Causal Effect Estimation with Context and Confounders

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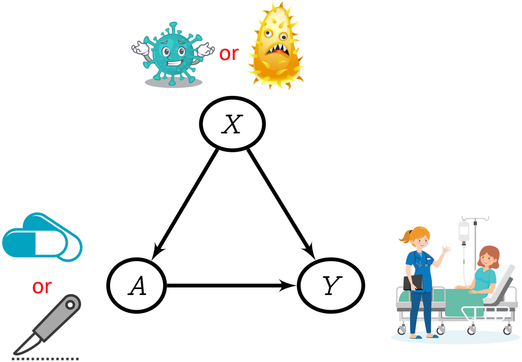
Deepmind

MLSS Okinawa, 2024

Observation vs intervention

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

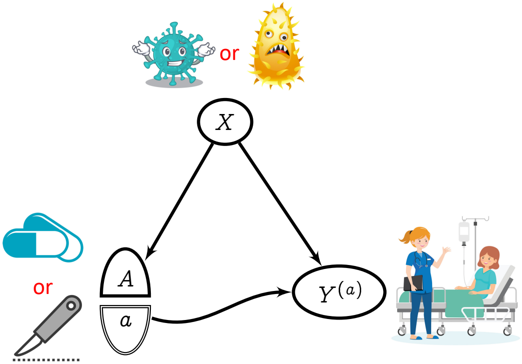


From our observations of historical hospital data:

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

Observation vs intervention

Average causal effect (intervention): $\mathbb{E}[Y^{(a)}] = \sum_x \mathbb{E}[Y \mid a, x]\,p(x)$

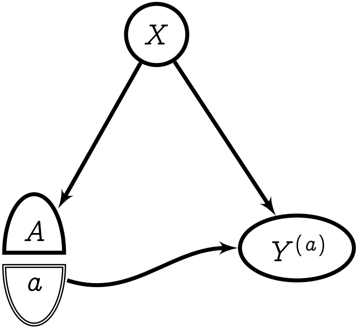


From our intervention (making all patients take a treatment):

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

Richardson, Robins (2013), Single World Intervention Graphs (SWIGs): A Unification of the Counterfactual and Graphical Approaches to Causality

Questions we will solve



Outline

First lecture: causal effect estimation, observed covariates:

- Average treatment effect (ATE), conditional average treatment effect (CATE), average treatment on treated (ATT), mediation effects.

Second lecture: causal effect estimation, hidden covariates:

- ... instrumental variables, proxy variables

What's new? What is it good for?

- Treatment A, covariates X, etc can be multivariate, complicated...
- ...by using kernel or adaptive neural net feature representations

Regression assumption: linear functions of features

All learned functions will take the form:

$$\begin{aligned} \gamma(x) &= \gamma^\top \varphi_\theta(x) \\ &\overset{\text{or}}{=} \langle \gamma, \varphi(x) \rangle_{\mathcal{H}} \end{aligned}$$

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Option 1: Finite dictionaries of learned neural net features $\varphi_\theta(x)$ (linear final layer γ)

Xu, G., A Neural mean embedding approach for back-door and front-door adjustment. (ICLR 23)

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

Option 2: Infinite dictionaries of fixed kernel features:

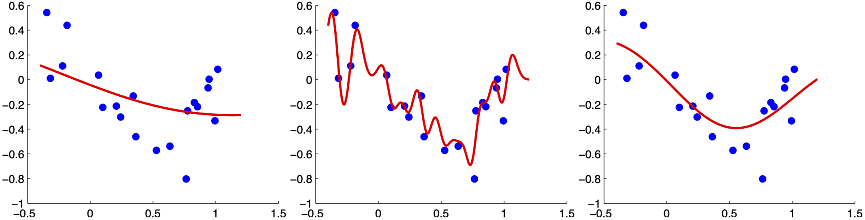
$$\langle \varphi(x_i), \varphi(x) \rangle_{\mathcal{H}} = k(x_i, x)$$

Kernel is feature dot product.

Singh, Xu, G. Kernel Methods for Causal Functions: Dose, Heterogeneous, and Incremental Response Curves. (Biometrika 23)

Singh, Sahani, G. Kernel Instrumental Variable Regression. (NeurIPS 19)

Kernel ridge regression: reminder



Kernel ridge regression

Approximate $\gamma_0(x) := \mathbb{E}[Y | X = x]$ using ridge regression

$$\hat{\gamma} = \operatorname*{argmin}_{\gamma \in \mathcal{H}} \sum_{i=1}^{n} (y_i - \langle \gamma, \varphi(x_i) \rangle_{\mathcal{H}})^2 + \lambda \|\gamma\|_{\mathcal{H}}^2$$

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Representer theorem:

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

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Solution is

$$\begin{aligned} \hat{\alpha} &= \underset{\alpha \in \mathbb{R}^d}{\operatorname{argmin}} \|y - K\alpha\|^2 + \lambda \alpha^\top K \alpha \\ &= (K + \lambda I_n)^{-1} y. \end{aligned}$$

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Prediction at new x: define $(k_{Xx})_i = k(x_i, x)$,

$$\hat{\gamma}(x) = \langle \hat{\gamma}, \varphi(x) \rangle_{\mathcal{H}} = \left\langle \sum_{i=1}^{n} \alpha_i \varphi(x_i), \varphi(x) \right\rangle_{\mathcal{H}} = \hat{\alpha}^\top k_{Xx}$$

Model fitting: ridge regression

Approximate $\gamma_0(x) := \mathbb{E}[\,Y\,|\,X = x]$ from features $\varphi(x_i)$ and y_i:

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

Kernel solution at x

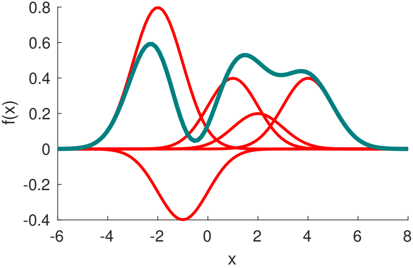
(as weighted sum of y)

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

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

$$(K_{XX})_{ij} = k(x_i, x_j) = \langle \varphi(x_i), \varphi(x_j)\rangle_{\mathcal{H}}$$

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



Observed covariates: (conditional) ATE

Kernel features (Biometrika 2023):

arXiv > econ > arXiv:2010.04855

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

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arXiv > cs > arXiv:2210.06610

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

Code for NN and kernel causal estimation with observed covariates:

`https://github.com/liyuan9988/DeepFrontBackDoor/`

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Average treatment effect

Potential outcome (intervention):

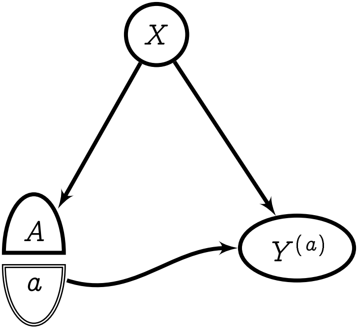
$$\mathbb{E}[Y^{(a)}] = \int \mathbb{E}[Y|a,x]\,dp(x)$$

(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

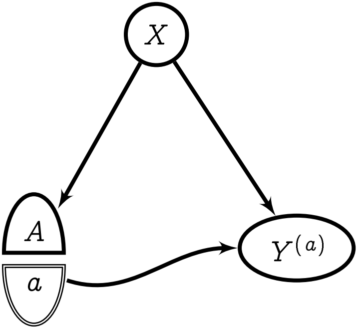
We may predict expected outcome from two inputs

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

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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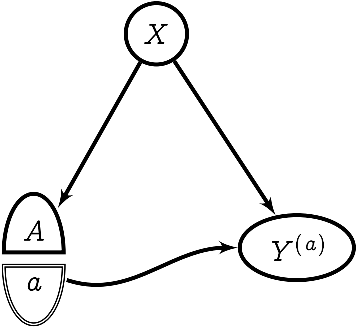

We use outer product of features ($\implies$ product of kernels):

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

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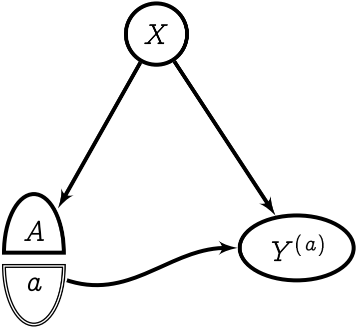

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Ridge regression solution:

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

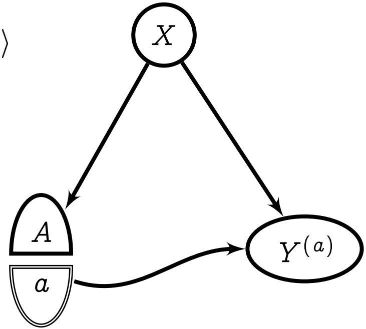
ATE (dose-response curve)

Well-specified setting:

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

ATE as feature space dot product:

$$\begin{aligned} \mathrm{ATE}(a) &= \mathbb{E}[\gamma_0(a,X)] \\ &= \mathbb{E}\left[\langle \gamma_0, \varphi(a) \otimes \varphi(X) \rangle\right] \end{aligned}$$



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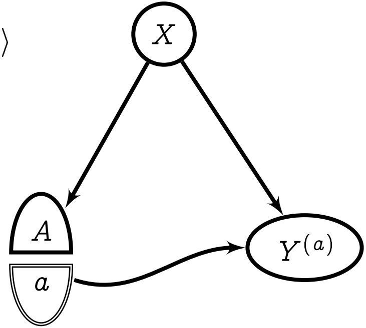


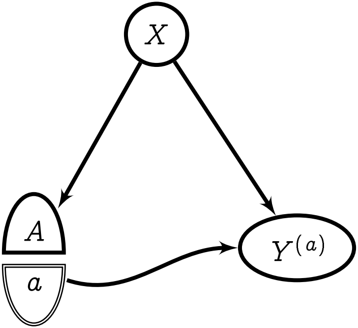
Feature map of probability $P(X)$,

$$\mu_X = [\ldots \mathbb{E}[\varphi_i(X)] \ldots]$$

ATE: example

US job corps: training for disadvantaged youths:

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



Empirical ATE:

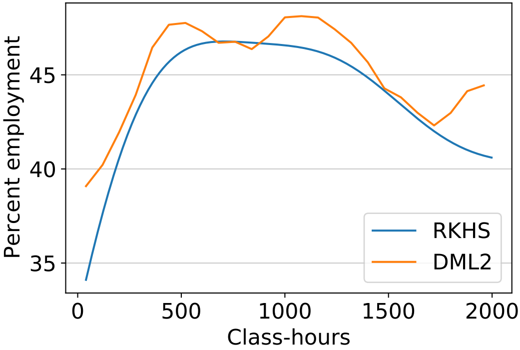
$$\widehat{\text{ATE}}(a) = \hat{\mathbb{E}}\left[\langle \hat{\gamma}_0, \varphi(X) \otimes \varphi(a)\rangle\right]$$

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

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 $\widehat{\mathrm{ATE}}(a)$.
- [DML2] Colangelo, Lee (2020), Double debiased machine learning nonparametric inference with continuous treatments.

Singh, Xu, G (2022a)

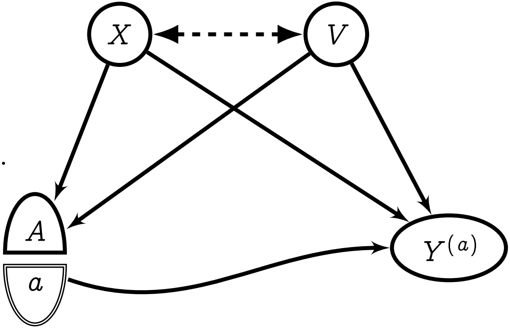
Conditional average treatment effect

Well-specified setting:

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

Conditional ATE

$$\mathrm{CATE}(a, v)$$
$$= \mathbb{E}\left[Y^{(a)} \middle| V = v \right]$$



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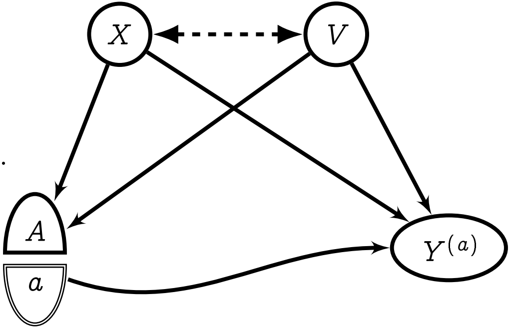

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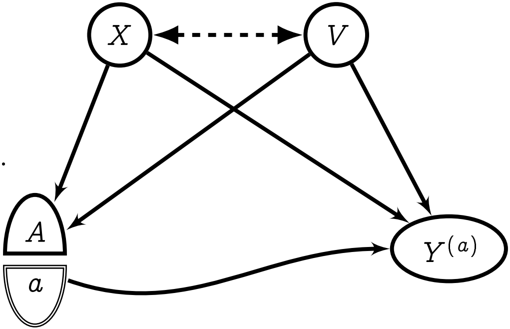

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$$= ...?$$

How to take conditional expectation?

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

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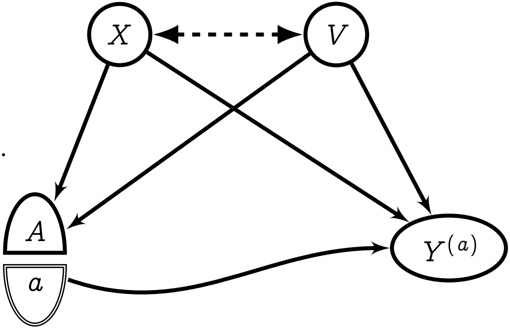

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$$= \langle \gamma_0, \varphi(a)\otimes \underbrace{\mathbb{E}[\varphi(X)|\,V=v]}_{\mu_{X|V=v}} \otimes\varphi(v)\rangle$$

Learn conditional mean embedding: $\mu_{X|V=v} := \mathbb{E}_X\left[\varphi(X)|\,V=v\right]$

Regressing from feature space to feature space

Our goal: an operator $F_0 : \mathcal{H}_{\mathcal{V}} \to \mathcal{H}_{\mathcal{X}}$ such that

$$F_0 \varphi(v) = \mu_{X|V=v}$$

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.

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

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

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Assume

$$F_0 \in \overline{\operatorname{span}\{\varphi(x) \otimes \varphi(v)\}} \iff F_0 \in \operatorname{HS}(\mathcal{H}_\mathcal{V}, \mathcal{H}_\mathcal{X})$$

Implied smoothness assumption:

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

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A Smooth Operator

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

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

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Ridge regression solution:

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

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

Consistency of conditional mean embedding

Assume problem well specified [B, 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.

[A] Li, Meunier, Mollenhauer, G (2022), Optimal Rates for Regularized Conditional Mean Embedding Learning

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

Earlier consistency proofs for finite dimensional $\varphi(x)$:

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

Caponnetto, De Vito (2007).

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Consistency [A, Theorem 2, Theorem 3]

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

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

[A] Li, Meunier, Mollenhauer, G (2022), Optimal Rates for Regularized Conditional Mean Embedding Learning

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

Earlier consistency proofs for finite dimensional $\varphi(x)$:

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

Caponnetto, De Vito (2007).

Consistency of CATE

Empirical CATE:

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

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Consistency: [A, Theorem 2]

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

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

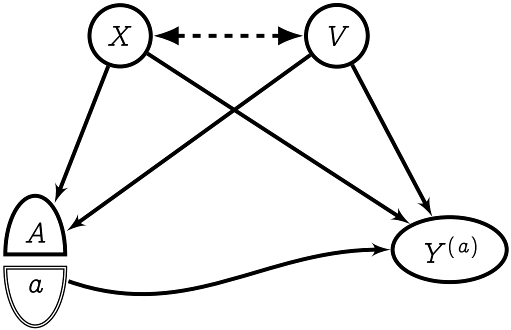
- $E_0 = G_1 \circ T_1^{\frac{c_1-1}{2}}$, $\|G_1\|_{HS}^2 \leq \zeta_1$,
- $\gamma_0 \in \mathcal{H}^c$.

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

Conditional ATE: example

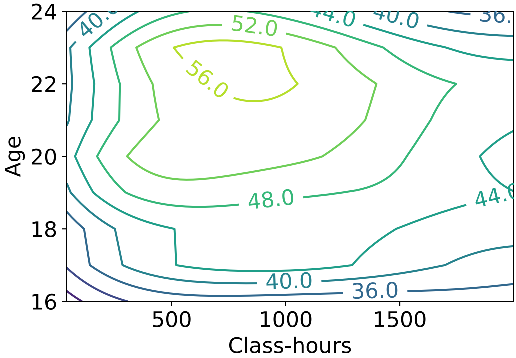
US job corps: training for disadvantaged youths:

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



Singh, Xu, G (2022a)

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)

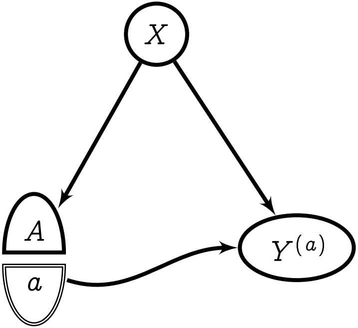
Counterfactual: average treatment on treated

Conditional mean:

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

Average treatment on treated:

$$\theta^{ATT}(a, a')$$
$$= \mathbb{E}[y^{(a')}|A = a]$$



Empirical ATT:

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

Counterfactual: average treatment on treated

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

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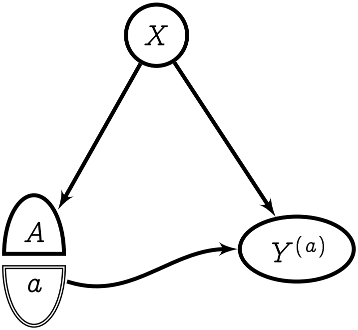

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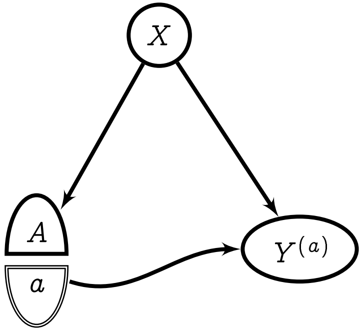
Average treatment on treated:

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



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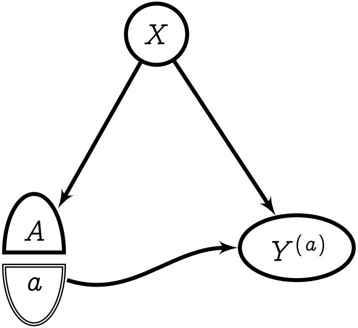

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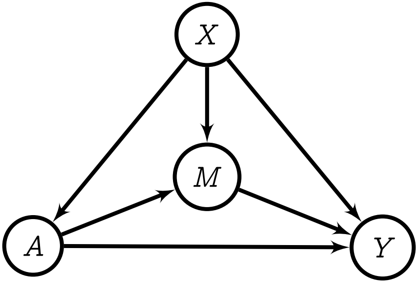
\end{aligned}$$

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?

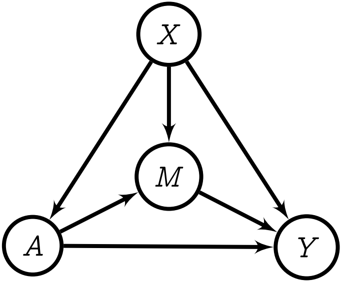


Mediation analysis: example

US job corps: training for disadvantaged youths:

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

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



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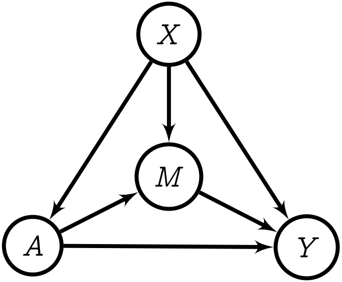

$\gamma_0(a, m, x) \approx \mathbb{E}[Y | A = a, M = m, X = x]$

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

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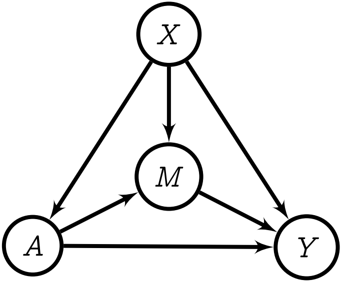

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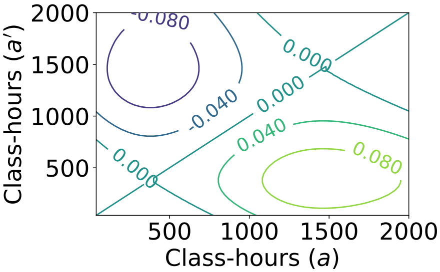
Singh, Xu, G (2022b). Kernel Methods for Multistage Causal Inference: Mediation Analysis and Dynamic Treatment Effects.

Mediation analysis: results

Total effect:

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

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



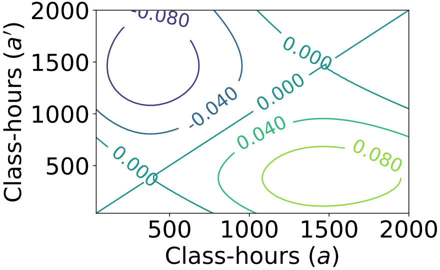
- $a' = 1600$ hours vs $a = 480$ means 0.1 reduction in arrests

Singh, Xu, G (2022b)

Mediation analysis: results

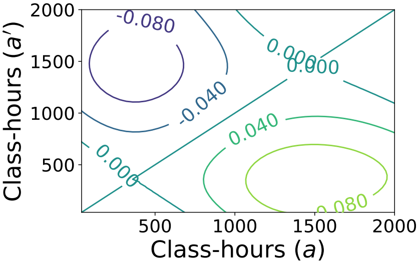
Total effect:

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



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

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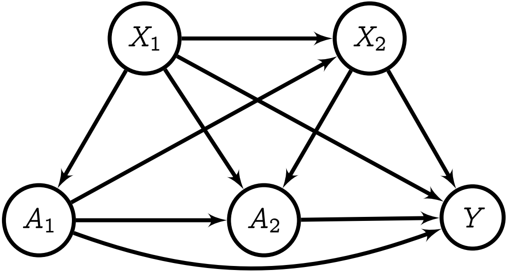
...dynamic treatment effect...

Dynamic treatment effect: sequence A_1, A_2 of treatments.



- potential outcomes $Y^{(a_1)}, Y^{(a_2)}, Y^{(a_1,a_2)}$,
- counterfactuals $\mathbb{E}\left[Y^{(a_1',a_2')} | A_1 = a_1, A_2 = a_2\right]$...

(c.f. the Robins G-formula)

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

Conclusions

Kernel and neural net solutions:

- ...for ATE, CATE, dynamic treatment effects
- ...with treatment A, covariates X, V, proxies (W, Z) multivariate, "complicated"
- Convergence guarantees for kernels and NN

Next lecture:

- Unobserved covariates/confounders (IV and proxy methods)

Code available for all methods

Research support

Work supported by:

The Gatsby Charitable Foundation

Google Deepmind

Questions?


THE KERNEL
BREWERY
LONDON
BALTIC PORTER
THE KERNEL
EXPORT STOUT