Causal Effect Estimation with Context and Confounders (Pt. 1)

Arthur Gretton

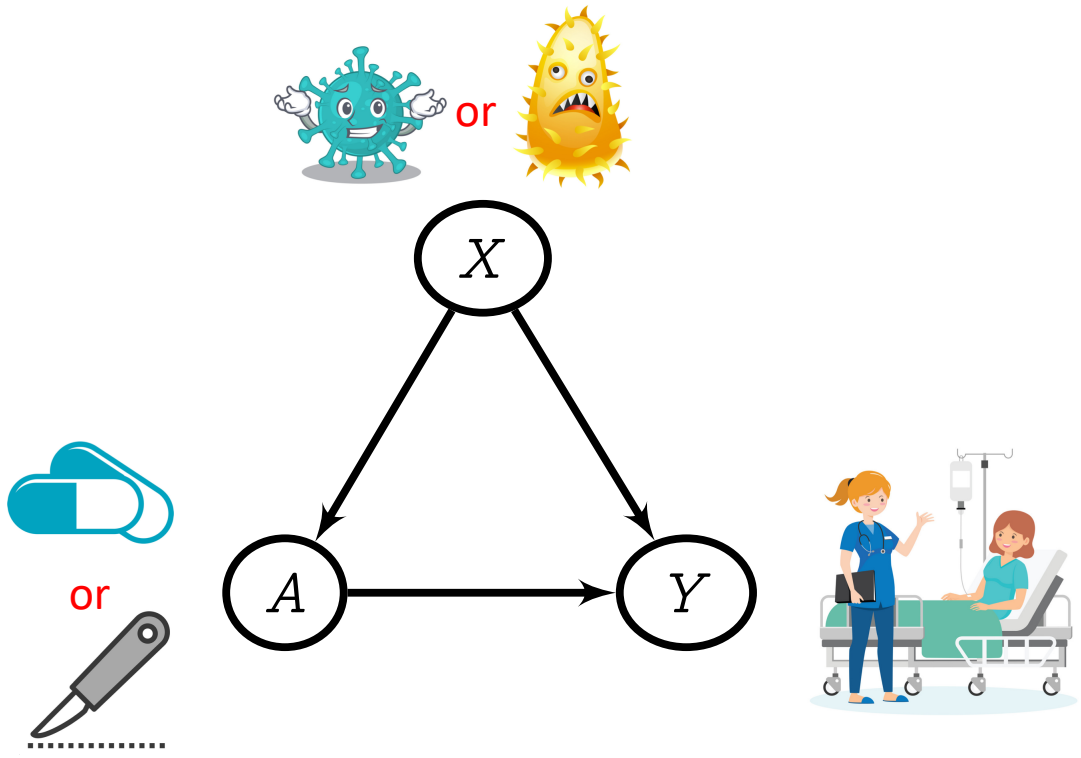
Gatsby Computational Neuroscience Unit,
Google DeepMind

MLSS, Tübingen 2026

MLSS 2003 Tübingen

Observation vs intervention

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

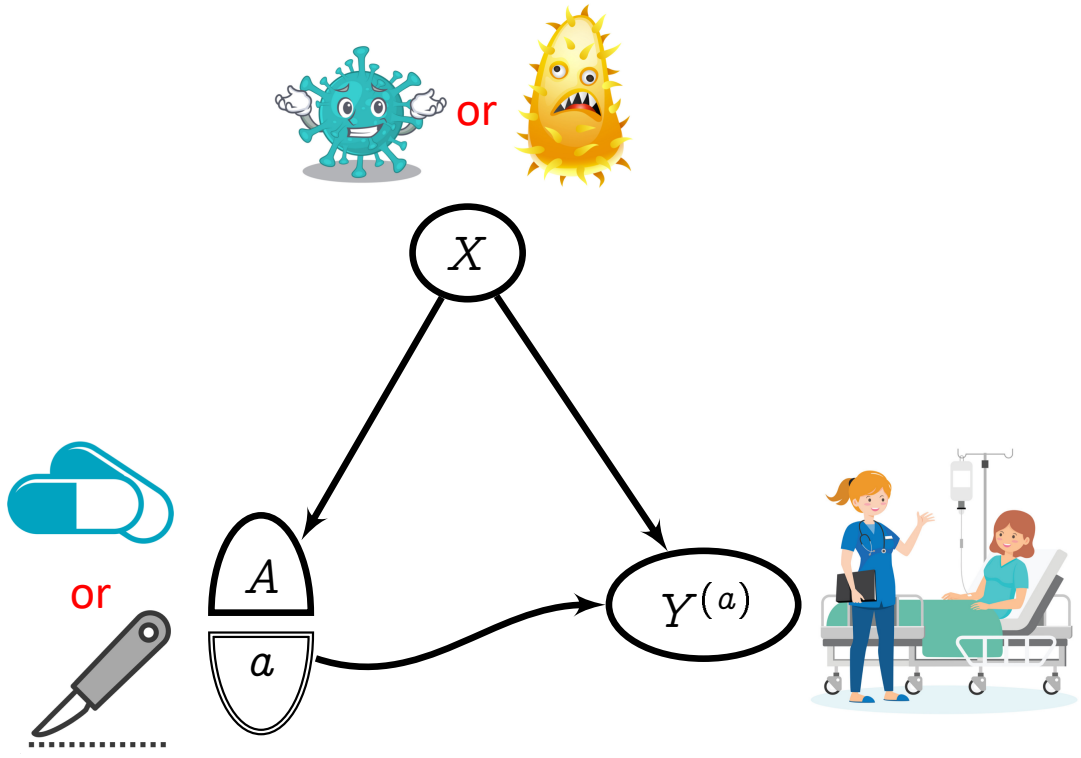


From our observations of historical hospital data:

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

Observation vs intervention

Dose-response curve (intervention): $\mathbb{E}[Y^{(a)}] = \sum_x \mathbb{E}[Y|a,x]p(x)$

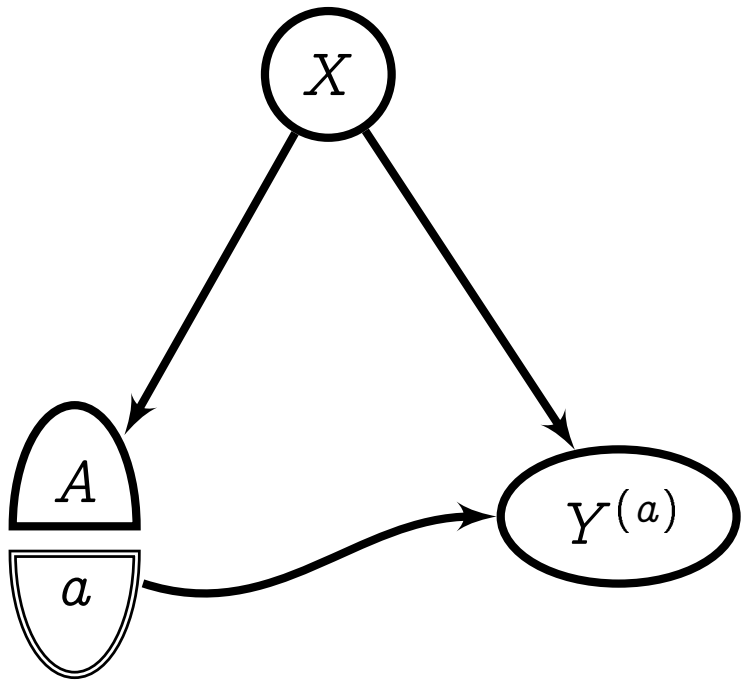


From our intervention (making all patients take a treatment):

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

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:

- Dose-response curve (DR), heterogeneous response curve (HR), 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:

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

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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.

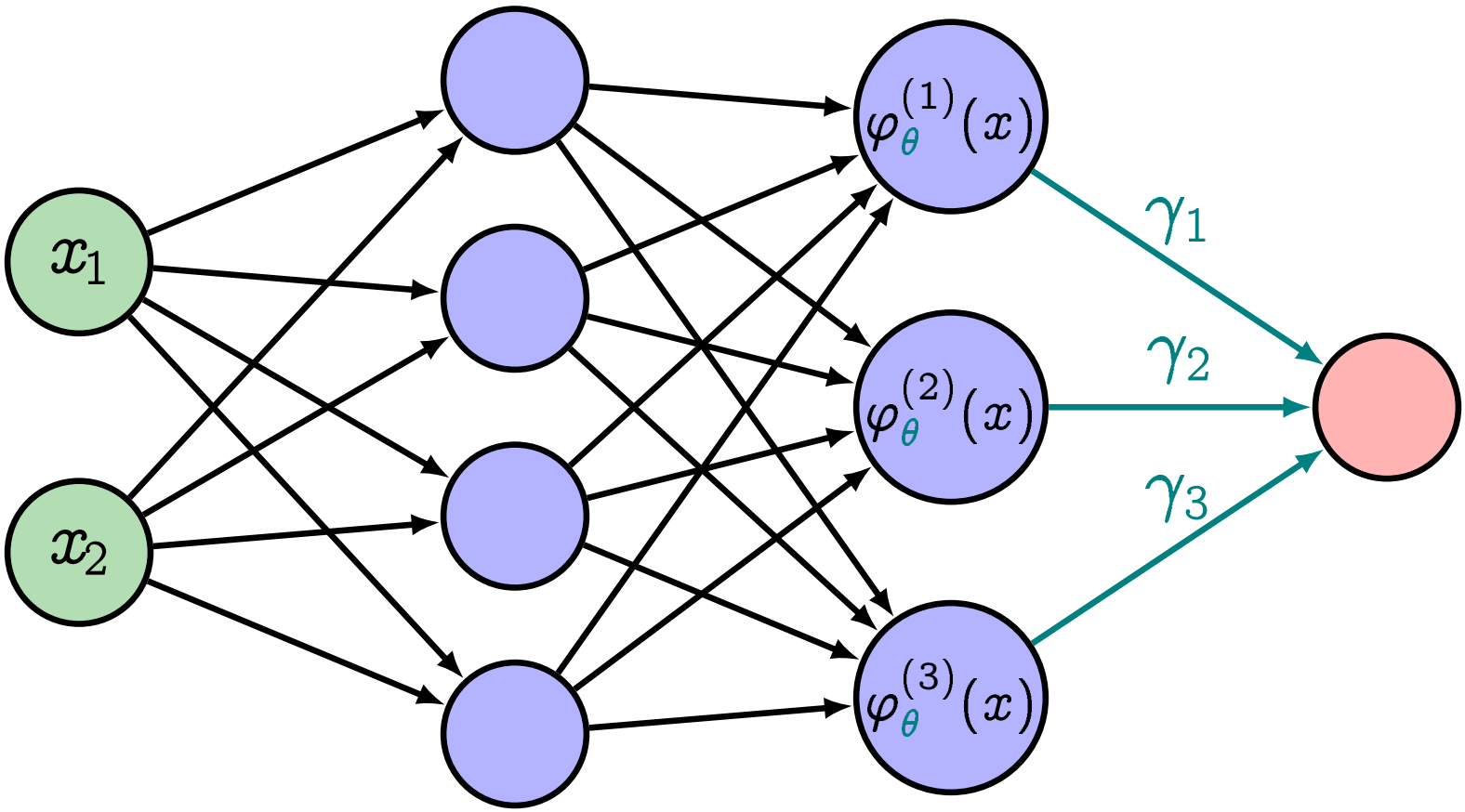
Singh, Xu, G. Kernel Methods for Causal Functions: Dose, Heterogeneous, and Incremental Response Curves. (Biometrika 23)

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

Model fitting: neural ridge regression

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

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



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Solution for linear final layer γ:

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

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

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

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How to solve for θ:

Substitute $\hat{\gamma}_\theta$ into (1), backprop for remaining θ.

More details: Galashov, Da Costa, Xu, Hennig, G, Closed-Form Last Layer Optimization (2025, arxiv:2510.04606)

Model fitting: kernel ridge regression

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

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

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Infinite dimensional solution at x:

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

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

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

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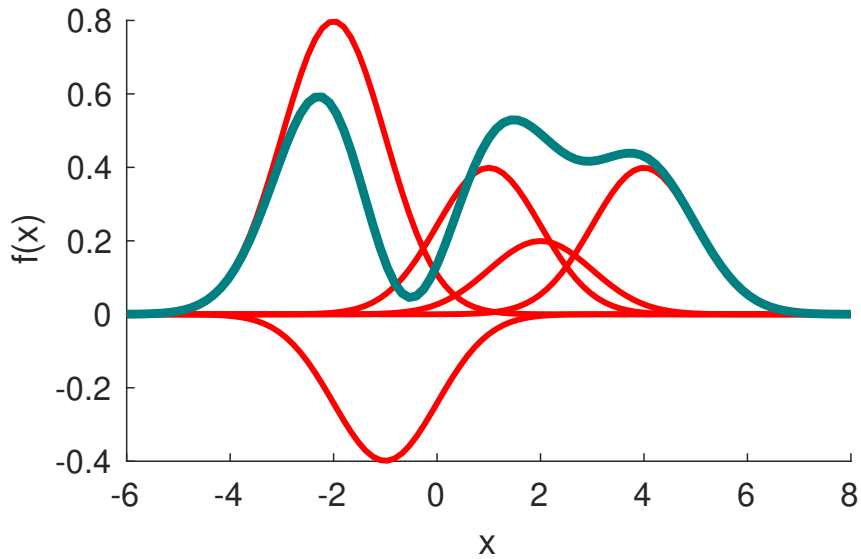
Kernel solution at x
(as weighted sum of y)

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

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

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

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



Causal effects, observed covariates

Kernels (Biometrika 2023):

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

NN features (ICLR 2023):

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

Computer Science > Machine Learning

[Submitted on 12 Oct 2022]

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

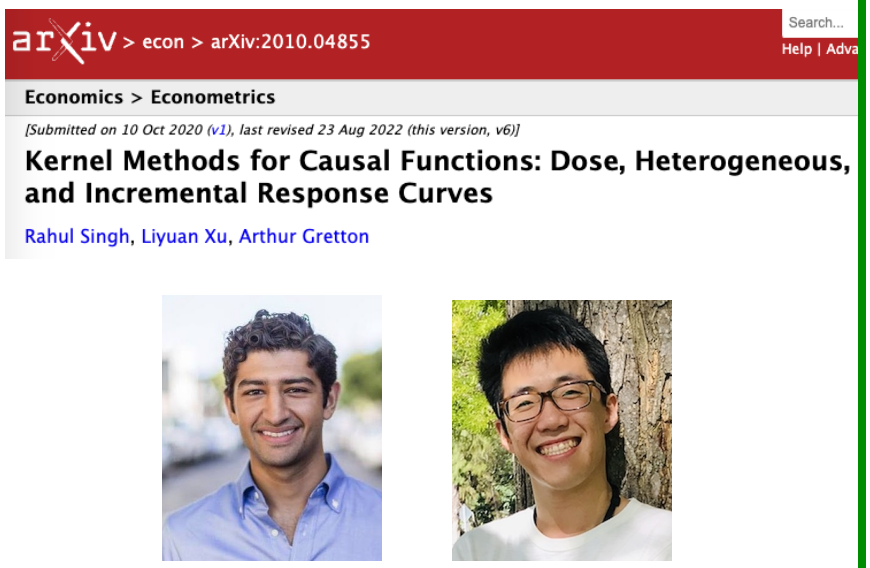
Liyuan Xu, Arthur Gretton

Code for NN and kernel causal estimation with observed covariates:

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

Causal effects, observed covariates

Kernel features (Biometrika 2023):



NN features (ICLR 2023):

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Dose-response curve

Potential outcome (intervention):

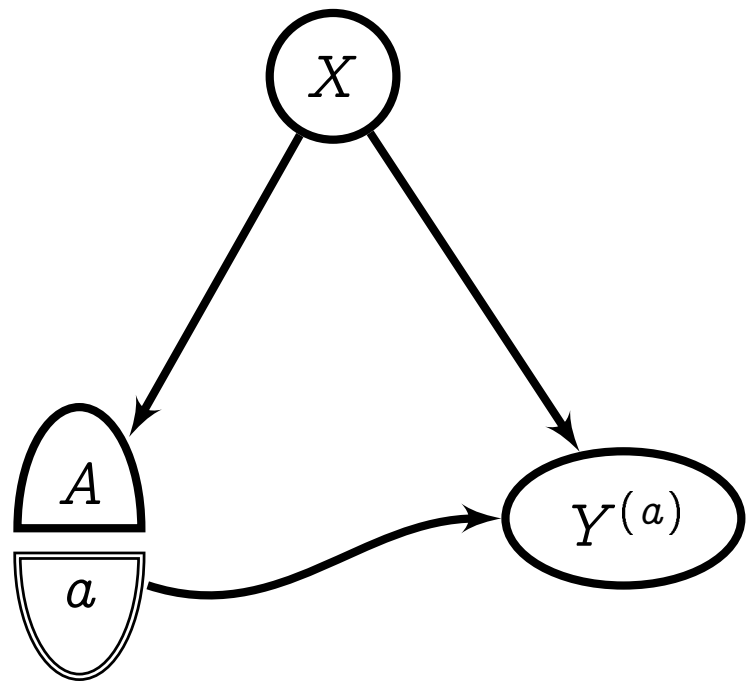
$$\mathrm{DR}(a) := \mathbb{E}[Y^{(a)}] = \int \mathbb{E}[Y|a,x]\,dp(x)$$

(the average structural function; 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:

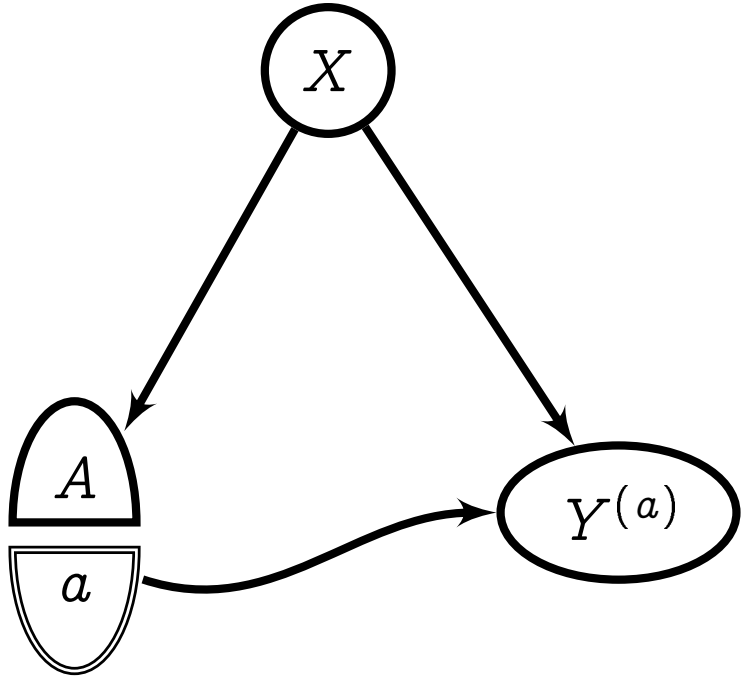
- A: treatment (training hours)
- Y: outcome (percentage employment)
- X: covariates (age, education, marital status, ...)



Multiple inputs via products of kernels

The expected output is a function of two arguments

$$\begin{aligned}
&\mathbb{E}[\,Y \,|\, a, x] \\
&= \gamma^\top [\varphi(a) \otimes \varphi(x)] \\
&= \gamma^\top \begin{bmatrix} \varphi_1(a)\varphi_1(x) \\ \varphi_1(a)\varphi_2(x) \\ \vdots \\ \varphi_2(a)\varphi_1(x) \\ \vdots \end{bmatrix}
\end{aligned}$$



(argument of kernel/feature map indicates feature space)

Multiple inputs via products of kernels

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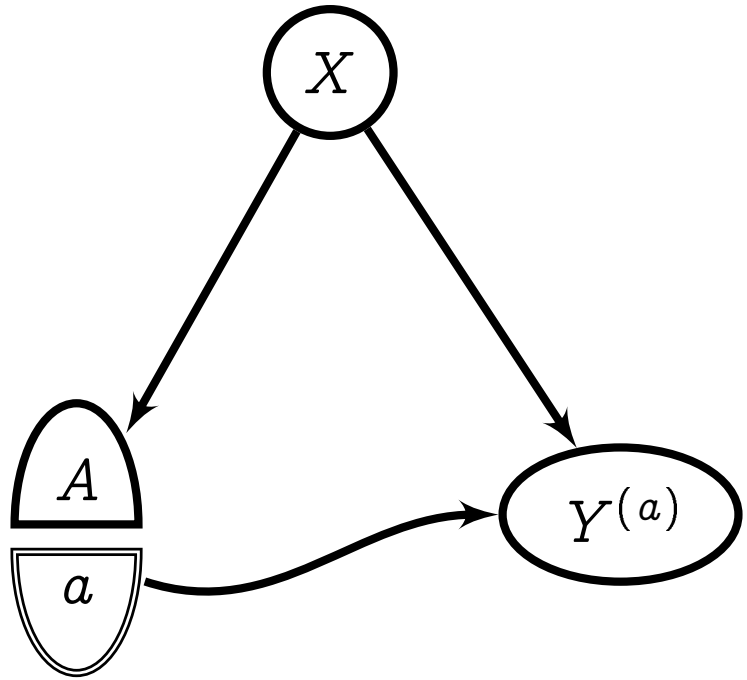
$$\mathbb{E}[Y|a,x] = \gamma^\top [\varphi(a) \otimes \varphi(x)] = \gamma^\top \begin{bmatrix} \varphi_1(a)\varphi_1(x) \\ \varphi_1(a)\varphi_2(x) \\ \vdots \\ \varphi_2(a)\varphi_1(x) \\ \vdots \end{bmatrix}$$



(argument of kernel/feature map indicates feature space)

Ridge regression solution:

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

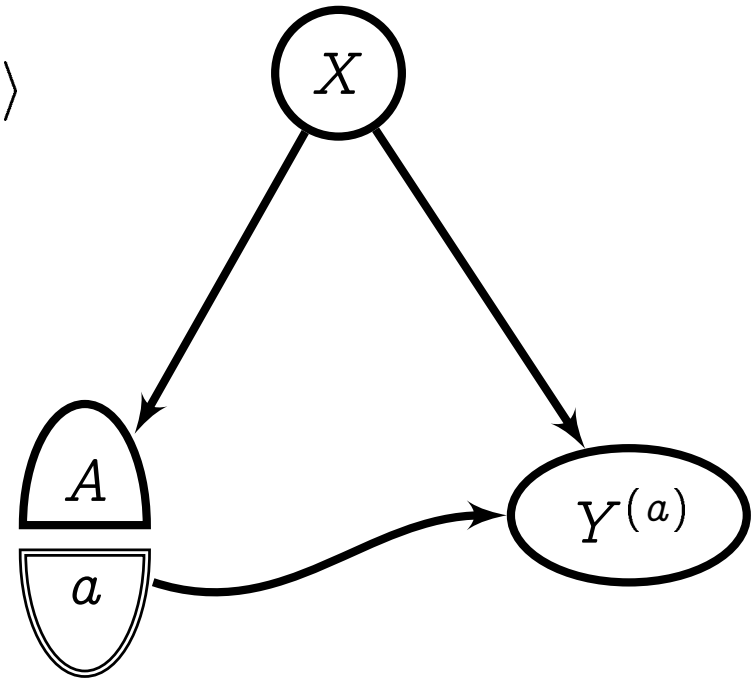
Dose-response curve

Well-specified setting:

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

DR as feature space dot product:

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



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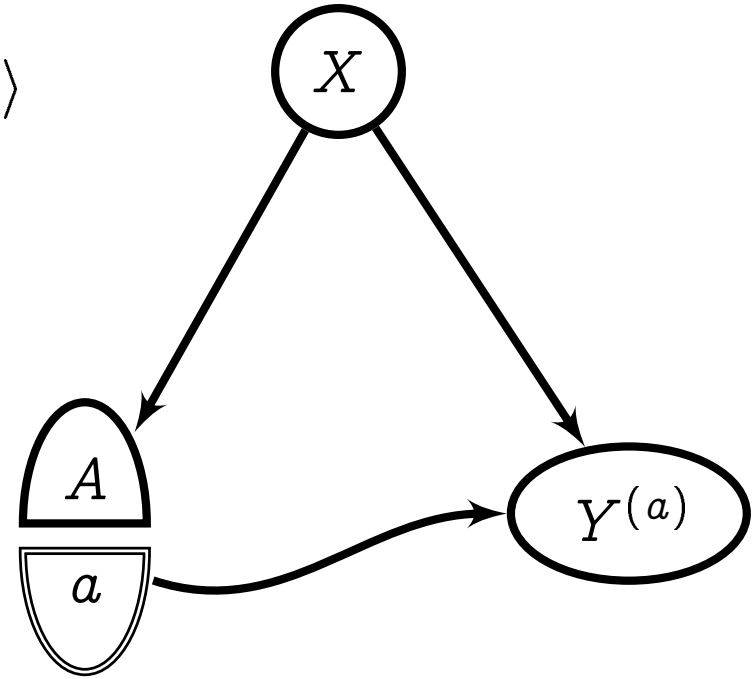


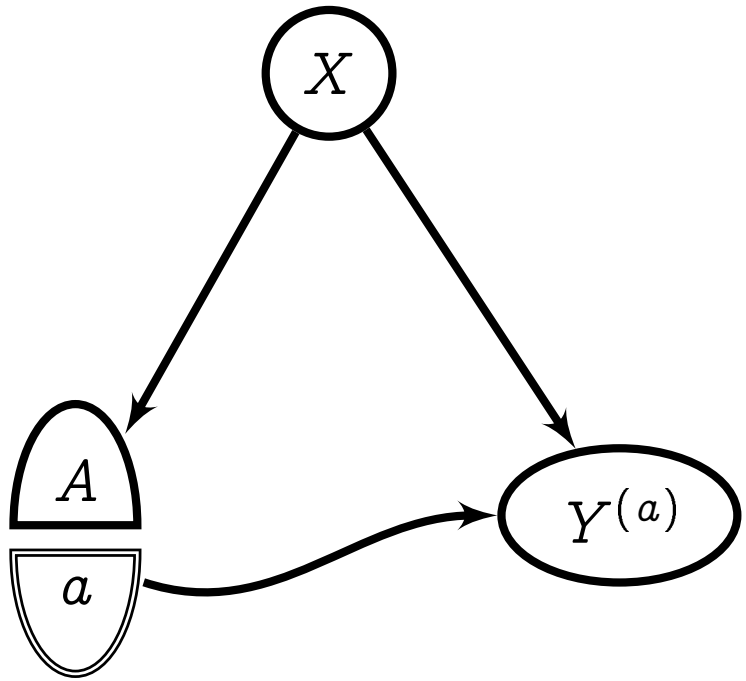
Feature map of probability $P(X)$,

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

DR: example

US job corps: training for disadvantaged youths:

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



Empirical DR:

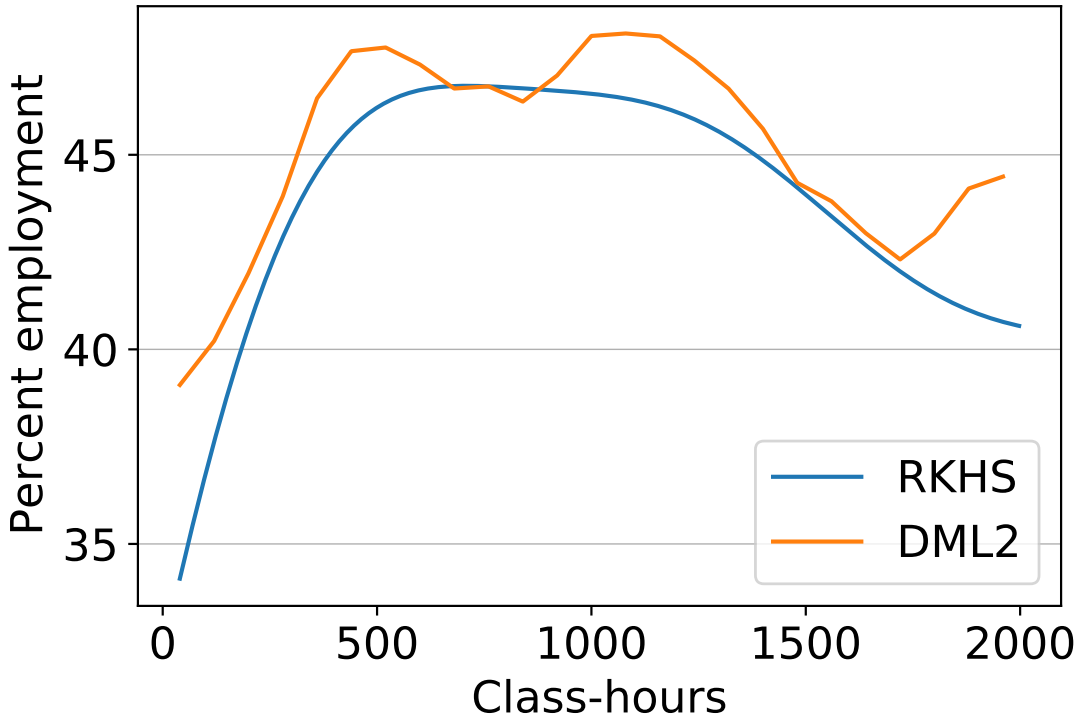
$$\widehat{\mathrm{DR}}(a) = \widehat{\mathbb{E}}\left[\langle \hat{\gamma}_0, \varphi(X) \otimes \varphi(a) \rangle\right]$$

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

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

Singh, Xu, G (2023).

DR: results



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

Singh, Xu, G (2023)

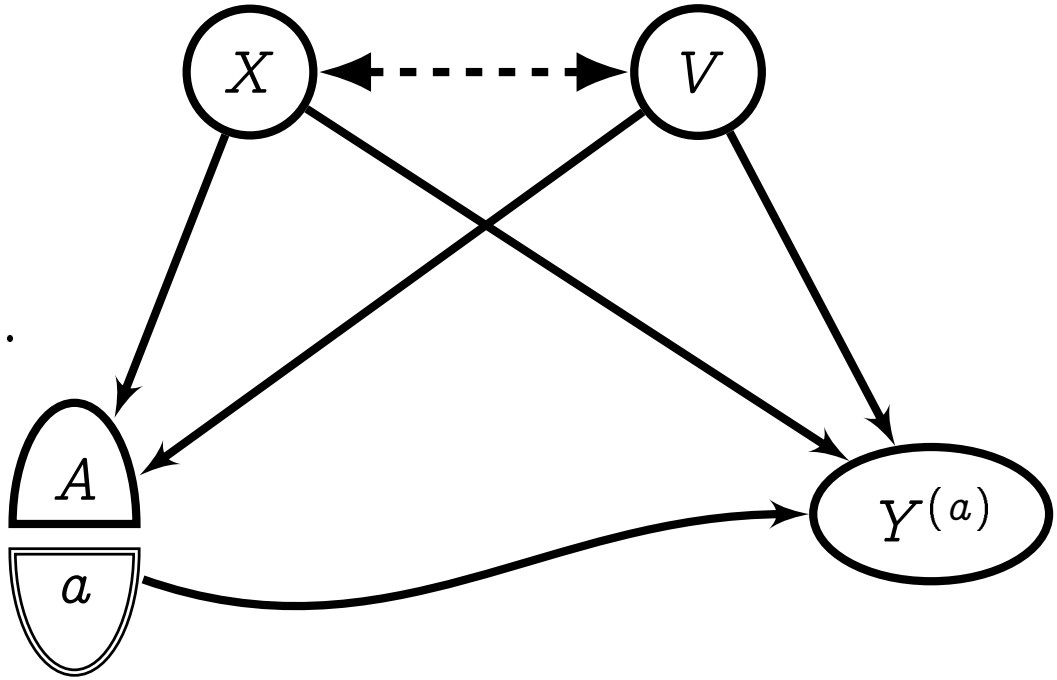
Heterogeneous response curve

Well-specified setting:

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

Heterogeneous response:

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



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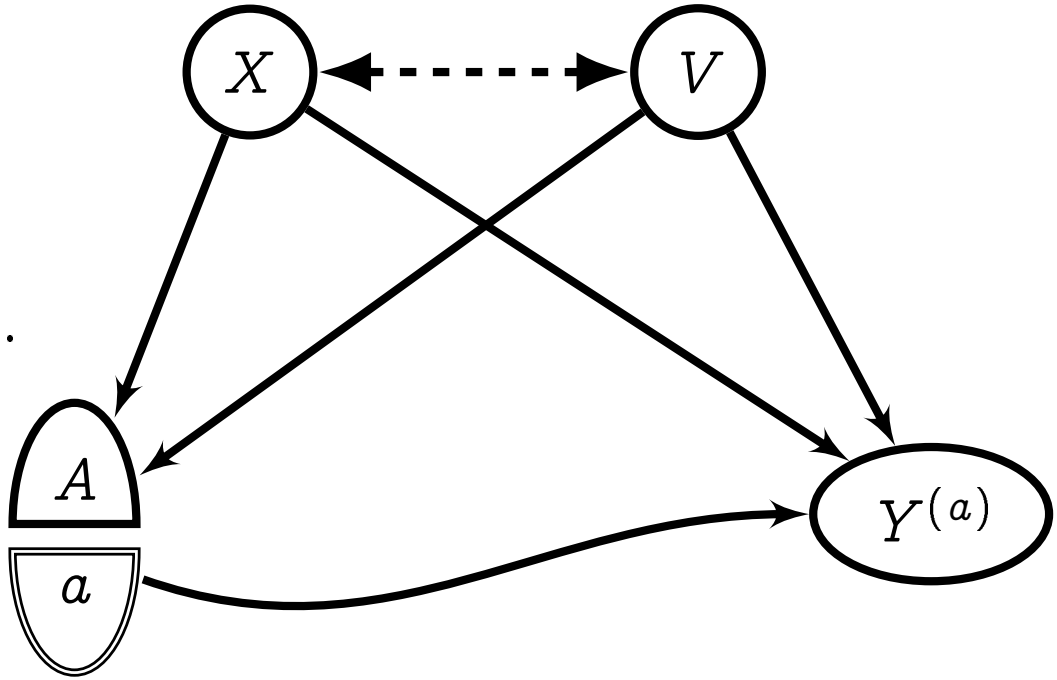

Heterogeneous response:

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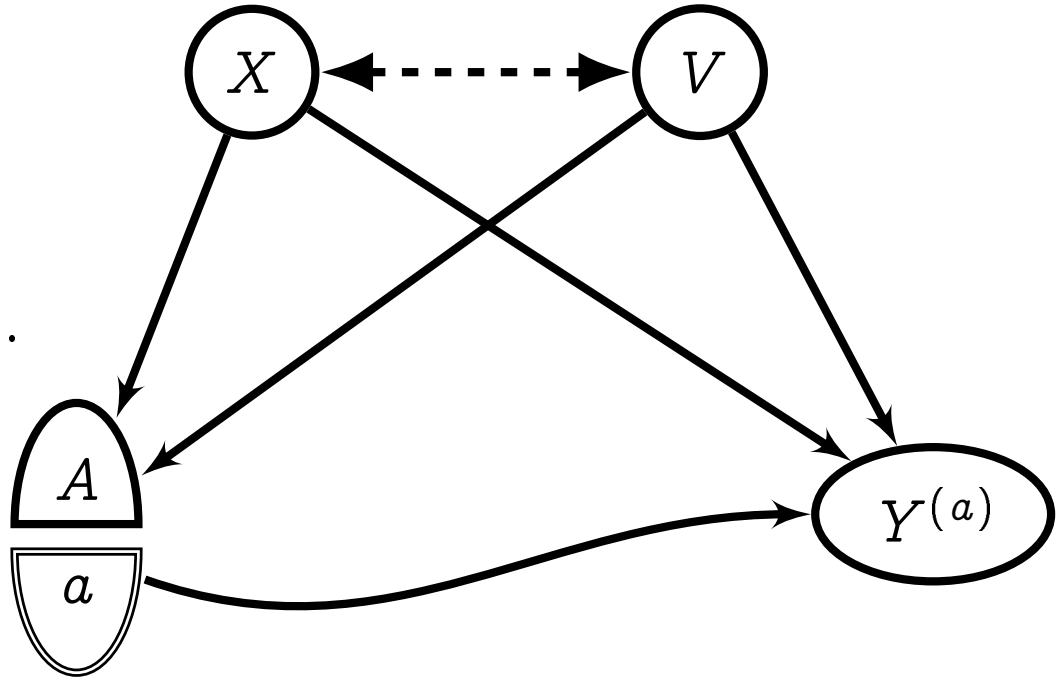

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$$= \ldots ?$$

How to take conditional expectation?

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

Heterogeneous response curve

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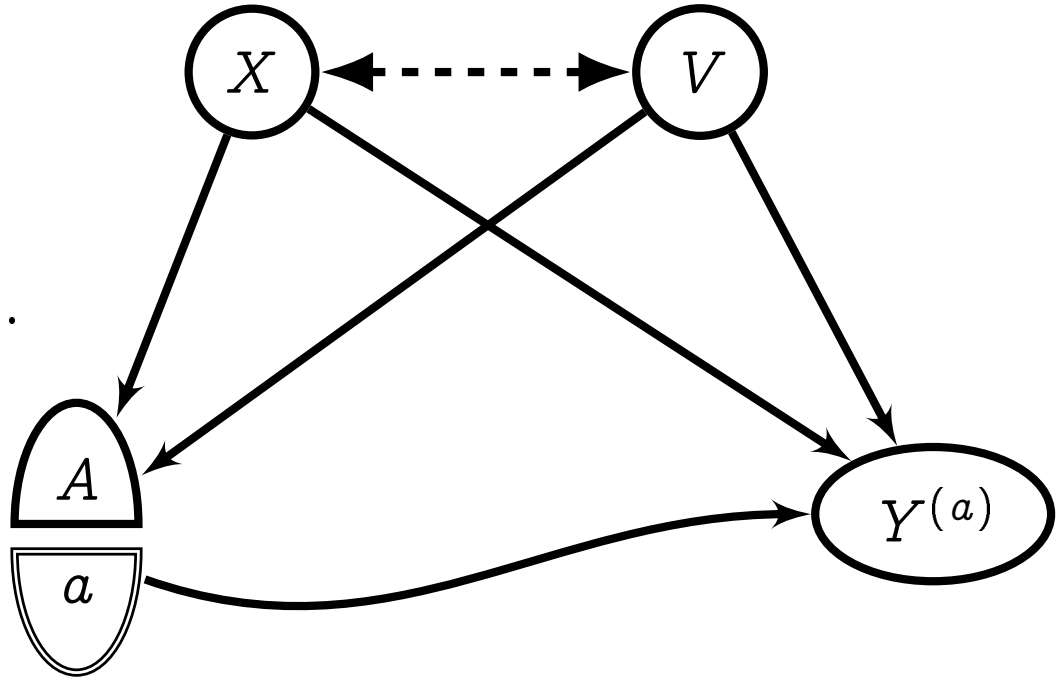

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$$= \mathbb{E}\left[\langle \gamma_0, \varphi(a) \otimes \varphi(X) \otimes \varphi(V) \rangle | V = v\right]$$
$$= \langle \gamma_0, \varphi(a) \otimes \underbrace{\mathbb{E}[\varphi(X)|V=v]}_{\mu_{X|V=v}} \otimes \varphi(v) \rangle$$

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

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

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

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 $\varphi(x)$:

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

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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 feature mean

Define C_V as covariance of features $\varphi(v)$

$$C_V = \mathbb{E}(\varphi(V) \otimes \varphi(V)), \qquad \mathbb{E}_V(f(V)g(V)) = \langle f, C_V g \rangle_{\mathcal{H}_\mathcal{V}}$$

$$C_V = \sum_{i=1}^{\infty} \eta_i \left(\sqrt{\eta_i} e_i\right) \otimes \left(\sqrt{\eta_i} e_i\right)$$

$\eta_i e_i(v) = \int k(v, v') e_i(v') dP_V(v'),$ assume for simplicity: $\text{supp}(P_V) = \mathcal{V}$

[A] Li, Meunier, Mollenhauer, G (2022), Optimal Rates for Regularized CME Learning
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Consistency of conditional feature mean

Define C_V as covariance of features $\varphi(v)$

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$$F_* \in S_2(\mathcal{H}_\mathcal{V}^{c_1}, \mathcal{H}_\mathcal{X}), \quad c_1 \in (1, 2]$$

larger $c_1 \implies$ smoother $F_* \implies$ easier problem.

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- Eigenspectrum of C_V decays as $\eta_j(C_V) \sim j^{-b_1}$, $b_1 \geq 1$.

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Heterogeneous Response from Samples

Consistency [A, Theorem 2, Theorem 3] (minimax)

$$\left\| \widehat{F} - F_* \right\|_{\mathrm{HS}}^2 = O_P\left(n^{-\frac{c_1 - 1}{c_1 + 1/b_1}} \right).$$

[A] Singh, Xu, G. (2023)

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Follows from consistency of $\widehat{F}$ and $\hat{\gamma}$

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Follows from consistency of $\widehat{F}$ and $\hat{\gamma}$

Empirical HR:

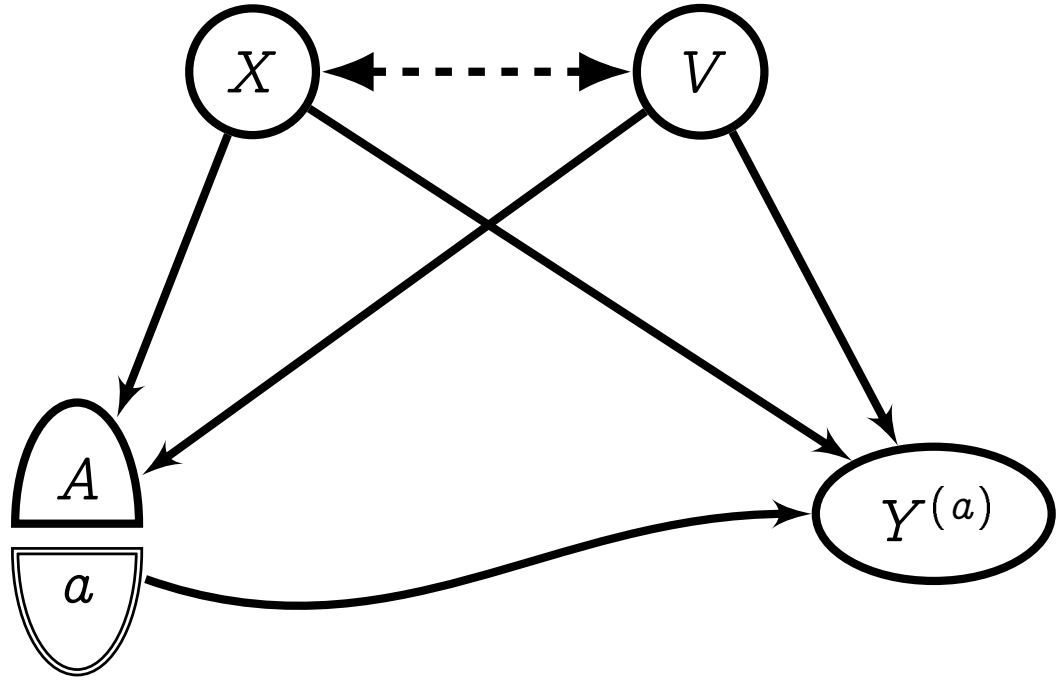
$$\widehat{\text{HR}}(a, v)$$
$$= Y^\top (K_{AA} \odot K_{XX} \odot K_{VV} + n\lambda I)^{-1} (K_{Aa} \odot \underbrace{K_{XX}(K_{VV} + n\lambda_1 I)^{-1} K_{Vv}}_{\text{from } \hat{\mu}_{X \mid V = v}} \odot K_{Vv})$$

[A] Singh, Xu, G. (2023)

Heterogeneous response: example

US job corps:

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

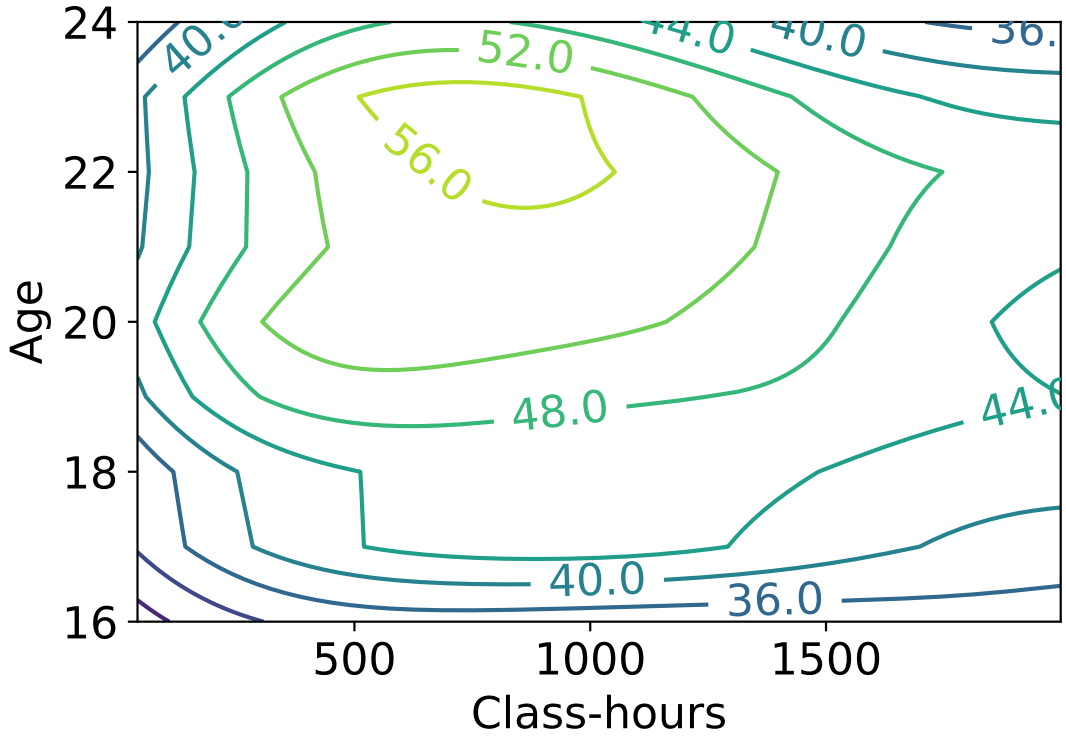


Empirical HR:

$$\widehat{\mathrm{HR}}(a, v) = \langle \hat{\gamma}_0, \varphi(a) \otimes \underbrace{\hat{F}\varphi(v)}_{\widehat{\mathbb{E}}[\varphi(X)\,|\,V=v]} \otimes \varphi(v) \rangle$$

Singh, Xu, G (2023)

Heterogeneous response: 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)

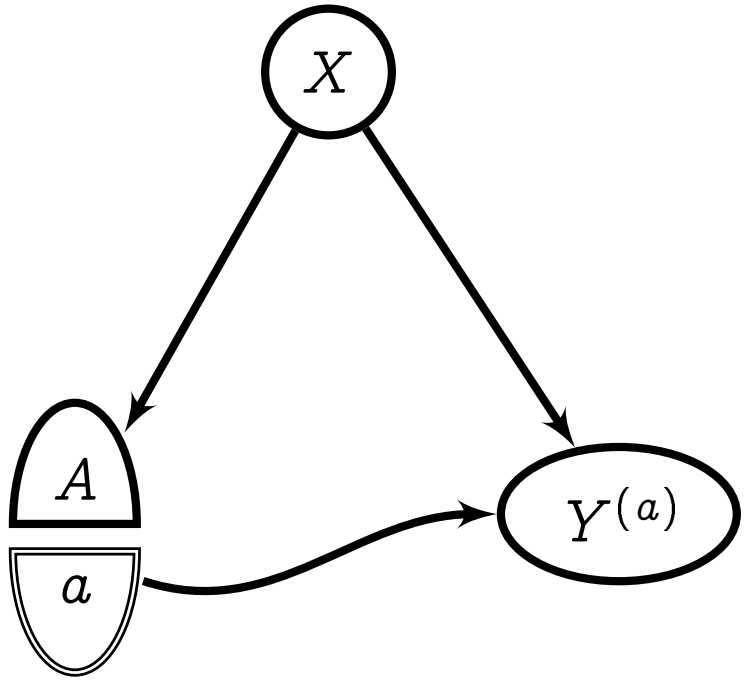
Counterfactual: average treatment on treated

Conditional mean:

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

Average treatment on treated:

$$\begin{aligned}&\mathrm{ATT}(a, a')\\ &= \mathbb{E}[y^{(a')}|A = a]\end{aligned}$$



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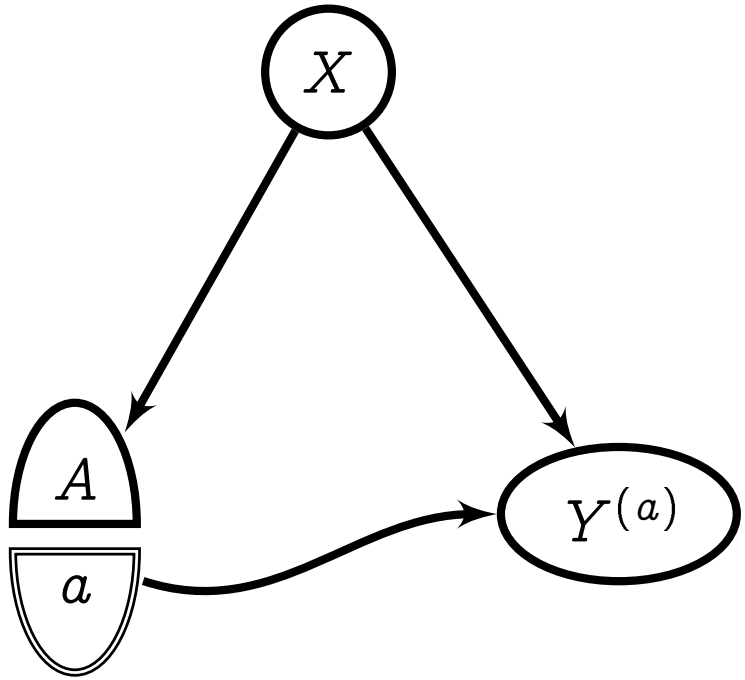

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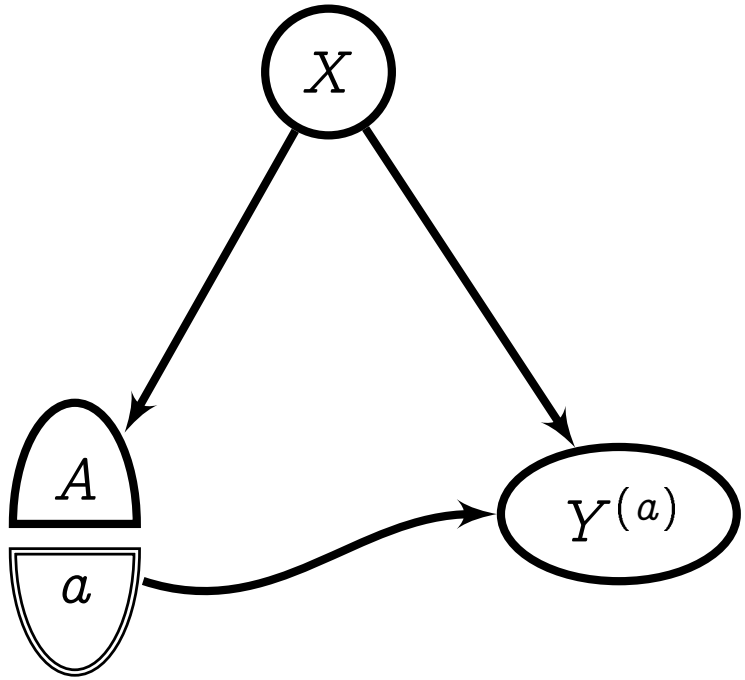

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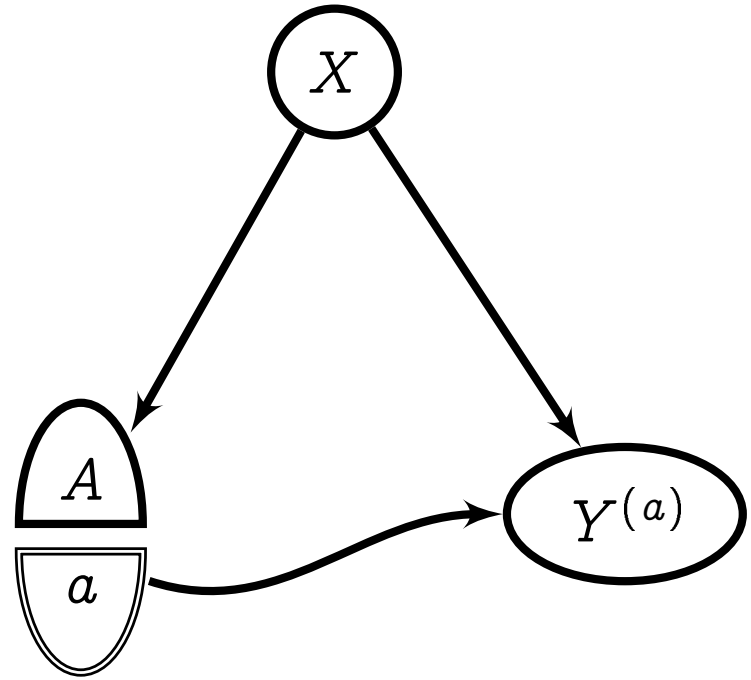

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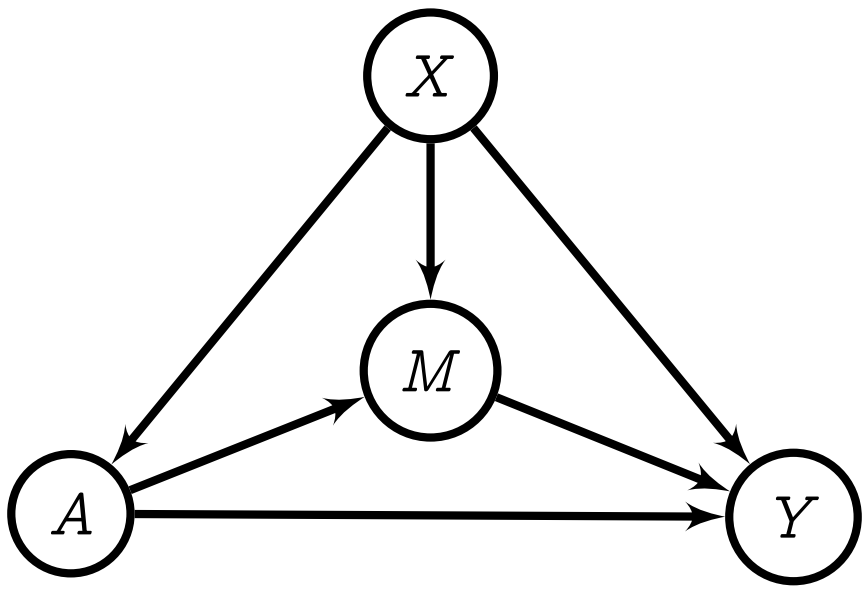
Mediation analysis

- 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, ...)
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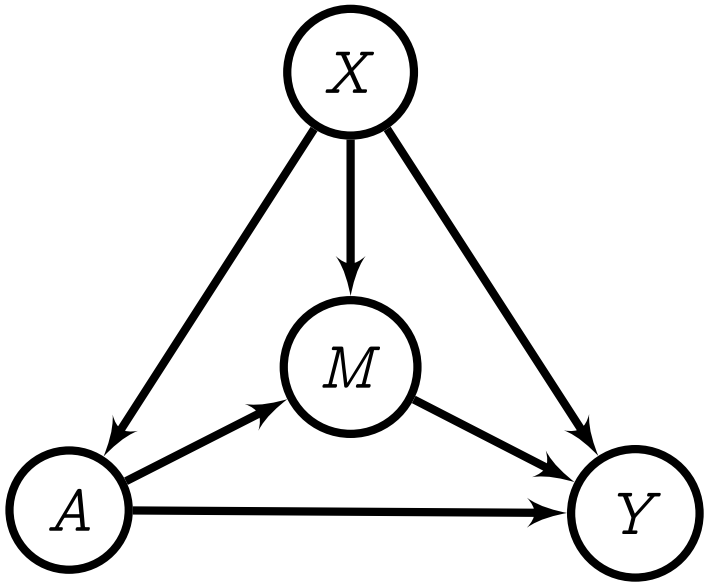

$\gamma_0(a, m, x) \approx \mathbb{E}[Y|A = a, M = m, X = x]$

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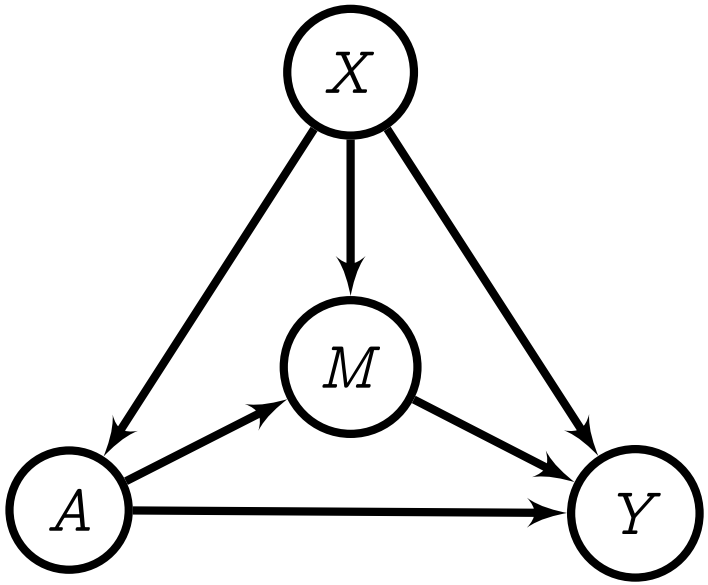

$$\gamma_0(a, m, x) \approx \mathbb{E}[Y|A = a, M = m, X = x]$$

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

Singh, Xu, G (2025). Kernel Methods for Multistage Causal Inference: Mediation Analysis and Dynamic Treatment Effects.

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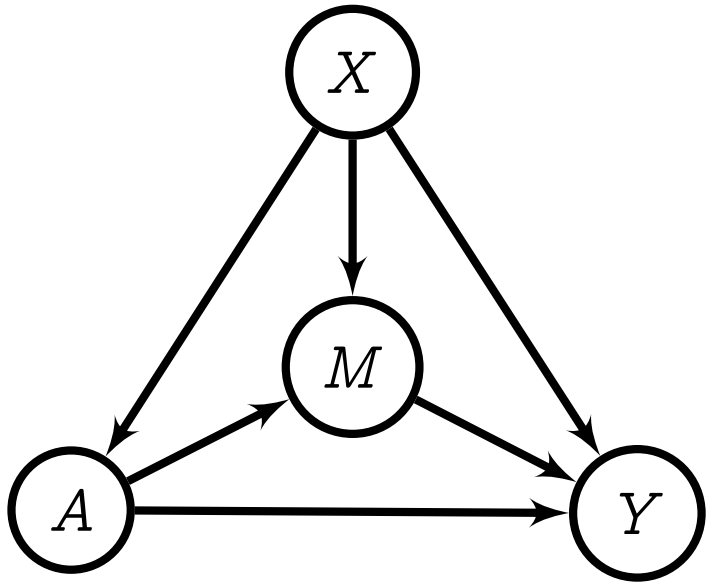

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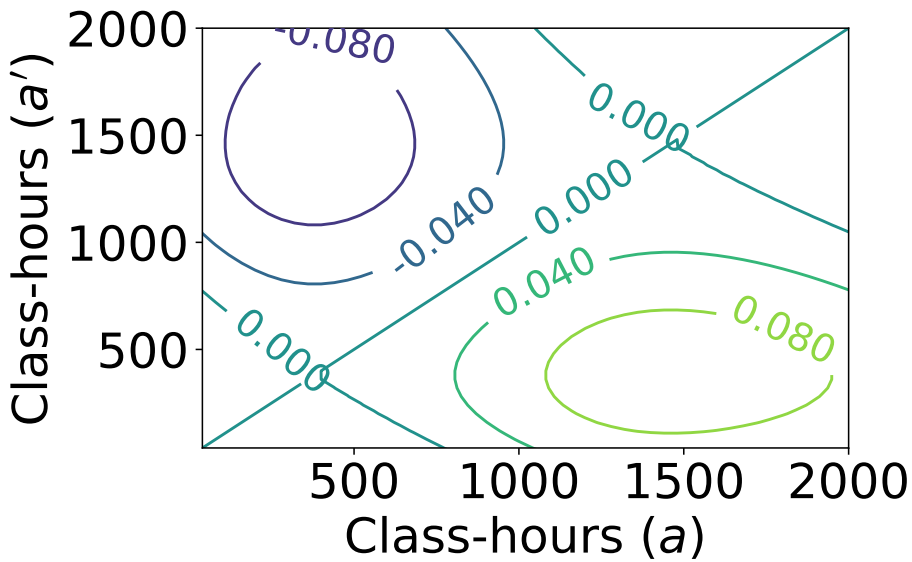
Mediation analysis: results

Total effect:

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



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

Singh, Xu, G (2025)

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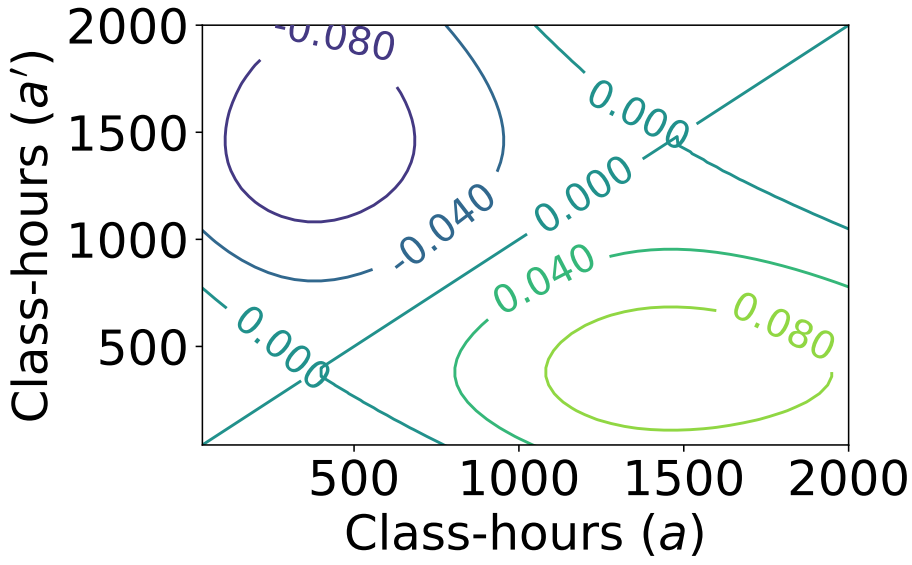
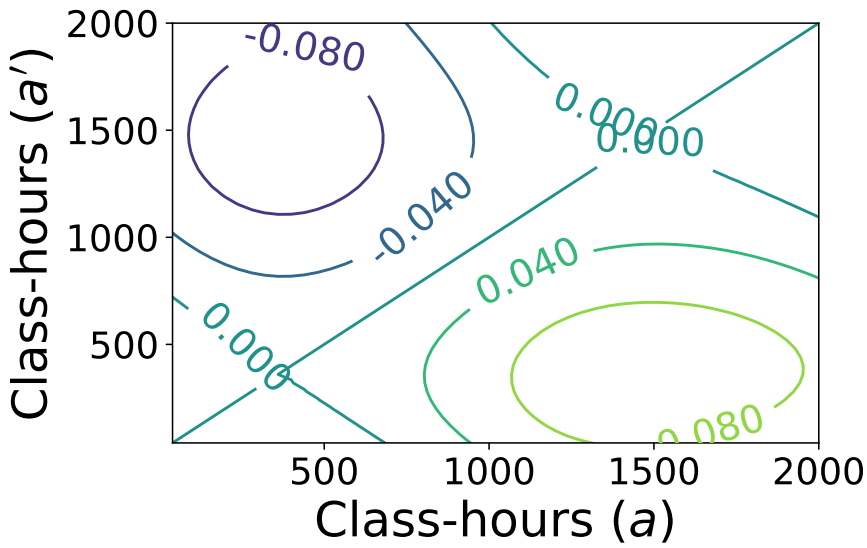


Direct effect:

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

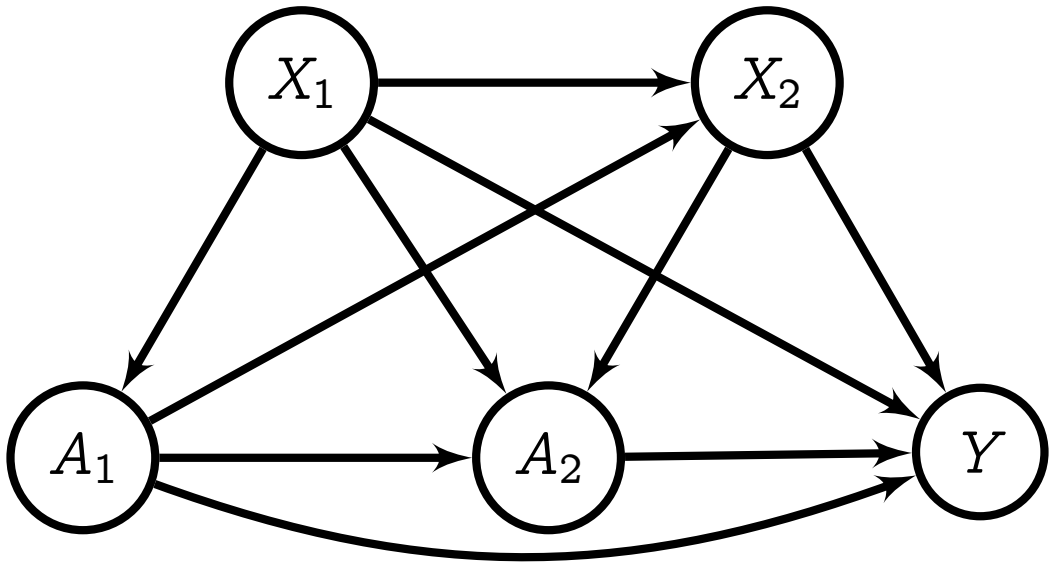


- $a' = 1600$ hours vs $a = 480$ means 0.1 reduction in arrests
- Indirect effect mediated via employment effectively zero

Singh, Xu, G (2025)

...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. (2025)

Conclusions

Kernel and neural net solutions:

- ...for dose-resoponse, heterogeneous response, dynamic treatment effects
- ...with treatment A, covariates X, V, 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

Google DeepMind

Questions?


THE KERNEL
BREWERY
LONDON
BALTIC PORTER
7.3% ABV
THE KERNEL
EXPORT STOUT