Causal Modelling with Kernels: Treatment Effects, Counterfactuals, Mediation, and Proxies








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Outline

Why a kernel approach:

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

Talk structure:

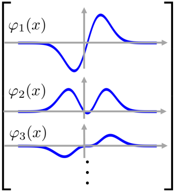
- Average treatment effect (ATE)
  - ...via kernel mean embedding (marginalization)
- Conditional average treatment effect (CATE)
  - via kernel conditional mean embedding
- Mediation effect
  - ...via a kernel mediation distribution embedding
- Proxy methods
  - ...when covariates are hidden

Main building block: kernel ridge regression

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

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

$$\gamma(x) = \langle \gamma, \varphi(x) \rangle_{\mathcal{H}} = \sum_{\ell=1}^{\infty} \gamma_\ell \varphi_\ell(x) = \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \\ \vdots \end{bmatrix}^{\top}$$



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By representer theorem:

$$\hat{\gamma} = \sum_{i=1}^{n} \alpha_i \varphi(x_i) \qquad\qquad \hat{\gamma}(x) = \sum_{i=1}^{n} \alpha_i \langle \varphi(x_i), \varphi(x) \rangle_{\mathcal{H}}$$

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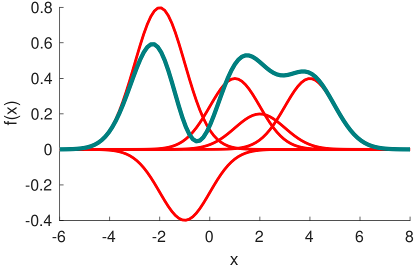

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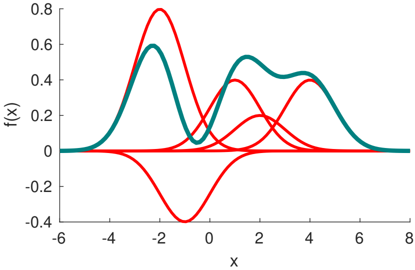
Solution expression at x:

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

$$\beta(x) = (K + \lambda I)^{-1} k_x$$

$(K_{XX})_{ij} = k(x_i, x_j)$,
$(k_{Xx})_i = k(x_i, x)$.



KRR: consistency in RKHS norm

Assume problem well specified

$$\gamma_0 = T^{\frac{c-1}{2}} g, \quad c \in (1,2], \quad \|g\|_{\mathcal{H}}^2 \leq \zeta,$$

T is covariance of features $\varphi(x)$:

- Larger $c \implies$ smoother $\gamma_0 \implies$ easier problem.
- Shorthand: $\gamma_0 \in \mathcal{H}^c$ where $\mathcal{H}^c \subset \mathcal{H}$

[A] Singh, Xu, G (2021a), Generalized Kernel Ridge Regression for Nonparametric Structural Functions and Semiparametric Treatment Effects.

Results from:

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Consistency [A, Prop. F.1]

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

best rate is $O_P(n^{-1/6})$.

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Average treatment effect

Average treatment effect

Potential outcome (intervention):

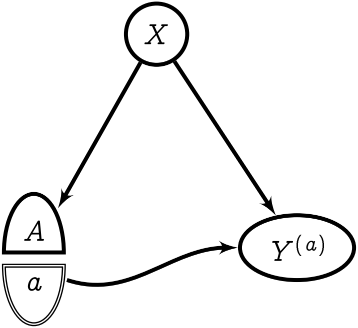
$$\mathrm{E}(Y^{(a)}) = \int E(y|a,x)\,dp(x)$$

(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

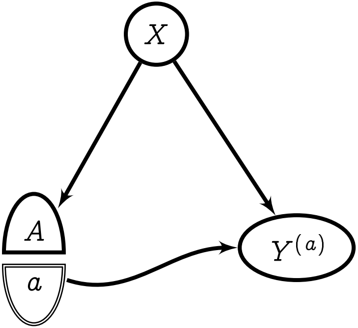
We may predict expected outcome from two inputs

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

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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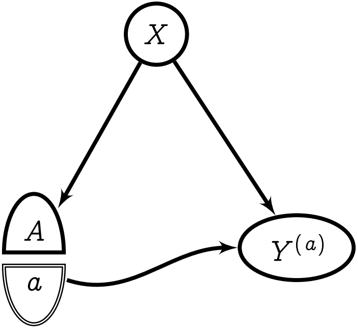

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We use outer product of features ($\implies$ product of kernels):

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

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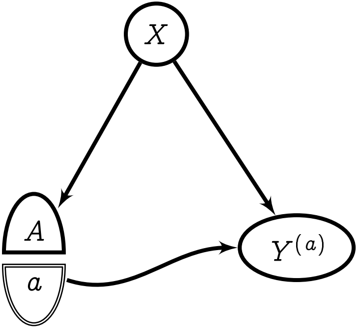

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Ridge regression solution:

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

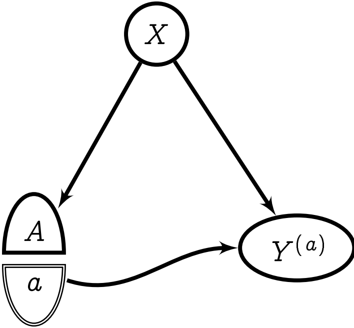
ATE (dose-response curve)

Well specified setting:

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

ATE as feature space dot product:

$$\begin{aligned}\theta_0^{\mathrm{ATE}}(a) &= \mathrm{E}_P[\gamma_0(a, X)] \\ &= \mathrm{E}_P \langle \gamma_0, \varphi(X) \otimes \varphi(a) \rangle_{\mathcal{H}_\mathcal{X} \otimes \mathcal{H}_\mathcal{A}}\end{aligned}$$



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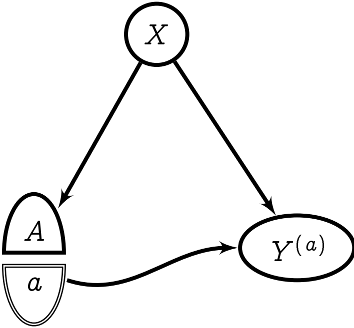

Feature map of probability P,

$$\mu_P = [\ldots \mathrm{E}_P[\varphi_i(X)]\ldots]$$

ATE (dose-response curve)

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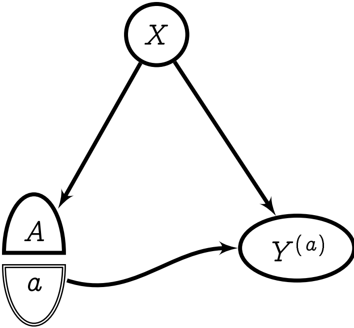

For characteristic kernels, μ_P is injective.

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

ATE: empirical estimate and consistency

Empirical estimate of ATE:

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

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Consistency:

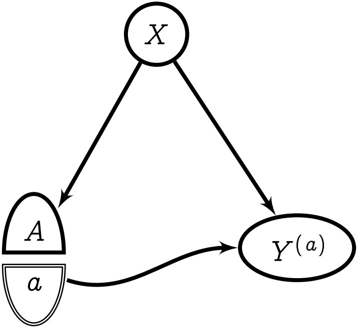
$$\left\| \hat{\theta}^{\text{ATE}} - \theta_o^{\text{ATE}} \right\|_{\infty} = O_P\left(n^{-\frac{1}{2}\frac{c-1}{c+1}} \right)$$

Follows from consistency of $\hat{\mu}_P$ and $\hat{\gamma}$, under smoothness assumption $\gamma_0 \in \mathcal{H}^c$.

ATE: example

US job corps: training for disadvantaged youths:

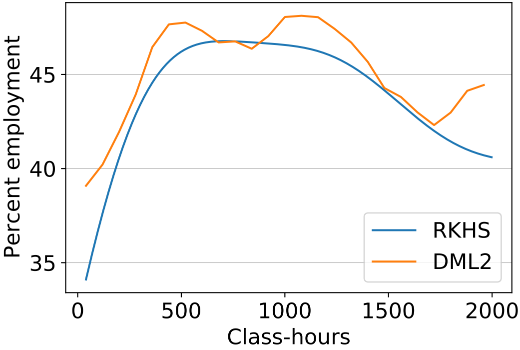
- X: confounder/context (age, education, marital status, ...)
- A: treatment (training hours)
- Y: outcome (percent employment)



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

Singh, Xu, G (2021a).

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 (2021a)

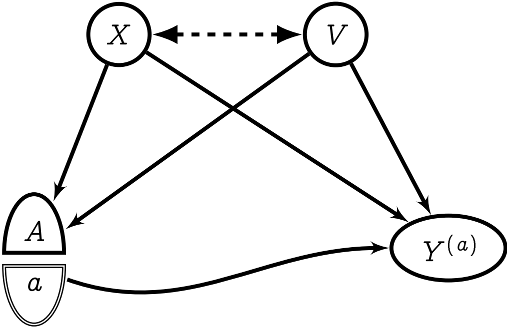
Conditional average treatment effect

Learned conditional mean:

$$\mathrm{E}[\,Y\,|\,a, x, v] \approx \gamma_0(a, x, v)$$
$$= \langle \gamma_0, \varphi(a) \otimes \varphi(x) \otimes \varphi(v) \rangle \,.$$

Conditional ATE

$$\theta_o^{\mathrm{CATE}}(a, v)$$
$$= \mathrm{E}(\,Y^{(a)} |\, V = v)$$



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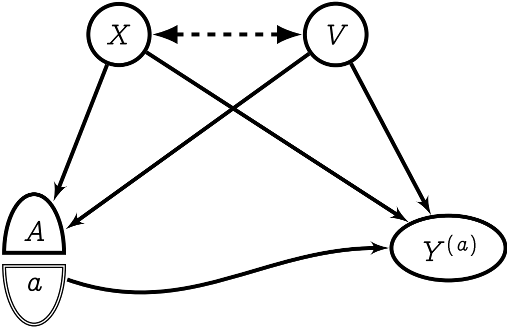

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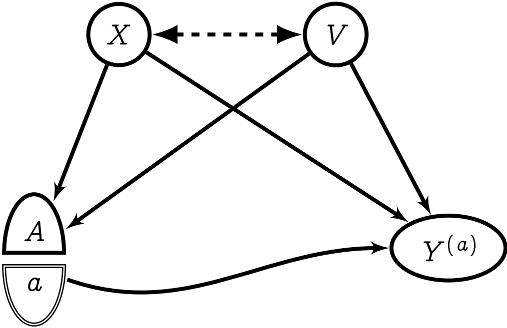
$$\theta_o^{\mathrm{CATE}}(a,v)$$
$$= \mathrm{E}(Y^{(a)}|V=v)$$
$$= \mathrm{E}_P\left(\langle\gamma_0,\varphi(a)\otimes\varphi(X)\otimes\varphi(V)\rangle\,|\,V=v\right)$$
$$= \ldots?$$



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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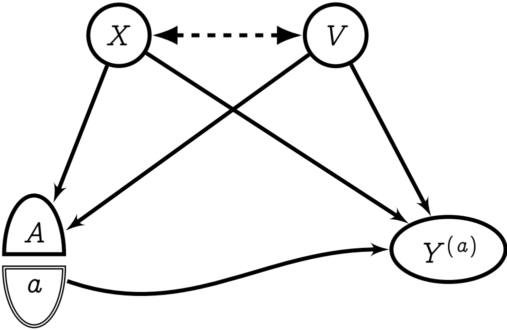
$$= \langle \gamma_0, \varphi(a) \otimes \underbrace{\mathrm{E}_P[\varphi(X)|\,V = v]}_{\mu_{X|\,V=v}} \otimes \varphi(v)\rangle$$



Learn conditional mean embedding: $\mu_{X|\,V=v} := \mathrm{E}_P\left(\varphi(X)|\,V = v\right)$

Regressing from feature space to feature space

Our goal: an operator $E_0 : \mathcal{H}_{\mathcal{V}} \to \mathcal{H}_{\mathcal{X}}$ such that

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

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.

Grunewalder, G, Shawe-Taylor (2013) Smooth operators.

Singh, Sahani, G (2019), Kernel Instrumental Variable Regression.

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$$E_0 \in \mathrm{HS}(\mathcal{H}_{\mathcal{V}}, \mathcal{H}_{\mathcal{X}}) \iff E_0 \in \overline{\mathrm{span}\left\{\varphi(x) \otimes \varphi(v)\right\}}$$

Implied smoothness assumption:

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

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A Smooth Operator

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

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

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Ridge regression solution:

$$\mu_{X|V=v} := \mathrm{E}_P[\varphi(X)|V = v] \approx \widehat{E}\varphi(v) = \sum_{\ell=1}^{n} \varphi(x_\ell)\beta_\ell(v)$$

$$\beta(v) = [K_{VV} + \lambda_2 I]^{-1} k_{Vv}$$

Consistency of conditional mean embedding

Assume problem well specified [A, Hypothesis 5]

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

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

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

[A] Singh, Sahani, G (2019)

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Consistency [A, Theorem 2]

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

best rate is $O_P(n^{-1/6})$.

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Consistency of CATE

Empirical CATE:

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

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Consistency:

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

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

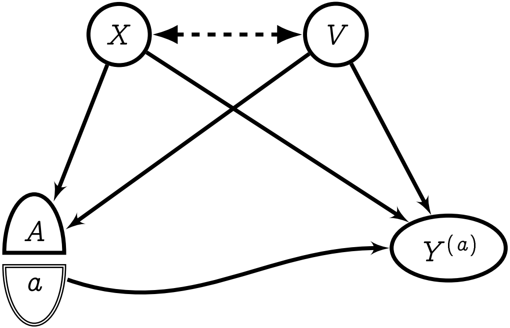
- $E_0^* = T_1^{\frac{c_1-1}{2}} \circ G_1^*$, $\|G_1\|_{HS}^2 \leq \zeta_1$,
- $\gamma_0 \in \mathcal{H}^c$.

Singh, Xu, G (2021a)

Conditional ATE: example

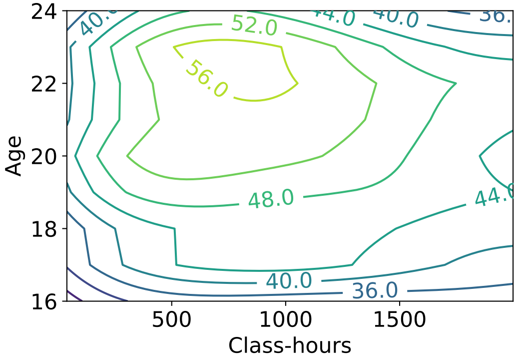
US job corps: training for disadvantaged youths:

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



Singh, Xu, G (2021a)

Conditional ATE: results



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

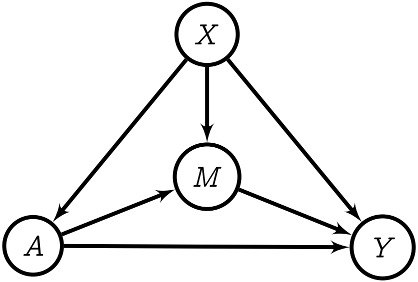
- 16 y/o: employment increases from 28% to at most 36%.
- 22 y/o: percent employment increases from 40% to 56%.

Singh, Xu, G (2021a)

Mediation analysis

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

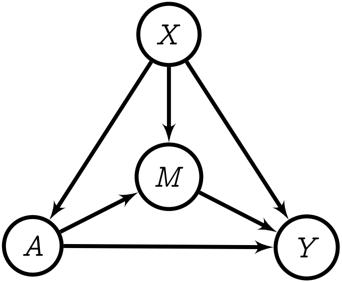
Is the effect Y mainly due to A? To M?



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)



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

Singh, Xu, G (2021b). Kernel Methods for Multistage Causal Inference: Mediation Analysis and Dynamic Treatment Effects.

Mediation analysis: example

US job corps: training for disadvantaged youths:

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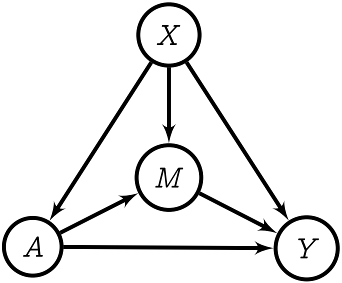

$\gamma_0(a, m, x) \approx \mathrm{E}[Y | A = a, M = m, X = x]$

A quantity of interest, the mediated effect:

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

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

Singh, Xu, G (2021b). Kernel Methods for Multistage Causal Inference: Mediation Analysis and Dynamic Treatment Effects.

Mediation analysis: example

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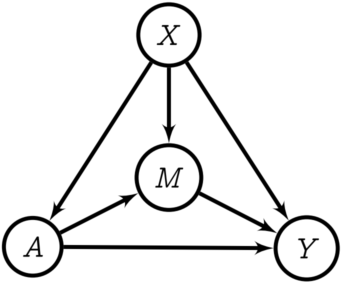


$\gamma_0(a, m, x) \approx \mathrm{E}[Y | A = a, M = m, X = x]$

A quantity of interest, the mediated effect:

$$Y^{\{a', M^{(a)}\}} = \int \gamma_0(a', M, X) \mathrm{d}\mathbb{P}(M | A = a, X) d\mathbb{P}(X)$$
$$= \langle \gamma_0, \varphi(a') \otimes \mathrm{E}_P\{\mu_{M|A=a,X} \otimes \varphi(X)\}\rangle$$

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

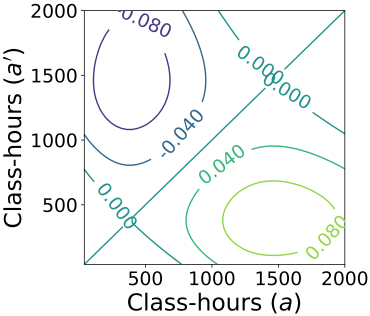
Singh, Xu, G (2021b). Kernel Methods for Multistage Causal Inference: Mediation Analysis and Dynamic Treatment Effects.

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

Singh, Xu, G (2021b)

Mediation analysis: results

Total effect:

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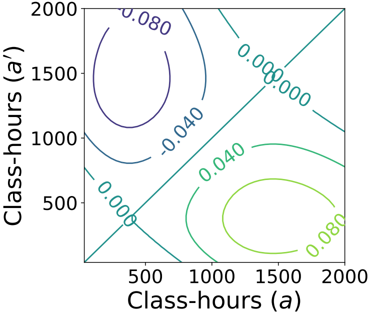
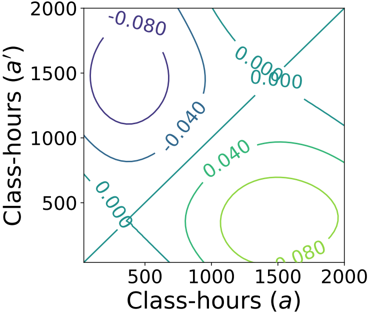


Direct effect:

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

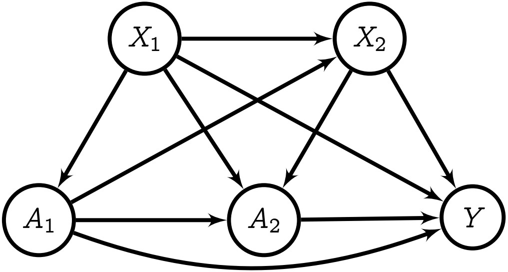


- $a' = 1600$ hours vs $a = 480$ means 0.1 reduction in arrests
- Indirect effect mediated via employment effectively zero

Singh, Xu, G (2021b)

...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 $\mathrm{E}(y^{(a_1',a_2')}|A_1 = a_1, A_2 = a_2)$...

(c.f. the Robins G-formula)

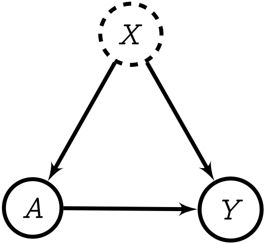
Unobserved confounders

The proxy correction

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

The definitions are:

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

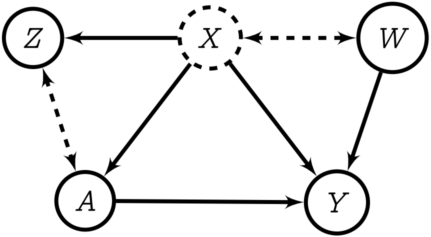


The proxy correction

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: causal link in either direction (or both).

Not all edges need be present.

Structural assumption:

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

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

Miao, Geng, Tchetgen Tchetgen (2018): Identifying causal effects with proxy variables of an unmeasured confounder.

The proxy correction

If X were observed,

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

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

Miao, Geng, Tchetgen Tchetgen (2018)

The proxy correction

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

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

...then potential outcome 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.

Miao, Geng, Tchetgen Tchetgen (2018)

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/

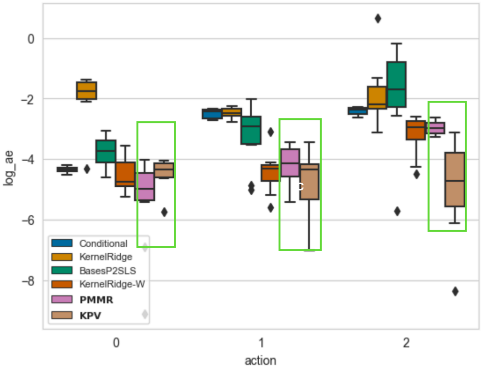
[A] Deaner (2021) Proxy controls and panel data.

[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:

- Doubly robust estimates for discrete A, V with automatic debiasing
- Elasticities
- Regression to potential outcome distributions over Y (not just $E(Y^{(a)}|\ldots)$)
- Instrumental variable regression

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

Selected papers

Observed confounders:

arXiv.org > econ > arXiv:2010.04855

Economics > Econometrics

[Submitted on 10 Oct 2020 (v1), last revised 14 Dec 2021 (this version, v4)]

Generalized Kernel Ridge Regression for Nonparametric Structural Functions and Semiparametric Treatment Effects

Rahul Singh, Liyuan Xu, Arthur Gretton

arXiv.org > stat > arXiv:2111.03950

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

Unobserved confounders:

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 J. Kusner, Arthur Gretton, Krikamol Muandet

NeurIPS 2021:

arXiv.org > cs > arXiv:2106.03907

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

Computer Science > Machine Learning

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

Kernel Instrumental Variable Regression

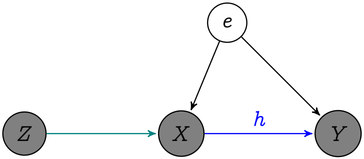
Rahul Singh, Maneesh Sahani, Arthur Gretton

Questions?


THE KERNEL
BREWERY
LONDON
BALTIC PORTER
THE KERNEL
EXPORT STOUT

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



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

Singh, Sahani, G., (NeurIPS 2019)
Xu, Chen, Srinivasan, de Freitas, Doucet, G. (ICLR 2021)

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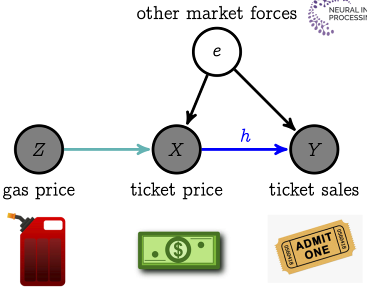
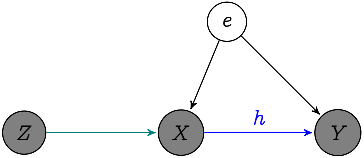


NEURAL INFORMATION PROCESSING SYSTEMS

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

Singh, Sahani, G., (NeurIPS 2019)
Xu, Chen, Srinivasan, de Freitas, Doucet, G. (ICLR 2021)

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)