

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

Arthur Gretton

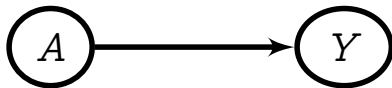
Gatsby Computational Neuroscience Unit,
University College London

Oxford, 2022

A medical treatment scenario



or

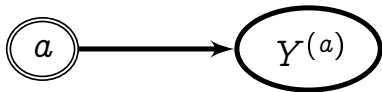
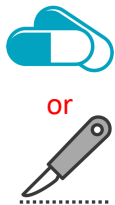


From our **observations** of historical hospital data:

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

Just recommend pills? Cheaper and more effective!

A medical treatment scenario



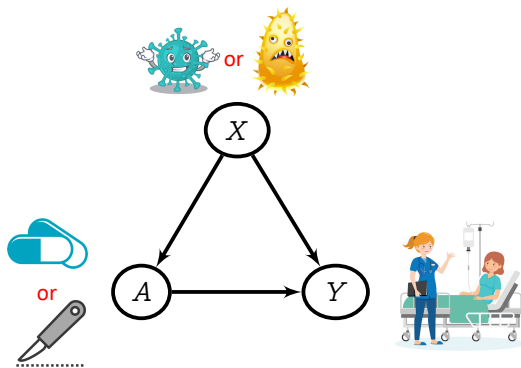
From our intervention (making all patients take a treatment):

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

What went wrong?

Observation vs intervention

Conditioning from observation: $E(Y|A = a) = \sum_x E(y|a, x)p(x|a)$

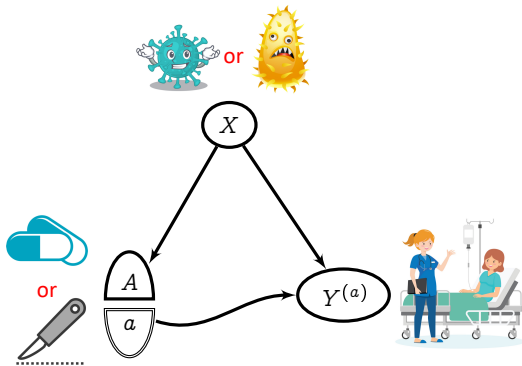


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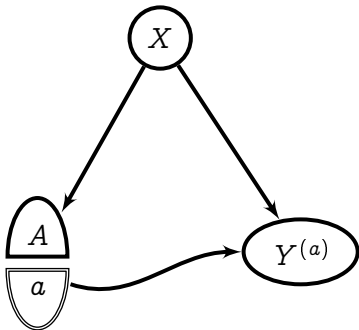
Average causal effect (**intervention**): $E(Y^{(a)}) = \sum_x E(y|a, x)p(x)$



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Questions we will solve



Outline

Talk structure:

- Average treatment effect (ATE)
 - ...via kernel mean embedding (marginalization)
- Conditional average treatment effect (CATE)
 - via kernel conditional mean embedding
- Average treatment on treated
- Mediation effect, dynamic treatment effect
- Proxy methods
 - ...when covariates are hidden

Advantages of the approach:

- Treatment A , covariates X , etc can be multivariate, complicated...
- Simple, robust implementation;
- Strong statistical guarantees under general smoothness assumptions

Methods also implemented for adaptive neural net features!

Key requirement: linear functions of features

All learned functions will take the form:

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

Option 1: Finite dictionaries of **learned** neural net features

Xu, Chen, Srinivasan, de Freitas, Doucet, G. "Learning Deep Features in Instrumental Variable Regression". (ICLR 21)

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

Xu, G. "A Neural Mean Embedding Approach for Back-door and Front-door Adjustment". (arXiv:2210.06610)

Option 2: Infinite dictionaries of **fixed** kernel features:

$$\langle \varphi(x_i), \varphi(x) \rangle_{\mathcal{H}} = k(x_i, x)$$

Kernel is feature dot product.

Primary focus of this talk.

Building block: kernel ridge regression

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

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

Kernel as feature dot product:

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Kernel as feature dot product:

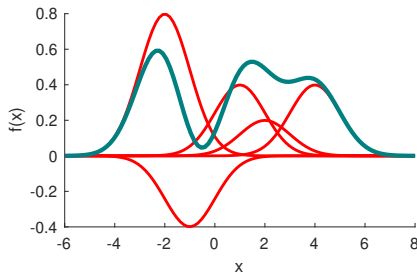
$$\langle \varphi(x_i), \varphi(x) \rangle_{\mathcal{H}} = k(x_i, x)$$

Solution at x :

$$\hat{\gamma}(x) = \sum_{i=1}^n \alpha_i k(x_i, x)$$

$$\alpha = (K_{XX} + \lambda I)^{-1} Y$$

$$(K_{XX})_{ij} = k(x_i, x_j),$$



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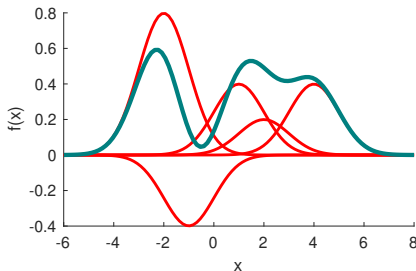
Solution at x (as weighted sum of y)

$$\hat{\gamma}(x) = \sum_{i=1}^n y_i \beta_i(x)$$

$$\beta(x) = (K_{XX} + \lambda I)^{-1} k_{Xx}$$

$$(K_{XX})_{ij} = k(x_i, x_j)$$

$$(k_{Xx})_i = k(x_i, x)$$



KRR: consistency in RKHS norm

Assume problem well specified

- Denote: $\gamma_0 \in \mathcal{H}^c$ where $\mathcal{H}^c \subset \mathcal{H}$, $c \in (1, 2]$
 - Larger $c \implies$ smoother $\gamma_0 \implies$ easier problem.
- Eigenspectrum decay of input feature covariance, $\eta_j \sim j^{-b}$, $b \geq 1$
 - Larger $b \implies$ easier problem

[A] Fischer, Steinwart (2020). Sobolev norm learning rates for regularized least-squares algorithms.

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Consistency [A, Theorem 1.ii]

$$\|\hat{\gamma} - \gamma_0\|_{\mathcal{H}} = O_P \left(n^{-\frac{1}{2} \frac{c-1}{c+1/b}} \right),$$

Best rate is $O_P(n^{-1/4})$ for $c = 2$, $b \rightarrow \infty$.

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(Conditional) average treatment effect,
average treatment on treated



Average treatment effect

Potential outcome (**intervention**):

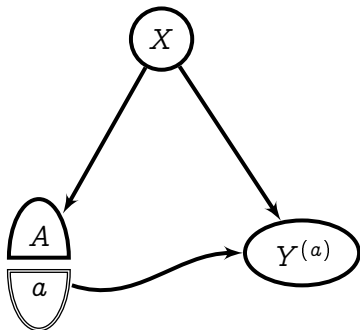
$$E(Y^{(a)}) = \int E(y|a, x) dp(x)$$

(the average structural function; in epidemiology, for continuous a , the dose-response curve).

Assume: (1) Stable Unit Treatment Value Assumption (aka “no interference”), (2) Conditional exchangeability $Y^{(a)} \perp\!\!\!\perp A|X$. (3) Overlap.

Example: US job corps, training for disadvantaged youths:

- A : treatment (training hours)
- Y : outcome (percentage employment)
- X : covariates (age, education, marital status, ...)



Multiple inputs via products of kernels

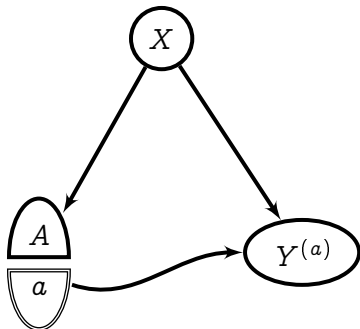
We may predict expected outcome
from two inputs

$$\gamma_0(a, x) := \mathbb{E}[Y | a, x]$$

Assume we have:

- covariate features $\varphi(x)$ with kernel $k(x, x')$
- treatment features $\varphi(a)$ with kernel $k(a, a')$

(argument of kernel/feature map indicates feature space)



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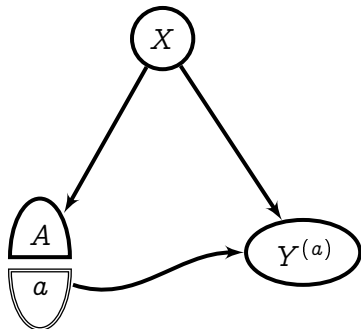
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We use outer product of features (\implies product of kernels):

$$\phi(x, a) = \varphi(a) \otimes \varphi(x) \quad \mathfrak{K}([a, x], [a', x']) = k(a, a')k(x, x')$$



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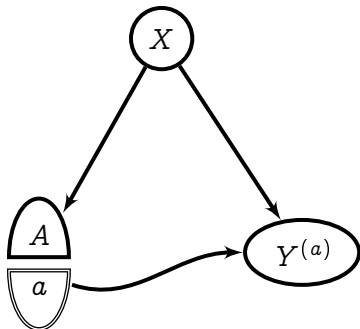
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Ridge regression solution:

$$\hat{\gamma}(x, a) = \sum_{i=1}^n y_i \beta_i(a, x), \quad \beta(a, x) = [K_{AA} \odot K_{XX} + \lambda I]^{-1} K_{Aa} \odot K_{Xx}$$



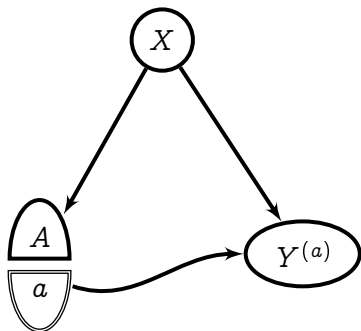
ATE (dose-response curve)

Well specified setting:

$$\gamma_0(a, x) = \mathbb{E}[Y | a, x].$$

ATE as feature space dot product:

$$\begin{aligned}\theta_0^{\text{ATE}}(a) &= \mathbb{E}_P[\gamma_0(a, X)] \\ &= \mathbb{E}_P \langle \gamma_0, \varphi(a) \otimes \varphi(X) \rangle\end{aligned}$$



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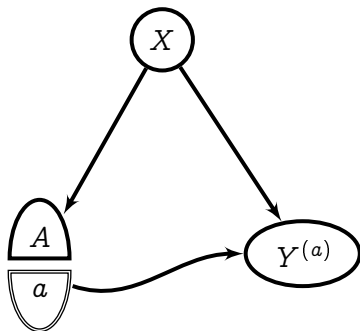
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Feature map of probability P ,

$$\mu_P = [\dots \mathbb{E}_P[\varphi_i(X)] \dots]$$



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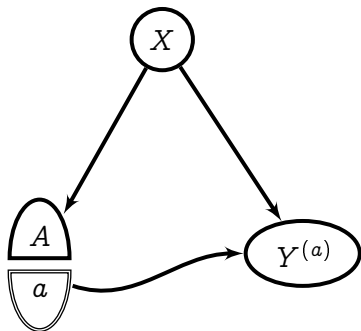
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For characteristic kernels, μ_P is injective.

Consistency: $\|\hat{\mu}_P - \mu_P\|_{\mathcal{H}} = O_P(n^{-1/2})$



ATE: empirical estimate and consistency

Empirical estimate of ATE:

$$\hat{\theta}^{\text{ATE}}(a) = \frac{1}{n} \sum_{i=1}^n Y^{\top} (K_{AA} \odot K_{XX} + n\lambda I)^{-1} (K_{Aa} \odot K_{Xx_i})$$

Singh, Xu, G (2022a), "Kernel Methods for Causal Functions: Dose, Heterogeneous, and Incremental Response Curves" (arXiv:2010.04855)

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Consistency:

$$\|\hat{\theta}^{\text{ATE}} - \theta_o^{\text{ATE}}\|_\infty = O_P \left(n^{-\frac{1}{2} \frac{c-1}{c+1/b}} \right)$$

Follows from consistency of $\hat{\mu}_P$ and $\hat{\gamma}$, under:

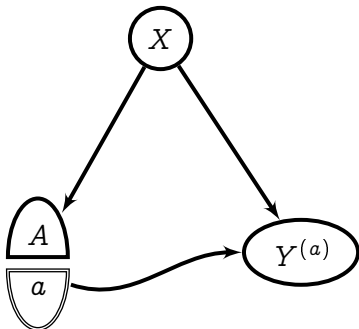
- smoothness assumption $\gamma_0 \in \mathcal{H}^c$, $c \in (1, 2]$
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ATE: example

US job corps: training for disadvantaged youths:

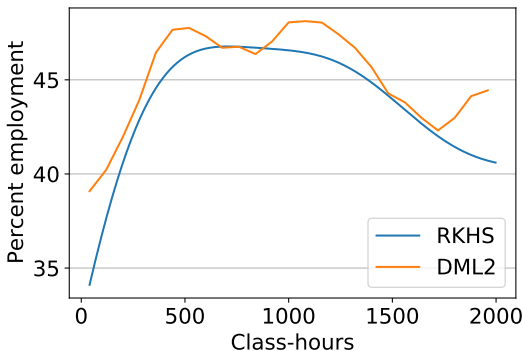
- X : covariate/context (age, education, marital status, ...)
- A : treatment (training hours)
- Y : outcome (percent employment)



Schochet, Burghardt, and McConnell (2008). Does Job Corps work? Impact findings from the national Job Corps study.

Singh, Xu, G (2022a).

ATE: results



- First 12.5 weeks of classes confer employment gain: from 35% to 47%.
- [RKHS] is our $\hat{\theta}^{\text{ATE}}(a)$
- [DML2] Colangelo, Lee (2020), Double debiased machine learning nonparametric inference with continuous treatments.

Singh, Xu, G (2022a)

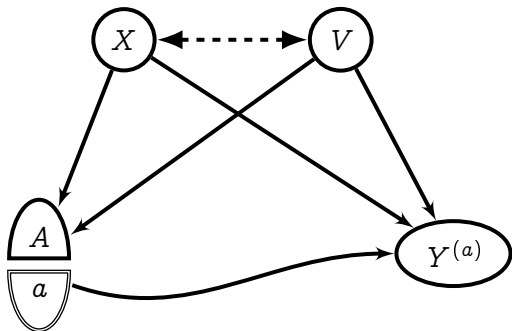
Conditional average treatment effect

Learned conditional mean:

$$\begin{aligned} \mathbb{E}[Y|a, x, v] &\approx \gamma_0(a, x, v) \\ &= \langle \gamma_0, \varphi(a) \otimes \varphi(x) \otimes \varphi(v) \rangle. \end{aligned}$$

Conditional ATE

$$\begin{aligned} \theta_o^{\text{CATE}}(a, v) \\ = \mathbb{E}(Y^{(a)} | V = v) \end{aligned}$$



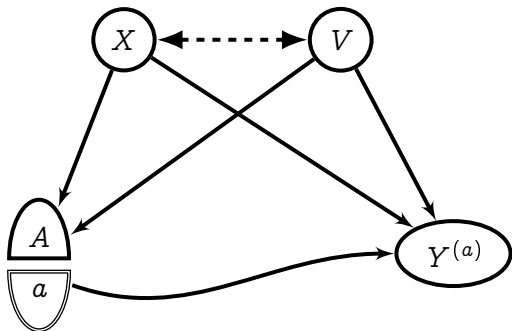
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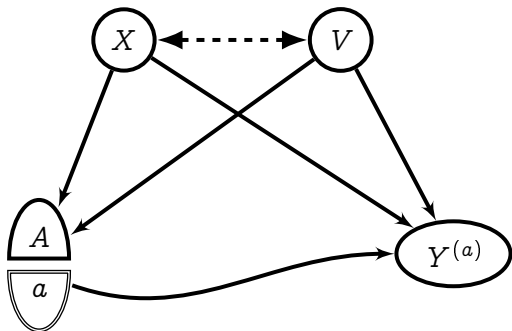
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How to take conditional expectation?

Density estimation for $p(X | V = v)$? Sample from $p(X | V = v)$?

Conditional average treatment effect

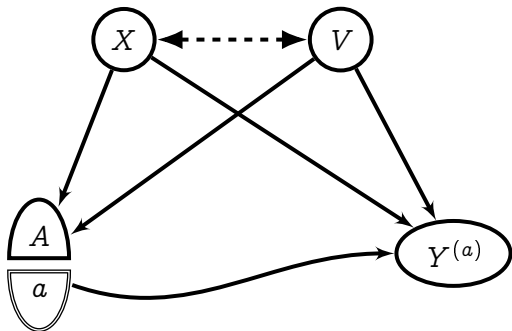
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Learn **conditional mean embedding**: $\mu_{X|V=v} := \mathbb{E}_P(\varphi(X) | V = v)$



Regressing from feature space to feature space

Our goal: an operator $E_0 : \mathcal{H}_V \rightarrow \mathcal{H}_X$ such that

$$E_0 \varphi(v) = \mu_{X|V=v}$$

Song, Huang, Smola, Fukumizu (2009). Hilbert space embeddings of conditional distributions with applications to dynamical systems.

Grunewalder, Lever, Baldassarre, Patterson, G, Pontil (2012). Conditional mean embeddings as regressors.

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$$E_0 \in \overline{\text{span}\{\varphi(x) \otimes \varphi(v)\}} \iff E_0 \in \text{HS}(\mathcal{H}_V, \mathcal{H}_X)$$

Implied smoothness assumption:

$$\mathbb{E}_P[h(X) | V = v] \in \mathcal{H}_V \quad \forall h \in \mathcal{H}_X$$

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A Smooth Operator

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

$$\hat{E} = \underset{E \in \text{HS}}{\text{argmin}} \sum_{\ell=1}^n \|\varphi(x_\ell) - E\varphi(v_\ell)\|_{\mathcal{H}_X}^2 + \lambda_2 \|E\|_{\text{HS}}^2$$

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Ridge regression solution:

$$\mu_{X|V=v} := \mathbb{E}_P[\varphi(X)|V=v] \approx \hat{E}\varphi(v) = \sum_{\ell=1}^n \varphi(x_\ell) \beta_\ell(v)$$
$$\beta(v) = [K_{VV} + \lambda_2 I]^{-1} k_{Vv}$$

Consistency of conditional mean embedding

Assume problem well specified [A, Assumption 6]

$$E_0 = G_1 \circ T_1^{\frac{c_1-1}{2}}, \quad c_1 \in (1, 2], \quad \|G_1\|_{HS}^2 \leq \zeta_1,$$

T_1 is covariance of features $\varphi(v)$:

- Eigenspectrum decays as $\eta_{1,j} \sim j^{-b_1}$, $b_1 \geq 1$.

Larger $c_1 \implies$ smoother $E_0 \implies$ easier problem.

Li, Meunier, Mollenhauer, G. Optimal Rates for Regularized Conditional Mean Embedding Learning, NeurIPS (2022)

Earlier consistency proofs (with slower rates or finite dimensional $\varphi(x)$):

Singh, Sahani, G (2019)

Grunewalder, Lever, Baldassarre, Patterson, G, Pontil (2012).

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Consistency [A, Proposition 3]

$$\left\| \widehat{E} - E_0 \right\|_{HS} = O_P \left(n^{-\frac{1}{2} \frac{c_1-1}{c_1+1/b_1}} \right),$$

best rate is $O_P(n^{-1/4})$, and is minimax optimal.

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Consistency of CATE

Empirical CATE:

$$\begin{aligned} & \hat{\theta}^{\text{CATE}}(a, v) \\ &= Y^\top (K_{AA} \odot K_{XX} \odot K_{VV} + n\lambda I)^{-1} (K_{Aa} \odot \underbrace{K_{XX}(K_{VV} + n\lambda_1 I)^{-1} K_{Vv}}_{\text{from } \hat{\mu}_{X|V=v}} \odot K_{Vv}) \end{aligned}$$

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Consistency: [A, Theorem 2]

$$\|\hat{\theta}^{\text{CATE}} - \theta_0^{\text{CATE}}\|_\infty = O_P \left(n^{-\frac{1}{2} \frac{c-1}{c+1/b}} + n^{-\frac{1}{2} \frac{c_1-1}{c_1+1/b_1}} \right).$$

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

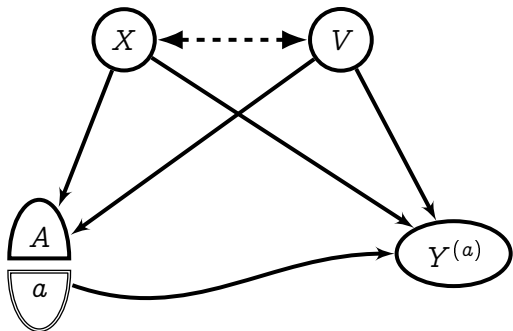
- $E_0 = G_1 \circ T_1^{\frac{c_1-1}{2}}$, $\|G_1\|_{HS}^2 \leq \zeta_1$,
- $\gamma_0 \in \mathcal{H}^c$.

[A] Singh, Xu, G (2022a)

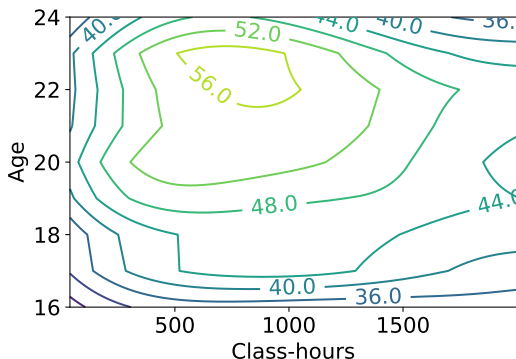
Conditional ATE: example

US job corps: training for disadvantaged youths:

- X : confounder/context (age, education, marital status, ...)
- A : treatment (training hours)
- Y : outcome (percent employed)
- V : age



Conditional ATE: results



Average percentage employment $Y^{(a)}$ for class hours a , **conditioned on age v** . Given around 12-14 weeks of classes:

- 16 y/o: employment increases from 28% to at most 36%.
- 22 y/o: percent employment increases from 40% to 56%.

Singh, Xu, G (2022a)

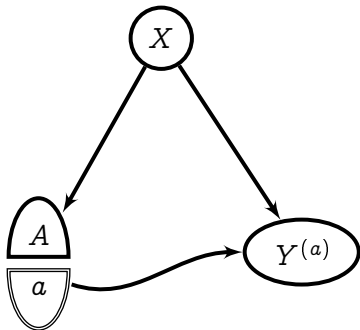
Counterfactual: average treatment on treated

Conditional mean:

$$E[Y|a, x] = \gamma_0(a, x)$$

Average treatment on treated:

$$\begin{aligned}\theta^{ATT}(a, a') \\ = E(y^{(a')} | A = a)\end{aligned}$$



Empirical ATT:

$$\hat{\theta}^{ATT}(a, a')$$

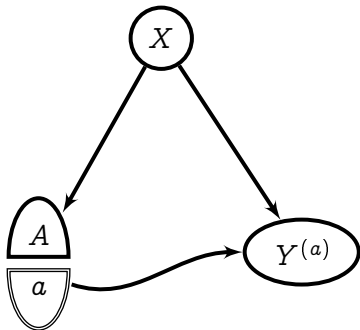
Counterfactual: average treatment on treated

Conditional mean:

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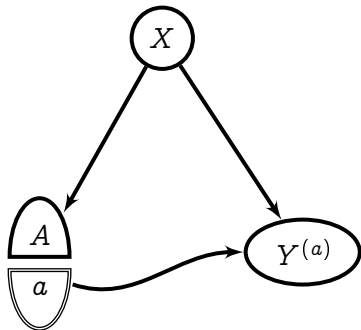
$$E[Y|a, x] = \gamma_0(a, x)$$

Average treatment on treated:

$$\begin{aligned}\theta^{ATT}(a, a') &= E(y^{(a')} | A = a) \\ &= E_P(\langle \gamma_0, \varphi(a') \rangle \otimes \varphi(X) | A = a) \\ &= \langle \gamma_0, \varphi(a') \rangle \otimes \underbrace{E_P[\varphi(X) | A = a]}_{\mu_{X|A=a}}\end{aligned}$$

Empirical ATT:

$$\hat{\theta}^{ATT}(a, a')$$



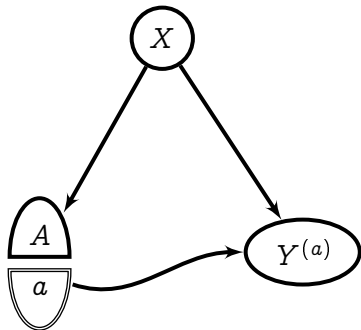
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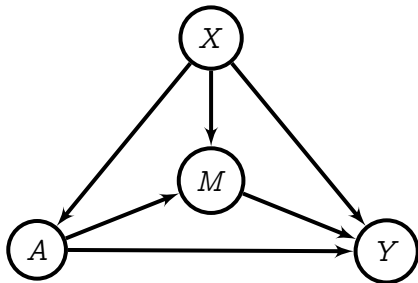
Empirical ATT:

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Mediation analysis

- Direct path from treatment A to effect Y
- Indirect path $A \rightarrow M \rightarrow Y$
- X : context

Is the effect Y mainly due to A ? To M ?

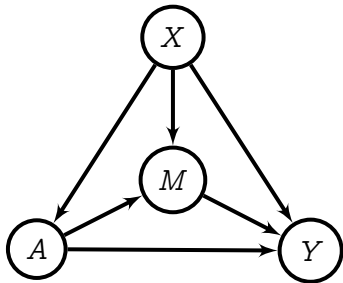


Mediation analysis: example

US job corps: training for disadvantaged youths:

- X : confounder/context (age, education, marital status, ...)
- A : treatment (training hours)
- Y : outcome (arrests)
- M : mediator (employment)

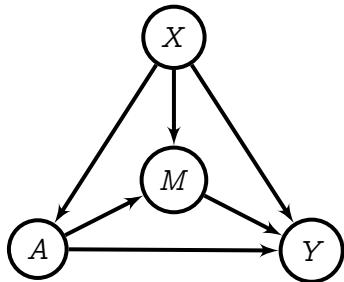
$$\gamma_0(a, m, x) \approx \mathbb{E}[Y | A = a, M = m, X = x]$$



Mediation analysis: example

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A quantity of interest, the **mediated effect**:

$$Y^{\{a', M^{(a)}\}} = \int \gamma_0(a', M, X) d\mathbb{P}(M | A = a, X) d\mathbb{P}(X)$$

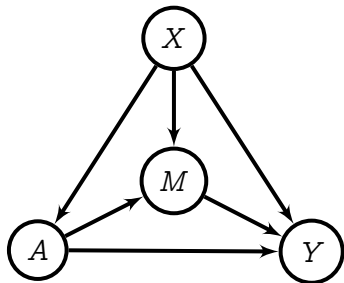
Effect of intervention a' , with $M^{(a)}$ as if intervention were a

Singh, Xu, G (2022b). Kernel Methods for Multistage Causal Inference: Mediation Analysis and Dynamic Treatment Effects. (arXiv:2111.03950)

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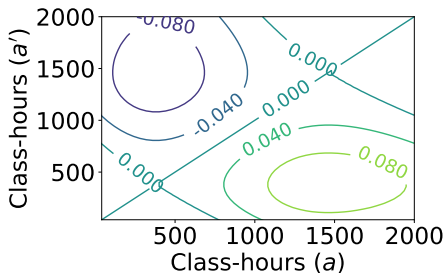
Effect of intervention a' , with $M^{(a)}$ as if intervention were a

Mediation analysis: results

Total effect:

$$\theta_0^{TE}(a, a')$$

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

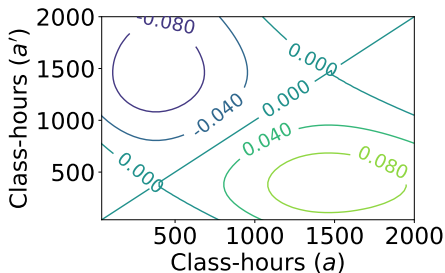


- $a' = 1600$ hours vs $a = 480$ means 0.1 reduction in arrests

Mediation analysis: results

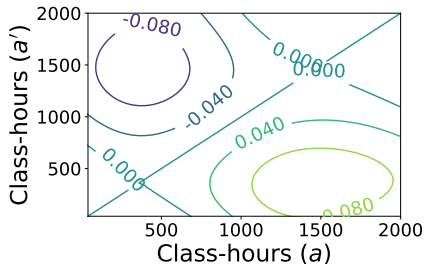
Total effect:

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Direct effect:

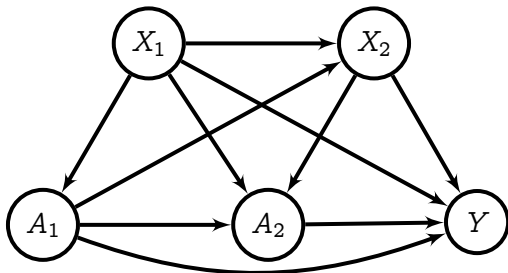
$$\theta_0^{DE}(a, a')$$
$$:= \mathbb{E}[Y\{a', M^{(a)}\} - Y\{a, M^{(a)}\}]$$



- $a' = 1600$ hours vs $a = 480$ hours means 0.1 reduction in arrests
- Indirect effect mediated via employment **effectively zero**

...dynamic treatment effect...

Dynamic treatment effect: sequence A_1, A_2 of treatments.



- potential outcomes $Y^{(a_1)}, Y^{(a_2)}, Y^{(a_1, a_2)}$,
- counterfactuals $E(y^{(a'_1, a'_2)} | A_1 = a_1, A_2 = a_2) \dots$

(c.f. the Robins G-formula)

Unobserved confounders



The proxy correction

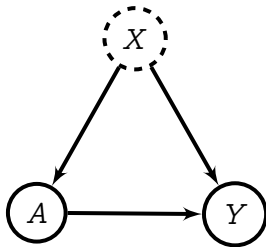
Unobserved X with (possibly) complex nonlinear effects on A , Y

The definitions are:

- X : unobserved confounder.
- A : treatment
- Y : outcome

If X were observed (which it isn't),

$$E(Y^{(a)}) = \int E(y|\mathbf{x}, a) dp(\mathbf{x})$$



The proxy correction

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

The definitions are:

- X : unobserved confounder.
- A : treatment
- Y : outcome
- Z : treatment proxy
- W outcome proxy

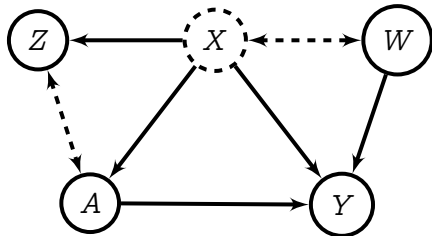
Bidirected arrow: possible confounding.

Structural assumption:

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

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

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



The proxy correction

If X were observed,

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

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

The proxy correction

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Main theorem: Assume we have solved...

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

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

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Main theorem: Assume we have solved...

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

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

...then **average causal effect** via $p(w)$:

$$E(y^{(a)}) = \int h_y(a, w)p(w)dw$$

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

Our solution

- Stage 1: ridge regression from $\phi(a) \otimes \phi(z)$ to $\phi(w)$
 - yields conditional mean embedding $\mu_{W|a,z}$
- Stage 2: ridge regression from $\mu_{W|a,z}$ and $\phi(a)$ to y
 - yields $h_y(w, a)$.
- Solved using sieves [A], kernel [B], or learned NN [C] features

Code available for kernel and NN solutions

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

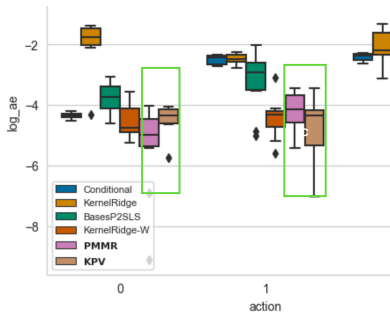
[A] Deaner (2021) Proxy controls and panel data.

[B] Mastouri*, Zhu*, Gultchin, Korba, Silva, Kusner, G,[†] Muandet[†] (2021); Proximal Causal Learning with Kernels: Two-Stage Estimation and Moment Restriction

[C] Xu, Kanagawa, G. (2021) Deep Proxy Causal Learning and its Application to Confounded Bandit Policy Evaluation

Grade retention and cognitive outcome

- X : unobserved confounder (“ability”)
- A : 0: no retention. 1: kindergarten retention. 2: early elementary retention.
- Y : math scores, age 11
- Z : cognitive test scores in elementary school
- W : cognitive test scores from kindergarten



J. Fruehwirth, S. Navarro, Y. Takahashi (2016). How the timing of grade retention affects outcomes: Identification and estimation of time-varying treatment effects.

Deaner (2021)

Conclusions

Kernel ridge regression:

- Solution for ATE, ATT, CATE, mediation analysis, dynamic treatment effects, proximal learning
- ...with treatment A , covariates X , V , mediator M , proxies (W , Z) multivariate, “complicated”
- Simple, robust implementation
- Strong statistical guarantees under general smoothness assumptions

In the papers, but not in this talk:

- Regression to potential outcome distributions over Y (not just $E(Y^{(a)}|\dots)$)
- Instrumental variable regression
- Same algorithms but with adaptive NN features

Selected papers

Observed confounders:

arXiv > econ > arXiv:2010.04855 Search...
Help | Advan

Economics > Econometrics

[Submitted on 10 Oct 2020 (v1), last revised 23 Aug 2022 (this version, v6)]

Kernel Methods for Causal Functions: Dose, Heterogeneous, and Incremental Response Curves

Rahul Singh, Liyuan Xu, Arthur Gretton

arXiv.org > stat > arXiv:2111.03950 Search...
Help | Ad

Statistics > Methodology

[Submitted on 6 Nov 2021]

Kernel Methods for Multistage Causal Inference: Mediation Analysis and Dynamic Treatment Effects

Rahul Singh, Liyuan Xu, Arthur Gretton

arXiv > cs > arXiv:2210.06610 Search...
Help | Ad

Computer Science > Machine Learning

[Submitted on 12 Oct 2022]

A Neural Mean Embedding Approach for Back-door and Front-door Adjustment

Liyuan Xu, Arthur Gretton

Unobserved confounders:

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

NeurIPS 2021:

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

Computer Science > Machine Learning

[Submitted on 7 Jun 2021 (v1), last revised 7 Dec 2021 (this version, v2)]

Deep Proxy Causal Learning and its Application to Confounded Bandit Policy Evaluation

Liyuan Xu, Heishiro Kanagawa, Arthur Gretton

NeurIPS 2019:

arXiv.org > cs > arXiv:1906.00232 Search...
Help | Advan

Computer Science > Machine Learning

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

Kernel Instrumental Variable Regression

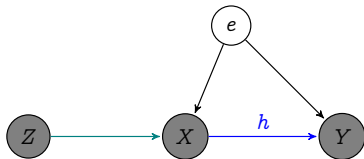
Rahul Singh, Maneesh Sahani, Arthur Gretton

Questions?



Instrumental variable setting (1)

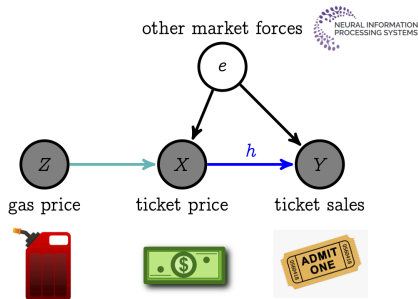
- **Unobserved** confounder $e \implies$ prediction \neq counterfactual prediction
- goal: learn causal relationship h between input X and output Y
 - if we intervened on X , what would be the effect on Y ?
- Instrument Z only influences Y via X , identifying h



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

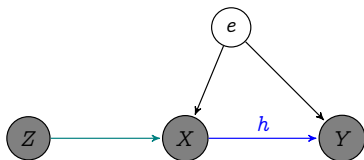
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Instrumental variable setting (2)



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

Singh, Sahani, G., (NeurIPS 2019)

Xu, Chen, Srinivasan, de Freitas, Doucet, G. (ICLR 2021)