# Doubly Robust Inference on Causal Derivative Effects for Continuous Treatments

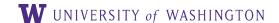
## Yikun Zhang

Joint work with Professor Yen-Chi Chen

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ENAR 2025 Spring Meeting March 25, 2025





#### The Role of Derivatives in Causal Inference

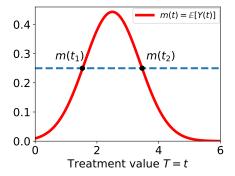
**Goal:** Study the causal effect of a treatment  $T \in \mathcal{T}$  on an outcome of interest  $Y \in \mathcal{Y}$ .

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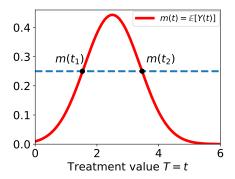
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- While  $m(t_1) = m(t_2)$ , the derivative effects  $m'(t_1)$ ,  $m'(t_2)$  are distinct!
- The **derivative effect curve**  $\theta(t) = m'(t) = \frac{d}{dt}\mathbb{E}[Y(t)]$  is a continuous generalization to the average treatment effect  $\mathbb{E}[Y(1)] \mathbb{E}[Y(0)]$ .

Our causal estimand of interest is the derivative effect curve

$$t\mapsto \theta(t)=m'(t)=rac{d}{dt}\mathbb{E}\left[Y(t)
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There are some closely related but distinct estimands:

• Incremental Causal/Treatment Effect (Kennedy, 2019; Rothenhäusler and Yu, 2019):

$$\mathbb{E}[Y(T+\delta)] - \mathbb{E}[Y(T)]$$
 for some deterministic  $\delta > 0$ .

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Average Derivative/Partial Effect (Powell et al., 1989; Newey and Stoker, 1993):

$$\mathbb{E}\left[\theta(T)\right] = \mathbb{E}\left[\frac{\partial}{\partial t}\mathbb{E}\left(Y|T,S\right)\right], \text{ where } S \in \mathcal{S} \subset \mathbb{R}^d \text{ is a covariate vector.}$$

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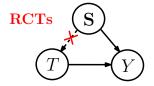
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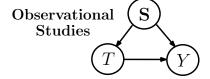
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Pros These estimands may have more realistic interpretations in the actual context.

Cons They quantify only the overall causal effects, not those at a specific level of interest.

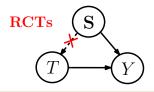
#### Identification Assumptions with Observational Data

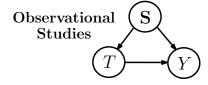




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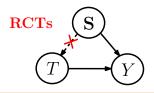


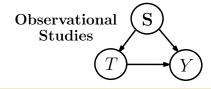
#### Assumption (Identification Conditions)

- **()** (Consistency) Y = Y(t) whenever  $T = t \in \mathcal{T}$ .
- ② (Ignorability) Y(t) is conditionally independent of T given S for all  $t \in \mathcal{T}$ .
- **(3)** (*Positivity*) The conditional density satisfies  $p_{T|S}(t|s) \ge p_{\min} > 0$  for all  $(t, s) \in T \times S$ .

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$$heta(t) = rac{d}{dt}\mathbb{E}\left[Y(t)
ight] \stackrel{ ext{(*)}^1}{=} \mathbb{E}\left[rac{\partial}{\partial t}\mathbb{E}(Y|T=t,S)
ight].$$

• The positivity condition is required for  $\frac{\partial}{\partial t}\mu(t,s) = \frac{\partial}{\partial t}\mathbb{E}\left(Y|T=t,S=s\right)$  to be well-defined on  $\mathcal{T}\times\mathcal{S}$ .

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## An Example of the Positivity Violation

#### Assumption (Positivity Condition)

There exists a constant  $p_{\min} > 0$  such that  $p_{T|S}(t|s) \ge p_{\min}$  for all  $(t, s) \in \mathcal{T} \times \mathcal{S}$ .

▶ Positivity is a very strong assumption with continuous treatments!

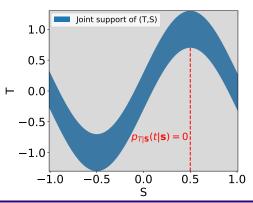
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$$T = \sin(\pi S) + E$$
,  $E \sim \text{Uniform}[-0.3, 0.3]$ ,  $S \sim \text{Uniform}[-1, 1]$ , and  $E \perp \!\!\! \perp S$ .



Note that  $p_{T|S}(t|s) = 0$  in the gray regions, and the positivity condition fails.

$$t \mapsto m(t) = \mathbb{E}[Y(t)]$$
 and  $t \mapsto \theta(t) = \frac{d}{dt}\mathbb{E}[Y(t)]$  for  $t \in \mathcal{T}$ .

#### Under the positivity condition:

• Propose a doubly robust (DR) estimator of  $\theta(t)$  via kernel smoothing.

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#### Without the positivity condition:

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$$Y(t) = \bar{m}(t) + \eta(S) + \epsilon. \tag{1}$$

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- **8** The usual IPW estimators of m(t) and  $\theta(t)$  are still biased even under model (1).
- ① Propose our bias-corrected IPW and DR estimators for m(t) and  $\theta(t)$ .
  - Has a novel connection to nonparametric support and level set estimation problems.

# Nonparametric Inference on $\theta(t)$ Under Positivity



## Recap of the Identification Under Positivity

#### Assumption (Identification Conditions)

- **()** (Consistency) Y = Y(t) whenever  $T = t \in \mathcal{T}$ .
- **2** (Ignorability) Y(t) is conditionally independent of T given S for all  $t \in T$ .
- **(8)** (Positivity) The conditional density satisfies  $p_{T|S}(t|s) \ge p_{\min} > 0$  for all  $(t, s) \in T \times S$ .

Given that 
$$\mu(t, s) = \mathbb{E}(Y|T = t, S = s)$$
, we have

**RA** or G-computation: 
$$\begin{cases} m(t) = \mathbb{E}\left[Y(t)\right] = \mathbb{E}\left[\mu(t,S)\right], \\ \theta(t) = \frac{d}{dt}\mathbb{E}\left[Y(t)\right] = \frac{d}{dt}\mathbb{E}\left[\mu(t,S)\right] = \mathbb{E}\left[\frac{\partial}{\partial t}\mu(t,S)\right]. \end{cases}$$

## Recap of the Identification Under Positivity

#### Assumption (Identification Conditions)

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IPW: 
$$\begin{cases} m(t) = \mathbb{E}\left[Y(t)\right] = \lim_{h \to 0} \mathbb{E}\left[\frac{Y}{p_{T|S}(T|S)} \cdot \frac{1}{h}K\left(\frac{T-t}{h}\right)\right], \\ \theta(t) = \frac{d}{dt}\mathbb{E}\left[Y(t)\right] = ???. \end{cases}$$

- $K: \mathbb{R} \to [0, \infty)$  is a kernel function, *e.g.*,  $K(u) = \begin{cases} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{u^2}{2}\right) & \text{(Gaussian),} \\ \frac{3}{4}(1-u^2) \cdot \mathbb{I}_{\{|u|<1\}} & \text{(Parabolic).} \end{cases}$
- h > 0 is a smoothing bandwidth parameter.

#### Dose-Response Curve Estimation Under Positivity

Given the observed data  $\{(Y_i, T_i, S_i)\}_{i=1}^n$ , there are three main strategies for estimating

$$m(t) = \mathbb{E}\left[Y(t)
ight] = \mathbb{E}\left[\mu(t,S)
ight] = \lim_{h o 0} \mathbb{E}\left[rac{Y \cdot K\left(rac{T-t}{h}
ight)}{h \cdot p_{T|S}(T|S)}
ight].$$

**1 RA Estimator** (Robins, 1986; Gill and Robins, 2001):

$$\widehat{m}_{\mathrm{RA}}(t) = \frac{1}{n} \sum_{i=1}^{n} \widehat{\mu}(t, S_i).$$

2 IPW Estimator (Hirano and Imbens, 2004; Imai and van Dyk, 2004):

$$\widehat{m}_{\mathrm{IPW}}(t) = \frac{1}{nh} \sum_{i=1}^{n} \frac{K\left(\frac{T_i - t}{h}\right)}{\widehat{p}_{T|S}(T_i|S_i)} \cdot Y_i.$$

3 DR Estimator (Kallus and Zhou, 2018; Colangelo and Lee, 2020):

$$\widehat{m}_{\mathrm{DR}}(t) = rac{1}{nh} \sum_{i=1}^n \left\{ rac{K\left(rac{T_i - t}{h}
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ight\}.$$

## RA and IPW Estimators for $\theta(t)$ Under Positivity

To estimate  $\theta(t) = \frac{d}{dt}\mathbb{E}[Y(t)] = \mathbb{E}\left[\frac{\partial}{\partial t}\mu(t, S)\right]$  from  $\{(Y_i, T_i, S_i)\}_{i=1}^n$ , we could also have three strategies:

RA Estimator:

$$\widehat{ heta}_{\mathrm{RA}}(t) = rac{1}{n} \sum_{i=1}^n \widehat{eta}(t, S_i) \quad ext{with} \quad eta(t, s) = rac{\partial}{\partial t} \mu(t, s).$$

**Question:** How can we generalize the IPW form  $m(t) = \lim_{h \to 0} \mathbb{E}\left[\frac{Y \cdot \mathbb{K}\left(\frac{T-t}{h}\right)}{h \cdot p_{T|S}(T|S)}\right]$  to identify and estimate  $\theta(t)$ ?

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IPW Estimator: Inspired by the derivative estimator in Mack and Müller (1989), we propose

$$\widehat{\theta}_{\mathrm{IPW}}(t) = \frac{1}{n} \sum_{i=1}^{n} \frac{Y_i \cdot \left(\frac{T_i - t}{h}\right) K\left(\frac{T_i - t}{h}\right)}{h^2 \cdot \kappa_2 \cdot \widehat{p}_{T|S}(T_i|S_i)} \quad \text{with} \quad \kappa_2 = \int u^2 \cdot K(u) \, du.$$

## Doubly Robust Estimator for $\theta(t)$ Under Positivity

Recall that 
$$\widehat{m}_{\mathrm{DR}}(t) = \frac{1}{nh} \sum_{i=1}^{n} \frac{K\left(\frac{T_i - t}{h}\right)}{\widehat{p}_{T|S}(T_i|S_i)} \cdot [Y_i - \widehat{\mu}(t, S_i)] + \frac{1}{n} \sum_{i=1}^{n} \widehat{\mu}(t, S_i).$$

$$\widehat{\theta}_{RA}(t) = \frac{1}{n} \sum_{i=1}^{n} \widehat{\beta}(t, S_i) \qquad "+" \qquad \widehat{\theta}_{IPW}(t) = \frac{1}{nh^2} \sum_{i=1}^{n} \frac{\left(\frac{T_i - t}{h}\right) K\left(\frac{T_i - t}{h}\right)}{\kappa_2 \cdot \widehat{p}_{T|S}(T_i|S_i)} \cdot Y_i \quad \Longrightarrow$$

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New IPW component

RA component

## Doubly Robust Estimator for $\theta(t)$ Under Positivity

Recall that 
$$\widehat{m}_{DR}(t) = \frac{1}{nh} \sum_{i=1}^{n} \frac{K\left(\frac{T_i - t}{h}\right)}{\widehat{p}_{T|S}(T_i|S_i)} \cdot [Y_i - \widehat{\mu}(t, S_i)] + \frac{1}{n} \sum_{i=1}^{n} \widehat{\mu}(t, S_i).$$

$$\widehat{\theta}_{\text{RA}}(t) = \frac{1}{n} \sum_{i=1}^{n} \widehat{\beta}(t, S_i) \qquad \text{"+"} \qquad \widehat{\theta}_{\text{IPW}}(t) = \frac{1}{nh^2} \sum_{i=1}^{n} \frac{\left(\frac{T_i - t}{h}\right) K\left(\frac{T_i - t}{h}\right)}{\kappa_2 \cdot \widehat{p}_{T|S}(T_i|S_i)} \cdot Y_i \implies$$

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The "New IPW component" leverages a local polynomial approximation to push the residual of the IPW component to (roughly) second order.

• Neyman orthogonality (Neyman, 1959; Chernozhukov et al., 2018) holds for this form of  $\hat{\theta}_{DR}(t)$  as  $h \to 0$ .

# Asymptotic Properties of $\widehat{\theta}_{DR}(t)$

#### Theorem (Theorem 1 in Zhang and Chen 2025)

Under some regularity assumptions and

- $igoplus \widehat{\mu}, \widehat{eta}, \widehat{p}_{T|S}$  are estimated on a dataset independent of  $\{(Y_i, T_i, S_i)\}_{i=1}^n$ ;
- at least one of the model specification conditions hold:
  - $\widehat{p}_{T|S}(t|s) \stackrel{P}{\to} \overline{p}_{T|S}(t|s) = p_{T|S}(t|s)$  (conditional density model),
  - $\widehat{\mu}(t,s) \stackrel{P}{\to} \overline{\mu}(t,s) = \mu(t,s)$  and  $\widehat{\beta}(t,s) \stackrel{P}{\to} \overline{\beta}(t,s) = \beta(t,s)$  (outcome model);
- $\sup_{|u-t|\leq h}\left|\left|\widehat{p}_{T|S}(u|S)-p_{T|S}(u|S)\right|\right|_{L_2}\left[\left|\left|\widehat{\mu}(t,S)-\mu(t,S)\right|\right|_{L_2}+h\left|\left|\widehat{\beta}(t,S)-\beta(t,S)\right|\right|_{L_2}\right]=o_P\left(\frac{1}{\sqrt{nh}}\right),$

we prove that

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- $\sup_{|u-t| \leq h} \left| \left| \widehat{p}_{T|S}(u|S) p_{T|S}(u|S) \right| \right|_{L_2} \left[ \left| \left| \widehat{\mu}(t,S) \mu(t,S) \right| \right|_{L_2} + h \left| \left| \widehat{\beta}(t,S) \beta(t,S) \right| \right|_{L_2} \right] = o_P \left( \frac{1}{\sqrt{nh}} \right),$

we prove that

$$ullet \sqrt{nh^3} \left[ \widehat{ heta}_{\mathrm{DR}}(t) - heta(t) 
ight] = rac{1}{\sqrt{n}} \sum_{i=1}^n \phi_{h,t} \left( Y_i, T_i, S_i; ar{\mu}, ar{eta}, ar{p}_{T|S} 
ight) + o_P(1).$$

$$\sqrt{nh^3}\left[\widehat{ heta}_{\mathrm{DR}}(t)- heta(t)-h^2B_{ heta}(t)
ight] \stackrel{d}{
ightarrow} \mathcal{N}\left(0,V_{ heta}(t)
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An asymptotically valid inference on  $\theta(t) = \frac{d}{dt}\mathbb{E}[Y(t)]$  can be conducted through

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lacksquare We estimate  $V_{ heta}(t) = \mathbb{E}\left[\phi_{h,t}^2\left(Y,T,S;ar{\mu},ar{ar{eta}},ar{p}_{T|S}
ight)
ight]$  with

$$\phi_{h,t}\left(Y,T,S;ar{\mu},ar{eta},ar{p}_{T|S}
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ight)}{\sqrt{h}\cdot\kappa_2\cdotar{p}_{T|S}(T|S)}\cdot\left[Y-ar{\mu}(t,S)-(T-t)\cdotar{eta}(t,S)
ight]$$

by 
$$\widehat{V}_{\theta}(t) = \frac{1}{n} \sum_{i=1}^{n} \phi_{h,t}^{2} (Y, T, S; \widehat{\mu}, \widehat{\beta}, \widehat{p}_{T|S}).$$

An asymptotically valid inference on  $\theta(t) = \frac{d}{dt}\mathbb{E}[Y(t)]$  can be conducted through

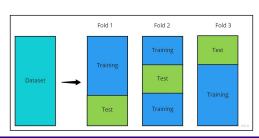
$$\sqrt{nh^3}\left[\widehat{\theta}_{\mathrm{DR}}(t)-\theta(t)-h^2\,B_{\theta}(t)\right]\overset{d}{
ightarrow}\mathcal{N}\left(0,\frac{V_{\theta}(t)}{}\right).$$

lacksquare We estimate  $V_{ heta}(t) = \mathbb{E}\left[\phi_{h,t}^2\left(Y,T,S;ar{\mu},ar{eta},ar{p}_{T|S}
ight)
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②  $\hat{\mu}$ ,  $\hat{\beta}$ ,  $\hat{p}_{T|S}$  can be estimated via sample-splitting or cross-fitting.



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- $\widehat{\mu}, \widehat{\beta}, \widehat{p}_{T|S}$  can be estimated via sample-splitting or cross-fitting.
- **(3)** The explicit form of  $B_{\theta}(t)$  is complicated, but  $h^2 B_{\theta}(t)$  is asymptotically negligible when  $h = O(n^{-\frac{1}{5}})$ .
  - This order aligns with the outputs from usual bandwidth selection methods (Wand and Jones, 1994; Wasserman, 2006).

# Nonparametric Efficiency Guarantee for $\widehat{\theta}_{\mathrm{DR}}(t)$

**Question:** Do we have a nonparametric efficiency lower bound for  $\widehat{\theta}_{DR}(t)$ ?

<sup>&</sup>lt;sup>2</sup>I acknowledge Ted Westling and Aaron Hudson for pointing out this direction.

# Nonparametric Efficiency Guarantee for $\widehat{\theta}_{\mathrm{DR}}(t)$

**Question:** Do we have a nonparametric efficiency lower bound for  $\widehat{\theta}_{DR}(t)$ ?

•  $t \mapsto \theta(t) := \Psi(P_0)(t)$  is *not* pathwise differentiable (Bickel et al., 1998; Hirano and Porter, 2012; Luedtke and van der Laan, 2016):

$$\forall t \in \mathcal{T}, \quad \exists \{ P_{\epsilon} : \epsilon \in \mathbb{R} \} \quad \text{ s.t. } \quad \lim_{\epsilon \to 0} \frac{\Psi(P_{\epsilon})(t) - \Psi(P_{0})(t)}{\epsilon} \quad \text{ does not exist. }$$

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• For a fixed h > 0, the smooth functional  $\Phi(P_0)(t) := \mathbb{E}\left[\frac{Y \cdot \left(\frac{T-t}{h}\right) K\left(\frac{T-t}{h}\right)}{h^2 \cdot \kappa_2 \cdot p_{T|S}(T|S)}\right]$  is pathwise differentiable (van der Laan et al., 2018; Takatsu and Westling, 2024).

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- Up to a shrinking bias  $O(h^2)$ , the efficient influence function for  $\Phi(P_0)(t)$  leads to

$$\widehat{ heta}_{ ext{EIF}}(t) = rac{1}{nh^2} \sum_{i=1}^n rac{\left(rac{T_i - t}{h}
ight) K\left(rac{T_i - t}{h}
ight)}{\kappa_2 \cdot \widehat{p}_{T|S}(T_i|S_i)} \left[Y_i - \widehat{\mu}(T_i, S_i)
ight] + rac{1}{n} \sum_{i=1}^n \widehat{eta}(t, S_i).$$

▶ The asymptotic variances of  $\hat{\theta}_{DR}(t)$  and  $\hat{\theta}_{EIF}(t)$  are the same (or differing by  $O(h^2)$ )!

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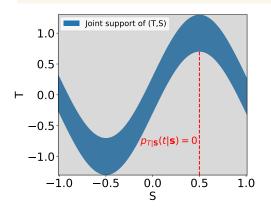
# Nonparametric Inference on $\theta(t)$ Without Positivity



# Identification Strategy Without Positivity

## Assumption (Identification Conditions)

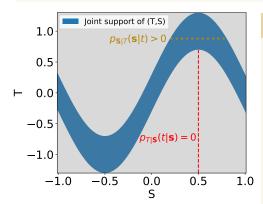
- **(1)** (Consistency) Y = Y(t) whenever  $T = t \in \mathcal{T}$ .
- ② (Ignorability) Y(t) is conditionally independent of T given S for all  $t \in T$ .
- **(3)** (Treatment Variation) Var(T|S = s) > 0 for all  $s \in S$ .



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# Assumption (Extrapolation; Zhang et al. 2024)

Assume  $(t, s) \mapsto \mathbb{E}[Y(t)|S = s]$  to be differentiable w.r.to t for any  $(t, s) \in \mathcal{T} \times \mathcal{S}$  with  $p_{S|T}(s|t) > 0$  and

$$\theta(t) = \frac{d}{dt} \mathbb{E} [Y(t)] = \mathbb{E} \left[ \frac{\partial}{\partial t} \mathbb{E} [Y(t)|S] \right]$$

$$\stackrel{*}{=} \mathbb{E} \left[ \frac{\partial}{\partial t} \mathbb{E} [Y(t)|S] \middle| T = t \right].$$

Additionally, it holds true that  $\mathbb{E}(Y) = \mathbb{E}[m(T)]$ .

$$\theta(t) = \frac{d}{dt} \mathbb{E}\left[Y(t)\right] = \mathbb{E}\left[\frac{\partial}{\partial t} \mathbb{E}\left[Y(t)|S\right]\right] \stackrel{\star}{=} \mathbb{E}\left[\frac{\partial}{\partial t} \mathbb{E}\left[Y(t)|S\right]|T = t\right].$$

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Proposition 2 in Zhang et al. (2024) shows that the above equality holds under an additive structural assumption

$$Y(t) = \bar{m}(t) + \eta(S) + \epsilon.$$

- $\bar{m}: \mathcal{T} \to \mathbb{R}$  and  $\eta: \mathcal{S} \to \mathbb{R}$  are deterministic functions.
- $\epsilon \in \mathbb{R}$  is an independent noise variable with  $\mathbb{E}(\epsilon) = 0$  and  $\text{Var}(\epsilon) > 0$ .

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- Identification:

$$m(t) = \mathbb{E}\left[Y + \int_{u=T}^{u=t} \theta(u) du\right]$$
 and  $\theta(t) = \int \frac{\partial}{\partial t} \mu(t, s) dF_{S|T}(s|t)$ .

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• RA estimators without positivity (Zhang et al., 2024):

$$\widehat{m}_{\mathrm{C,RA}}(t) = \frac{1}{n} \sum_{i=1}^{n} \left[ Y_i + \int_{\widetilde{t}=T_i}^{\widetilde{t}=t} \widehat{\theta}_{\mathrm{C,RA}}(\widetilde{t}) d\widetilde{t} \right] \quad \text{and} \quad \widehat{\theta}_{\mathrm{C,RA}}(t) = \int \widehat{\beta}(t,s) d\widehat{F}_{S|T}(s|t).$$

**Question:** How about IPW and DR estimators for  $\theta(t)$  without positivity?

• For identification, we assume  $Y(t) = \overline{m}(t) + \eta(S) + \epsilon$ .

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- For identification, we assume  $Y(t) = \overline{m}(t) + \eta(S) + \epsilon$ .
- Recall the standard (oracle) IPW estimators for m(t) and  $\theta(t)$ :

$$\widetilde{m}_{\mathrm{IPW}}(t) = \frac{1}{nh} \sum_{i=1}^{n} \frac{Y_i \cdot K\left(\frac{T_i - t}{h}\right)}{p_{T|S}(T_i|S_i)} \quad \text{and} \quad \widetilde{\theta}_{\mathrm{IPW}}(t) = \frac{1}{nh^2} \sum_{i=1}^{n} \frac{Y_i \cdot \left(\frac{T_i - t}{h}\right) K\left(\frac{T_i - t}{h}\right)}{\kappa_2 \cdot p_{T|S}(T_i|S_i)}.$$

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# Proposition (Proposition 2 in Zhang and Chen 2025)

$$\lim_{h\to 0}\mathbb{E}\left[\widetilde{m}_{\mathrm{IPW}}(t)\right]=\bar{m}(t)\cdot\rho(t)+\omega(t)\neq m(t),\qquad \text{with}\quad \rho(t)=\mathbb{P}\left(S\in\mathcal{S}(t)\right),$$

$$\lim_{h\to 0} \mathbb{E}\left[\widetilde{\theta}_{\mathrm{IPW}}(t)\right] = \begin{cases} \bar{m}'(t)\cdot\rho(t) & \neq \theta(t), \\ \infty & \end{cases} \text{ and } \omega(t) = \mathbb{E}\left[\eta(S)\mathbb{1}_{\{S\in\mathcal{S}(t)\}}\right].$$

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▶ **Key Issue:** The conditional support S(t) of  $p_{S|T}(s|t)$  and the marginal support S of  $p_S(s)$  are different under the violations of positivity!!

$$\lim_{h\to 0} \mathbb{E}\left[\widetilde{\theta}_{\mathrm{IPW}}(t)\right] = \lim_{h\to 0} \mathbb{E}\left[\frac{Y\left(\frac{T-t}{h}\right)K\left(\frac{T-t}{h}\right)}{h^2 \cdot \kappa_2 \cdot p_{T|S}(T|S)}\right] = \begin{cases} \bar{m}'(t) \cdot \rho(t) \\ \infty \end{cases} \neq \theta(t),$$

where 
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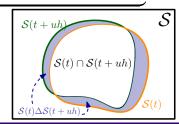
where  $\rho(t) = \mathbb{P}\left(S \in \mathcal{S}(t)\right)$  and  $\omega(t) = \mathbb{E}\left[\eta(S)\mathbb{1}_{\left\{S \in \mathcal{S}(t)\right\}}\right]$ .

• We first want to disentangle  $\theta(t) = \bar{m}'(t)$  from the bias term:

$$\mathbb{E}\left[\frac{Y\cdot\left(\frac{T-t}{h}\right)K\left(\frac{T-t}{h}\right)\cdot p_{S|T}(S|t)}{h^2\cdot\kappa_2\cdot p_{T|S}(T|S)\cdot p_S(S)}\right] = \bar{m}'(t) + O(h^2)$$

$$+\int_{\mathbb{R}}\mathbb{E}\left\{\left[\bar{m}(t+uh) + \eta(S)\right]\left[\mathbb{1}_{\left\{S\in\mathcal{S}(t+uh)\setminus\mathcal{S}(t)\right\}} - \mathbb{1}_{\left\{S\in\mathcal{S}(t)\setminus\mathcal{S}(t+uh)\right\}}\right]\Big|T=t\right\}u\cdot K(u)\,du\,.$$

Non-vanishing Bias

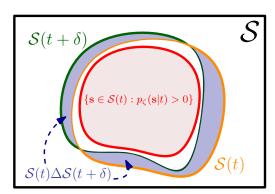


$$\mathbb{E}\left[\frac{Y\cdot\left(\frac{T-t}{h}\right)K\left(\frac{T-t}{h}\right)p_{S|T}(S|t)}{h^2\cdot\kappa_2\cdot p_{T|S}(T|S)\cdot p_S(S)}\right] = \bar{m}'(t) + O(h^2) + \text{"Non-vanishing Bias"}.$$

$$\mathbb{E}\left[\frac{Y\cdot\left(\frac{T-t}{h}\right)K\left(\frac{T-t}{h}\right)p_{S|T}(S|t)}{h^2\cdot\kappa_2\cdot p_{T|S}(T|S)\cdot p_S(S)}\right] = \bar{m}'(t) + O(h^2) + \text{"Non-vanishing Bias"}.$$

Description We replace  $p_{S|T}(s|t)$  with a ζ-interior conditional density  $p_{\zeta}(s|t)$  so that

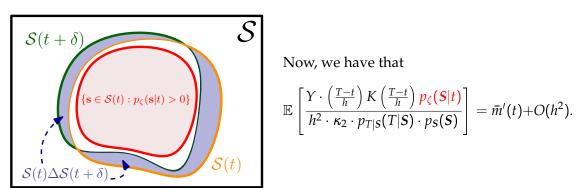
$${s \in \mathcal{S}(t) : p_{\zeta}(s|t) > 0} \subset \mathcal{S}(t+\delta)$$
 for any  $\delta \in [-h,h]$ .



$$\mathbb{E}\left[\frac{Y\cdot\left(\frac{T-t}{h}\right)K\left(\frac{T-t}{h}\right)p_{S|T}(S|t)}{h^2\cdot\kappa_2\cdot p_{T|S}(T|S)\cdot p_S(S)}\right] = \bar{m}'(t) + O(h^2) + \text{"Non-vanishing Bias"}.$$

We replace  $p_{S|T}(s|t)$  with a  $\zeta$ -interior conditional density  $p_{\zeta}(s|t)$  so that

$${s \in S(t) : p_{\zeta}(s|t) > 0} \subset S(t+\delta)$$
 for any  $\delta \in [-h,h]$ .



Now, we have that

$$\mathbb{E}\left|\frac{Y\cdot\left(\frac{T-t}{h}\right)K\left(\frac{T-t}{h}\right)p_{\zeta}(S|t)}{h^2\cdot\kappa_2\cdot p_{T|S}(T|S)\cdot p_S(S)}\right|=\bar{m}'(t)+O(h^2)$$

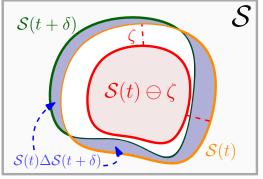
# ζ-Interior Conditional Density

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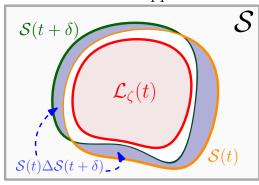
Support shrinking approach



$$\mathcal{S}(t) \ominus \zeta = \left\{ s \in \mathcal{S}(t) : \inf_{\mathbf{x} \in \partial \mathcal{S}(t)} \left| \left| s - \mathbf{x} \right| \right|_2 \ge \zeta \right\},$$

$$p_{\zeta}(s|t) = \frac{p_{S|T}(s|t) \cdot \mathbb{1}_{\{s \in \mathcal{S}(t) \ominus \zeta\}}}{\int_{\mathcal{S}(t) \ominus \zeta} p_{S|T}(s_1|t) ds_1}.$$

Level set approach



$$\mathcal{L}_{\zeta}(t) = \left\{ s \in \mathcal{S}(t) : p_{S|T}(s|t) \geq \zeta 
ight\},$$

$$p_{\zeta}(s|t) = \frac{p_{S|T}(s|t) \cdot \mathbb{1}_{\{s \in \mathcal{L}_{\zeta}(t)\}}}{\int_{\mathcal{L}_{\zeta}(t)} p_{S|T}(s_1|t) ds_1}.$$

**▶** Bias-Corrected IPW Estimator Without Positivity:

$$\widehat{\theta}_{\text{C,IPW}}(t) = \frac{1}{nh^2} \sum_{i=1}^{n} \frac{Y_i \cdot \left(\frac{T_i - t}{h}\right) K\left(\frac{T_i - t}{h}\right) \widehat{p}_{\zeta}(S_i | t)}{\kappa_2 \cdot \widehat{p}(T_i, S_i)},$$

•  $\widehat{p}(t, s)$ ,  $\widehat{p}_{\zeta}(s|t)$  are estimators of p(t, s),  $p_{\zeta}(s|t)$  and  $\zeta = 0.5 \cdot \max\{\widehat{p}_{S|T}(S_i|t) : i = 1, ..., n\}$ .

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- **▶** Bias-Corrected DR Estimator Without Positivity:

$$\widehat{\theta}_{\text{C,DR}}(t) = \underbrace{\frac{1}{nh^2} \sum_{i=1}^{n} \frac{\left(\frac{T_i - t}{h}\right) K\left(\frac{T_i - t}{h}\right) \widehat{p}_{\zeta}(S_i | t)}{\kappa_2 \cdot \widehat{p}(T_i, S_i)} \left[ Y_i - \widehat{\mu}(t, S_i) - (T_i - t) \cdot \widehat{\beta}(t, S_i) \right]}_{\text{IPW component}} + \underbrace{\int \widehat{\beta}(t, s) \cdot \widehat{p}_{\zeta}(s | t) \, ds}_{\text{RA component}}.$$

# Asymptotic Properties of $\widehat{\theta}_{C,DR}(t)$ Without Positivity

## Theorem (Theorem 5 in Zhang and Chen 2025)

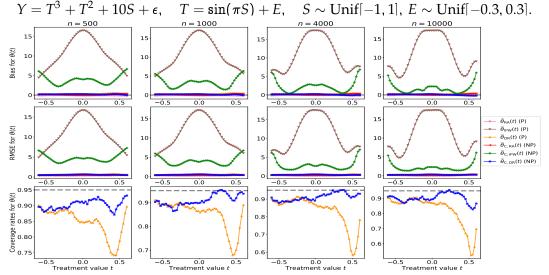
Under some regularity assumptions and

- **1**  $\widehat{\mu}$ ,  $\widehat{\beta}$ ,  $\widehat{p}$ ,  $\widehat{p}_{\zeta}$  are estimated on a dataset independent of  $\{(Y_i, T_i, S_i)\}_{i=1}^n$ ;
- 3 at least one of the model specification conditions hold:
  - $\widehat{p}(t,s) \stackrel{P}{\to} \overline{p}(t,s) = p(t,s)$  (joint density model),
  - $\widehat{\mu}(t,s) \stackrel{P}{\to} \overline{\mu}(t,s) = \mu(t,s)$  and  $\widehat{\beta}(t,s) \stackrel{P}{\to} \overline{\beta}(t,s) = \beta(t,s)$  (outcome model);
- $\sup_{|u-t|\leq h}||\widehat{p}(u,S)-p(u,S)||_{L_2}\left[||\widehat{\mu}(t,S)-\mu(t,S)||_{L_2}+h\left|\left|\widehat{\beta}(t,S)-\beta(t,S)\right|\right|_{L_2}\right]=o_P\left(\frac{1}{\sqrt{nh}}\right),$ we prove that
- $\sqrt{nh^3}\left[\widehat{\theta}_{C,DR}(t) \theta(t)\right] = \frac{1}{\sqrt{n}}\sum_{i=1}^n \phi_{C,h,t}\left(Y_i,T_i,S_i;\bar{\mu},\bar{\beta},\bar{p}_{T|S}\right) + o_P(1).$
- $\sqrt{nh^3} \left[ \widehat{\theta}_{\mathsf{C},\mathsf{DR}}(t) \theta(t) h^2 \cdot B_{\mathsf{C},\theta}(t) \right] \overset{d}{\to} \mathcal{N} \left( 0, V_{\mathsf{C},\theta}(t) \right).$

# **Experiments and Discussion**



# Simulations for $\hat{\theta}_{C,RA}(t)$ , $\hat{\theta}_{C,IPW}(t)$ , $\hat{\theta}_{C,DR}(t)$ Without Positivity



**Note:**  $\beta(t, s) = \frac{\partial}{\partial t} \mu(t, s)$  is estimated via automatic differentiation of a well-trained neural network (inspired by Luedtke 2024).

# A Case Study Under Positivity

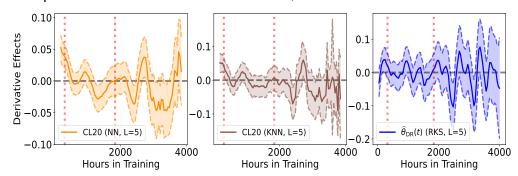
We compare our proposed DR estimator  $\hat{\theta}_{DR}(t)$  under positivity with the finite-difference method (Colangelo and Lee 2020; CL20) on the U.S. Job Corps program (Schochet et al., 2001).

- Y is the proportion of weeks employed in  $2^{nd}$  year after enrollment.
- *T* is the total hours of academic and vocational training received.
- *S* comprises 49 socioeconomic characteristics, and n = 4024.

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$$\sqrt{nh^3}\left[\widehat{\theta}_{\mathrm{DR}}(t)-\theta(t)-h^2B_{\theta}(t)\right]\overset{d}{\to}\mathcal{N}\left(0,V_{\theta}(t)\right).$$

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- Without the positivity condition:
  - Our bias-corrected IPW and DR estimators  $\hat{\theta}_{C,IPW}(t)$ ,  $\hat{\theta}_{C,DR}(t)$  reveal interesting connections to nonparametric level set estimation problems (Bonvini et al., 2023):

Causal Inference ←⇒ Geometric Data Analysis (https://uwgeometry.github.io/)!

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- § Future Works:
  - Sensitivity analysis on unmeasured confounding (Chernozhukov et al., 2022).
  - Generalize our derivative estimators to other causal estimands:
    - instantaneous causal effect  $\frac{d}{dt}\mathbb{E}\left[Y(t)|S=s\right]$  (Stolzenberg, 1980);
    - direct and indirect effects in mediation analysis (Huber et al., 2020; Xu et al., 2021)?

# Thank you!

#### More details can be found in

[1] Y. Zhang and Y.-C. Chen. Doubly Robust Inference on Causal Derivative Effects for Continuous Treatments. *arXiv preprint*, 2025. https://arxiv.org/abs/2501.06969.

All the code and data are available at <a href="https://github.com/zhangyk8/npDRDeriv">https://github.com/zhangyk8/npDRDeriv</a>.

Python Package: npDoseResponse.

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# Detailed Regularity Assumptions

# Assumption (Differentiability of the conditional mean outcome function)

For any  $(t, s) \in \mathcal{T} \times \mathcal{S}$  and  $\mu(t, s) = \mathbb{E}(Y|T = t, S = s)$ , it holds that

- $0 \mu(t, s)$  is at least four times continuously differentiable with respect to t.
- (0)  $\mu(t, s)$  and all of its partial derivatives are uniformly bounded on  $T \times S$ .

Let  $\mathcal{J}$  be the support of the joint density p(t, s).

# Assumption (Differentiability of the density functions)

For any  $(t, s) \in \mathcal{J}$ , it holds that

- **1** The joint density p(t, s) and the conditional density  $p_{T|S}(t|s)$  are at least three times continuously differentiable with respect to t.
- p(t, s),  $p_{T|S}(t|s)$ ,  $p_{S|T}(s|t)$ , as well as all of the partial derivatives of p(t, s) and  $p_{T|S}(t|s)$  are bounded and continuous up to the boundary  $\partial \mathcal{J}$ .
- § The support T of the marginal density  $p_T(t)$  is compact and  $p_T(t)$  is uniformly bounded away from 0 within T.

# **Detailed Regularity Assumptions**

# Assumption (Regular kernel conditions)

A kernel function  $K : \mathbb{R} \to [0, \infty)$  is bounded and compactly supported on [-1, 1] with  $\int_{\mathbb{R}} K(t) dt = 1$  and K(t) = K(-t). In addition, it holds that

- $oldsymbol{0} \kappa_j := \int_{\mathbb{R}} u^j K(u) \, du < \infty$  and  $u_j := \int_{\mathbb{R}} u^j K^2(u) \, du < \infty$  for all j=1,2,...
- @ K is a second-order kernel, i.e.,  $\kappa_1=0$  and  $\kappa_2>0$ .
- **(3)**  $K = \left\{ t' \mapsto \left( \frac{t'-t}{h} \right)^{k_1} K\left( \frac{t'-t}{h} \right) : t \in \mathcal{T}, h > 0, k_1 = 0, 1 \right\}$  is a bounded VC-type class of measurable functions on  $\mathbb{R}$ .

# Assumption (Smoothness condition on S(t))

For any  $\delta \in \mathbb{R}$  and  $t \in \mathcal{T}$ , there exists an absolute constant  $A_0 > 0$  such that either (i) " $S(t) \ominus (A_0|\delta|) \subset S(t+\delta)$ " for the support shrinking approach or (ii) " $\mathcal{L}_{A_0|\delta|}(t) \subset S(t+\delta)$ " for the level set approach.

### Self-Normalized IPW and DR Estimators

The self-normalizing technique can reduce the instability of IPW and DR estimators (Kallus and Zhou, 2018):

Self-Normalized Estimators Under Positivity:

$$\widehat{ heta}_{ ext{IPW}}^{ ext{norm}}(t) = rac{\widehat{ heta}_{ ext{IPW}}(t)}{rac{1}{nh}\sum\limits_{j=1}^{n}rac{K\left(rac{T_{j}-t}{h}
ight)}{\widehat{p}_{T|S}(T_{j}|S_{j})}} = rac{\sum\limits_{i=1}^{n}rac{Y_{i}\left(rac{T_{i}-t}{h}
ight)K\left(rac{T_{i}-t}{h}
ight)}{\widehat{p}_{T|S}(T_{i}|S_{i})}}{\kappa_{2}h\sum\limits_{j=1}^{n}rac{K\left(rac{T_{j}-t}{h}
ight)}{\widehat{p}_{T|S}(T_{j}|S_{j})}},$$

and

$$\widehat{ heta}_{ ext{DR}}^{ ext{norm}}(t) = rac{\sum\limits_{i=1}^{n}rac{\left[Y_{i}-\widehat{\mu}(t,S_{i})-(T_{i}-t)\cdot\widehat{eta}(t,S_{i})
ight]\left(rac{T_{i}-t}{h}
ight)K\left(rac{T_{i}-t}{h}
ight)}{\widehat{p}_{T\mid S}(T_{i}\mid S_{i})}}{\kappa_{2}h\sum\limits_{i=1}^{n}rac{K\left(rac{T_{i}-t}{h}
ight)}{\widehat{p}_{T\mid S}(T_{j}\mid S_{j})}}+rac{1}{n}\sum\limits_{i=1}^{n}\widehat{eta}(t,S_{i}).$$

### Self-Normalized IPW and DR Estimators

Self-Normalized Estimators Without Positivity:

$$\widehat{\theta}_{\text{C,IPW}}^{\text{norm}}(t) = \frac{\widehat{\theta}_{\text{C,IPW}}(t)}{\frac{1}{nh} \sum\limits_{j=1}^{n} \frac{K\left(\frac{T_{j}-t}{h}\right) \cdot \widehat{p}_{\zeta}(S_{j}|t)}{\widehat{p}(T_{j},S_{j})}} = \frac{\sum\limits_{i=1}^{n} \frac{Y_{i}\left(\frac{T_{i}-t}{h}\right) K\left(\frac{T_{i}-t}{h}\right) \cdot \widehat{p}_{\zeta}(S_{i}|t)}{\widehat{p}(T_{i},S_{i})}}{\kappa_{2}h \sum\limits_{j=1}^{n} \frac{K\left(\frac{T_{j}-t}{h}\right) \cdot \widehat{p}_{\zeta}(S_{j}|t)}{\widehat{p}(T_{j},S_{j})}},$$

and

$$\begin{split} \widehat{\theta}_{\mathrm{C,DR}}^{\mathrm{norm}}(t) &= \frac{\sum\limits_{i=1}^{n} \frac{\left[Y_{i} - \widehat{\mu}(t, S_{i}) - (T_{i} - t) \cdot \widehat{\beta}(t, S_{i})\right] \left(\frac{T_{i} - t}{h}\right) K\left(\frac{T_{i} - t}{h}\right) \cdot \widehat{p}_{\zeta}(S_{i} | t)}{\widehat{p}(T_{i}, S_{i})} \\ & \kappa_{2} h \sum\limits_{j=1}^{n} \frac{K\left(\frac{T_{j} - t}{h}\right) \cdot \widehat{p}_{\zeta}(S_{j} | t)}{\widehat{p}(T_{j}, S_{j})} \\ & + \int \widehat{\beta}(t, s) \cdot \widehat{p}_{\zeta}(s | t) \, ds. \end{split}$$

# Simulations Under the Positivity Condition

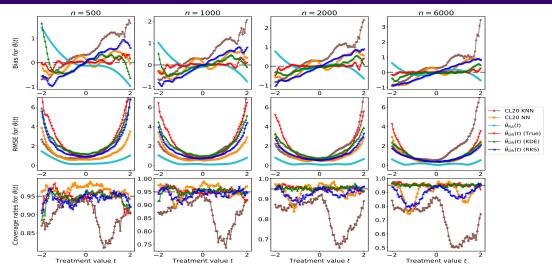
We generate i.i.d. observations  $\{(Y_i, T_i, S_i)\}_{i=1}^n$  from the following data-generating model (Colangelo and Lee, 2020):

$$Y = 1.2 T + T^2 + TS_1 + 1.2 \boldsymbol{\xi}^T S + \epsilon \sqrt{0.5 + F_{\mathcal{N}(0,1)}(S_1)}, \quad \epsilon \sim \mathcal{N}(0,1),$$
 $T = F_{\mathcal{N}(0,1)} \left(3 \boldsymbol{\xi}^T S\right) - 0.5 + 0.75 E, \quad S = (S_1, ..., S_d)^T \sim \mathcal{N}_d \left(\mathbf{0}, \Sigma\right), \ E \sim \mathcal{N}(0,1),$ 

#### where

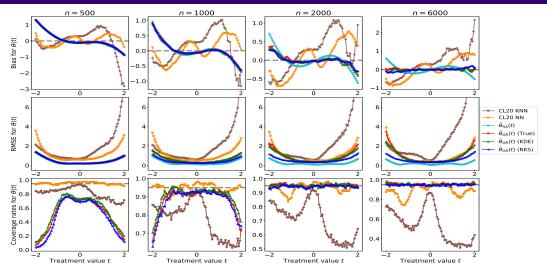
- $F_{\mathcal{N}(0,1)}$  is the CDF of  $\mathcal{N}(0,1)$  and d=20.
- $\boldsymbol{\xi} = (\xi_1, ..., \xi_d)^T \in \mathbb{R}^d$  has its entry  $\xi_j = \frac{1}{j^2}$  for j = 1, ..., d and  $\Sigma_{ii} = 1, \Sigma_{ij} = 0.5$  when |i j| = 1, and  $\Sigma_{ij} = 0$  when |i j| > 1 for i, j = 1, ..., d.
- The dose-response curve is given by  $m(t) = 1.2t + t^2$ , and our parameter of interest is the derivative effect curve  $\theta(t) = 1.2 + 2t$ .

# Simulations for Estimating $\theta(t)$ Under Positivity



Comparisons between our proposed estimators and the finite-difference approaches by Colangelo and Lee (2020) ("CL20") under positivity and with 5-fold cross-fitting across various sample sizes.

# Simulations for Estimating $\theta(t)$ Under Positivity



Comparisons between our proposed estimators and the finite-difference approaches by Colangelo and Lee (2020) ("CL20") under positivity and without cross-fitting across various sample sizes.