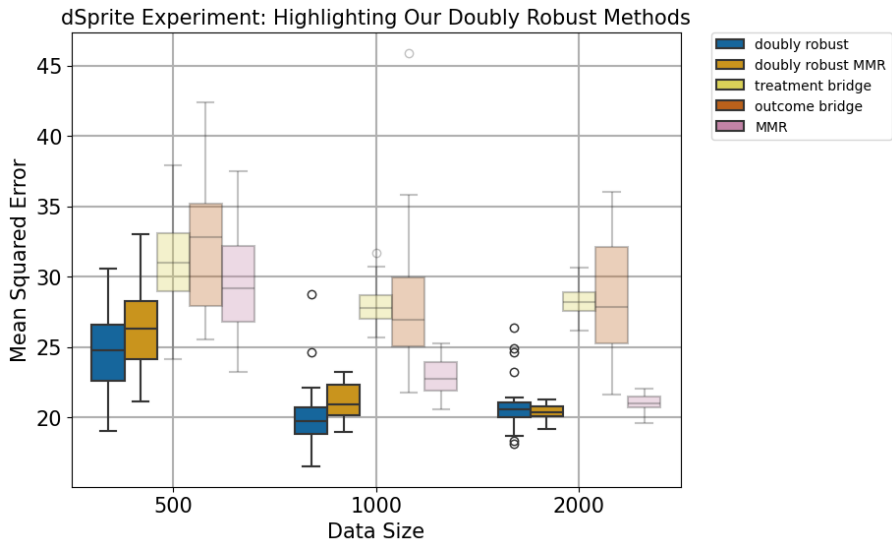


Synthetic experiment, results

dSprite Experiment: Treatment and Outcome Bridge-based Methods



Synthetic experiment, results

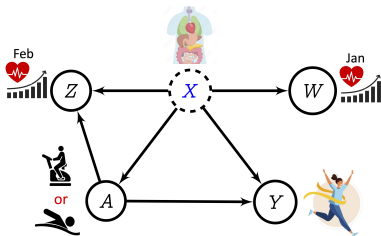


Conclusion

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)

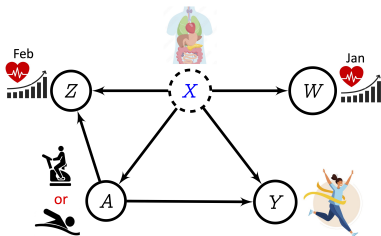


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Key messages:

- 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/>

<https://github.com/BariscanBozkurt/>

Doubly-Robust-Kernel-Proxy-Variable-Algorithm

Research support

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The Gatsby Charitable Foundation



Google DeepMind



Questions?



Failures of completeness assumptions (1)

Recall (one of the) completeness assumptions:

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

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 $p(X|z)$

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

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

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

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

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