Doubly Robust Inference on Causal Derivative Effects for Continuous Treatments

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The Notion of Derivative

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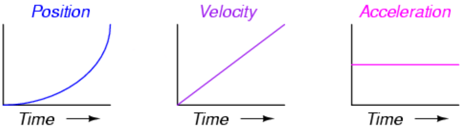

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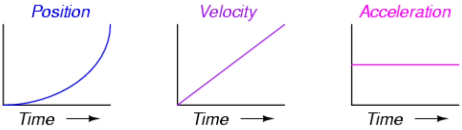

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- **Economics:** marginal cost, marginal revenue, marginal propensity to consume (Haavelmo, 1947) are all related to derivatives.

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*“**The fundamental causal laws must use present properties and past neighborhood properties to determine future neighborhood properties** ... the fundamental laws ... must involve some neighbourhood properties as well. And **the most natural sort of neighbourhood property appears to be derivative.**”*

Brit. J. Phil. Sci. **65** (2014), 845–862

Why Physics Uses Second Derivatives

Kenny Easwaran

Quoted from pp.857 of Easwaran (2014). This view is also defended in Chapter 1 of Lange (2002).

The Role of Derivatives in Causal Inference

Goal: We want to study the causal effect of a treatment $T \in \mathcal{T}$ on an outcome of interest $Y \in \mathcal{Y}$.

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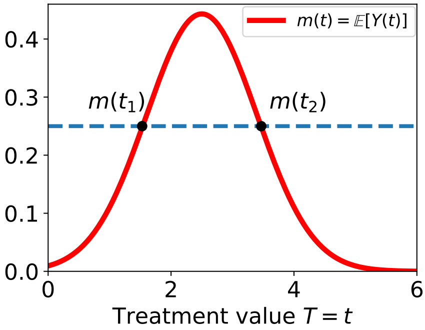

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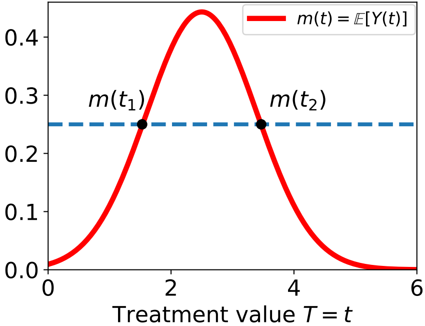

- While $m(t_1) = m(t_2)$, the derivative effects $m'(t_1), m'(t_2)$ are distinct!
- The derivative effect curve $\theta(t) = m'(t) = \frac{d}{dt}\mathbb{E}[Y(t)]$ is a continuous generalization to the average treatment effect $\mathbb{E}[Y(1)] - \mathbb{E}[Y(0)]$.

Estimand of Interest and its Alternatives

Our causal estimand of interest is the **derivative effect curve**

$$t \mapsto \theta(t) = m'(t) = \frac{d}{dt}\mathbb{E}\left[Y(t)\right] \quad \text{for} \quad t \in \mathcal{T}.$$

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There are some closely related but distinct estimands:

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

$$\mathbb{E}\left[Y(T+\delta)\right] - \mathbb{E}\left[Y(T)\right]$$

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

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

  where $\boldsymbol{S} \in \mathcal{S} \subset \mathbb{R}^d$ is a covariate vector.

To identify and estimate $\theta(t)$ from the observed data $\{(Y_i, T_i, \boldsymbol{S}_i)\}_{i=1}^n$, the following assumptions are generally imposed.

Assumption (Identification Conditions)

1. *(Consistency)* $Y_i = Y_i(t)$ *whenever* $T_i = t \in \mathcal{T}$.
2. *(Ignorability or Unconfoundedness)* $Y_i(t) \perp\!\!\!\perp T_i \,\big|\, \boldsymbol{S}_i$ *for all* $t \in \mathcal{T}$.
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2. Positivity is a strong assumption with continuous treatments!

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An Example of the Positivity Violation

Assumption (Positivity Condition)

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

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

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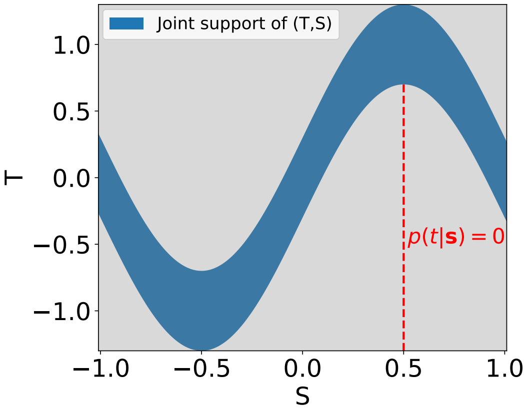

- **Note:** $p(t|s) = 0$ in the gray regions, and the positivity condition fails.

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4. We propose our bias-corrected IPW and DR estimators of $\theta(t)$.
   - Our approach establishes an interesting connection to nonparametric support and level set estimation problems.

Recap of the Identification Under Positivity

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

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

Here, $K : \mathbb{R} \to [0, \infty)$ is a kernel function and $h > 0$ is a smoothing bandwidth parameter.

Dose-Response Curve Estimation Under Positivity

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

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

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

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

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

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

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

Challenges of Deriving a DR Estimator of $\theta(t)$

The usual approach to construct a DR (or AIPW) estimator is as follows:

$$\widehat{m}_{\mathrm{RA}}(t) = \frac{1}{n}\sum_{i=1}^{n}\widehat{\mu}(t, \boldsymbol{S}_i) \qquad \text{“+”} \qquad \widehat{m}_{\mathrm{IPW}}(t) = \frac{1}{nh}\sum_{i=1}^{n}\frac{K\left(\frac{T_i - t}{h}\right)}{\widehat{p}_{T|\boldsymbol{S}}(T_i|\boldsymbol{S}_i)} \cdot Y_i$$

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This “naive” combining approach does not work for constructing a DR estimator of $\theta(t)$:

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

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$\Longrightarrow$

- $\widehat{\theta}_{\mathrm{AIPW},1}(t) = \frac{1}{nh^2}\sum_{i=1}^{n}\frac{\left(\frac{T_i - t}{h}\right)K\left(\frac{T_i - t}{h}\right)}{\kappa_2\cdot\widehat{p}_{T|\boldsymbol{S}}(T_i|\boldsymbol{S}_i)}\left[Y_i - \widehat{\beta}(t, \boldsymbol{S}_i)\right] + \frac{1}{n}\sum_{i=1}^{n}\widehat{\beta}(t, \boldsymbol{S}_i)$;
- $\widehat{\theta}_{\mathrm{AIPW},2}(t) = \frac{1}{nh}\sum_{i=1}^{n}\frac{K\left(\frac{T_i - t}{h}\right)}{\widehat{p}_{T|\boldsymbol{S}}(T_i|\boldsymbol{S}_i)}\left[\frac{Y_i}{h\cdot\kappa_2}\left(\frac{T_i - t}{h}\right) - \widehat{\beta}(t, \boldsymbol{S}_i)\right] + \frac{1}{n}\sum_{i=1}^{n}\widehat{\beta}(t, \boldsymbol{S}_i)$; etc.

Remark: All these AIPW estimators are, at best, singly robust!!

Doubly Robust Estimator of $\theta(t)$ Under Positivity

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1. The “IPW component” leverages a local polynomial approximation to push the residual to (roughly) second order.
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1. The “IPW component” leverages a local polynomial approximation to push the residual to (roughly) second order.
   - Neyman orthogonality (Neyman, 1959; Chernozhukov et al., 2018) holds as $h \to 0$.
2. Different from $\widehat{m}_{\mathrm{IPW}}(t)$ and $\widehat{m}_{\mathrm{DR}}(t)$, we must compute the inverse probability weights as $\frac{1}{\widehat{p}_{T|\boldsymbol{S}}(T_i|\boldsymbol{S}_i)}$ but not $\frac{1}{\widehat{p}_{T|\boldsymbol{S}}(t|\boldsymbol{S}_i)}$ for $i = 1, ..., n$.

Theorem (Theorem 1 in Zhang and Chen 2025)

Under some regularity assumptions and

1. $\widehat{\mu}, \widehat{\beta}, \widehat{p}_{T|S}$ *are estimated on a dataset independent of* $\{(Y_i, T_i, \boldsymbol{S}_i)\}_{i=1}^n$;
2. *at least one of the model specification conditions hold:*
   - $\widehat{p}_{T|S}(t|\boldsymbol{s}) \xrightarrow{P} \bar{p}_{T|S}(t|\boldsymbol{s}) = p_{T|S}(t|\boldsymbol{s})$ *(conditional density model),*
   - $\widehat{\mu}(t,\boldsymbol{s}) \xrightarrow{P} \bar{\mu}(t,\boldsymbol{s}) = \mu(t,\boldsymbol{s})$ *and* $\widehat{\beta}(t,\boldsymbol{s}) \xrightarrow{P} \bar{\beta}(t,\boldsymbol{s}) = \beta(t,\boldsymbol{s})$ *(outcome model);*
3. $$\sup_{|u-t|\le h} \left|\left|\widehat{p}_{T|S}(u|\boldsymbol{S}) - p_{T|S}(u|\boldsymbol{S})\right|\right|_{L_2} \left[\left|\left|\widehat{\mu}(t,\boldsymbol{S}) - \mu(t,\boldsymbol{S})\right|\right|_{L_2} + h\left|\left|\widehat{\beta}(t,\boldsymbol{S}) - \beta(t,\boldsymbol{S})\right|\right|_{L_2}\right] = o_P\left(\frac{1}{\sqrt{nh}}\right),$$

we prove that

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

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we prove that

- $$\sqrt{nh^3}\left[\widehat{\theta}_{\text{DR}}(t) - \theta(t)\right] = \frac{1}{\sqrt{n}}\sum_{i=1}^n \phi_{h,t}\left(Y_i, T_i, \boldsymbol{S}_i; \bar{\mu}, \bar{\beta}, \bar{p}_{T|S}\right) + o_P(1).$$
- $$\sqrt{nh^3}\left[\widehat{\theta}_{\text{DR}}(t) - \theta(t) - h^2 B_\theta(t)\right] \xrightarrow{d} \mathcal{N}\left(0, V_\theta(t)\right).$$

We can conduct asymptotically valid inference on $\theta(t) = \frac{d}{dt}\mathbb{E}\left[Y(t)\right]$ using

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

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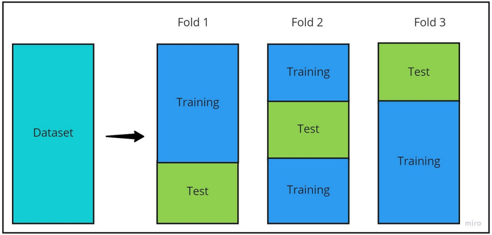
2. $\widehat{\mu}, \widehat{\beta}, \widehat{p}_{T|\boldsymbol{S}}$ can be estimated via sample-splitting or cross-fitting.



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2. $\widehat{\mu}, \widehat{\beta}, \widehat{p}_{T|\boldsymbol{S}}$ 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 $h = O\left(n^{-\frac{1}{5}}\right)$.
   - This order aligns with the outputs from usual bandwidth selection methods (Wand and Jones, 1994; Wasserman, 2006).

Why Do We Need Positivity?

Assumption (Identification Conditions)

1. *(Consistency)* $Y = Y(t)$ *whenever* $T = t \in \mathcal{T}$.
2. *(Ignorability or Unconfoundedness)* $Y(t) \perp\!\!\!\perp T \,\big|\, \boldsymbol{S}$ *for all* $t \in \mathcal{T}$.
3. *(**Positivity**)* $p_{T|\boldsymbol{S}}(t|\boldsymbol{s}) \geq p_{\min} > 0$ *for all* $(t, \boldsymbol{s}) \in \mathcal{T} \times \mathcal{S}$.

The RA (or G-computation) formulae are given by

$$m(t) = \mathbb{E}\left[Y(t)\right] = \mathbb{E}\left[\mu(t, \boldsymbol{S})\right] \quad \text{and} \quad \theta(t) = \frac{d}{dt}\mathbb{E}\left[Y(t)\right] = \mathbb{E}\left[\frac{\partial}{\partial t}\mu(t, \boldsymbol{S})\right].$$

The IPW approaches also rely on the following identities:

$$\lim_{h\to 0} \mathbb{E}\left[\frac{Y \cdot K\left(\frac{T-t}{h}\right)}{h \cdot p_{T|\boldsymbol{S}}(T|\boldsymbol{S})}\right] = \mathbb{E}\left[\mu(t, \boldsymbol{S})\right] \quad \text{and} \quad \lim_{h\to 0} \mathbb{E}\left[\frac{Y\left(\frac{T-t}{h}\right) K\left(\frac{T-t}{h}\right)}{\kappa_2\, h^2\, p_{T|\boldsymbol{S}}(T|\boldsymbol{S})}\right] = \mathbb{E}\left[\frac{\partial}{\partial t}\mu(t, \boldsymbol{S})\right].$$

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Identification Issue: Without positivity, $\mu(t, \boldsymbol{s}) = \mathbb{E}\left(Y | T = t, \boldsymbol{S} = \boldsymbol{s}\right)$ is *not well-defined* outside the support $\mathcal{J} \subset \mathcal{T} \times \mathcal{S}$ of the joint density $p(t, \boldsymbol{s})$.

Identification Strategy Without Positivity

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Assumption (Extrapolation Condition; Zhang et al. 2024)

Suppose that at least one of the following conditions are valid.

1. *The function* $\mathbb{E}\left[Y(t)|\boldsymbol{S} = \boldsymbol{s}\right]$ *is continuously differentiable with respect to* t *for any* $(t, \boldsymbol{s}) \in \mathcal{T} \times \mathcal{S}$ *with* $p_{S|T}(\boldsymbol{s}|t) > 0$ *and*

$$\theta(t) = \mathbb{E}\left[\frac{\partial}{\partial t}\mathbb{E}\left[Y(t)|\boldsymbol{S}\right]\right] = \mathbb{E}\left[\frac{\partial}{\partial t}\mathbb{E}\left[Y(t)|\boldsymbol{S}\right] \Big| T = t\right].$$

2. *The potential outcome* $Y(t)$ *is continuously differentiable with respect to* t *and*

$$\theta(t) = \mathbb{E}\left[\mathbb{E}\left[\frac{\partial}{\partial t}Y(t)\Big|\boldsymbol{S}\right]\right] = \mathbb{E}\left[\mathbb{E}\left[\frac{\partial}{\partial t}Y(t)\Big|\boldsymbol{S}\right] \Big| T = t\right].$$

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

Identification Strategy Without Positivity

If $\theta(t) = \frac{d}{dt}\mathbb{E}\left[Y(t)\right] = \mathbb{E}\left[\frac{\partial}{\partial t}\mathbb{E}\left[Y(t)|\boldsymbol{S}\right]\right] = \mathbb{E}\left[\frac{\partial}{\partial t}\mathbb{E}\left[Y(t)|\boldsymbol{S}\right]\middle|T = t\right]$ holds true, then

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&\overset{(*)}{=} \mathbb{E}\left[\frac{\partial}{\partial t}\mathbb{E}[Y(t)|T=t,\boldsymbol{S}]\Big|T=t\right] && \text{(*) Ignorability} \\
&\overset{(**)}{=} \mathbb{E}\left[\frac{\partial}{\partial t}\mathbb{E}(Y|T=t,\boldsymbol{S})\Big|T=t\right] && \text{(**) Consistency} \\
&= \mathbb{E}\left[\frac{\partial}{\partial t}\mu(t,\boldsymbol{S})\Big|T=t\right] := \theta_C(t).
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- For any $t \in \mathcal{T}$, the fundamental theorem of calculus reveals that

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- Taking the expectation on both sides of the above equality yields that

$$m(t) = \mathbb{E}(Y) + \mathbb{E}\left\{\int_{\widetilde{t}=T}^{\widetilde{t}=t} \mathbb{E}\left[\frac{\partial}{\partial t}\mu(\widetilde{t}, \boldsymbol{S})\Big|T = \widetilde{t}\right] d\widetilde{t}\right\}.$$

Validity of Our Identification Strategies Without Positivity

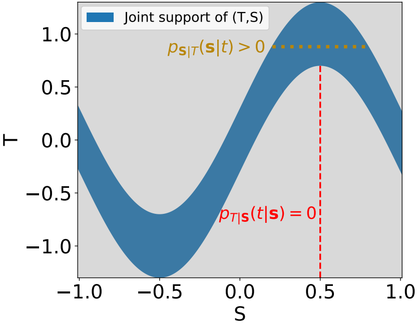
We identify $\theta(t)$ through

$$\theta_C(t) = \mathbb{E}\left[\frac{\partial}{\partial t}\mathbb{E}(Y|T=t,\boldsymbol{S})\middle|T=t\right] = \mathbb{E}\left[\frac{\partial}{\partial t}\mu(t,\boldsymbol{S})\middle|T=t\right].$$

- In contrast to the identification via $\mathbb{E}\left[\frac{\partial}{\partial t}\mu(t,\boldsymbol{S})\right]$ under positivity, we only need

$$\frac{\partial}{\partial t}\mu(t,\boldsymbol{s}) = \frac{\partial}{\partial t}\mathbb{E}(Y|T=t,\boldsymbol{s})$$

  to be well-defined when $p_{\boldsymbol{S}|T}(\boldsymbol{s}|t) > 0$.



Key Example: Additive Confounding Model

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

- $\bar{m} : \mathcal{T} \to \mathbb{R}$ and $\eta : \mathcal{S} \to \mathbb{R}$ are deterministic functions.
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- **RA estimator without positivity** (Zhang et al., 2024):

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

Estimation Biases of IPW Estimators Without Positivity

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

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$$\lim_{h\to 0} \mathbb{E}\left[\widetilde{m}_{\text{IPW}}(t)\right] = \bar{m}(t)\cdot\rho(t) + \omega(t) \neq m(t),$$

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Key Issue: The conditional support $\mathcal{S}(t)$ of $p_{\boldsymbol{S}|T}(\boldsymbol{s}|t)$ and the marginal support $\mathcal{S}$ of $p_{\boldsymbol{S}}(\boldsymbol{s})$ are different!!

Bias-Corrected IPW Estimator of $\theta(t)$

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

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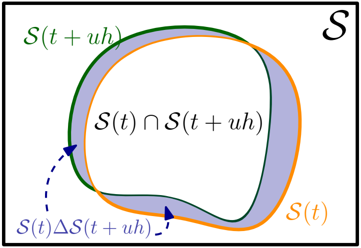
1. We first want to disentangle $\theta(t) = \bar{m}'(t)$ from the bias term:

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

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



Bias-Corrected IPW Estimator of $\theta(t)$

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

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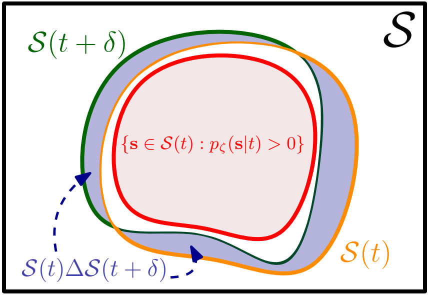
2. We replace $p_{S|T}(s|t)$ with a ζ-interior conditional density $p_\zeta(s|t)$ so that

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



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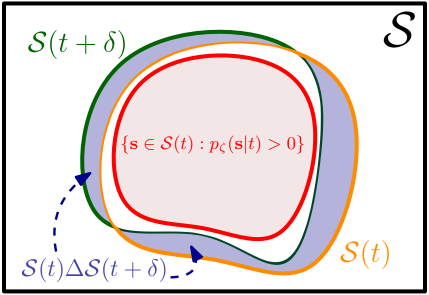

- Now, we have that $\mathbb{E}\left[\frac{Y\left(\frac{T-t}{h}\right)K\left(\frac{T-t}{h}\right)p_\zeta(\boldsymbol{S}|T)}{h^2\cdot\kappa_2\cdot p_{T|S}(T|\boldsymbol{S})\cdot p_S(\boldsymbol{S})}\right] = \bar{m}'(t) + O(h^2).$

ζ-Interior Conditional Density

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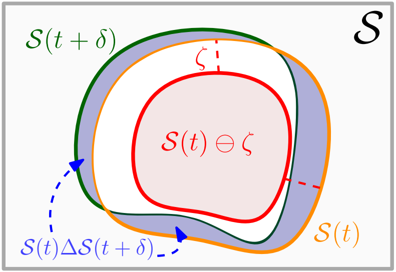
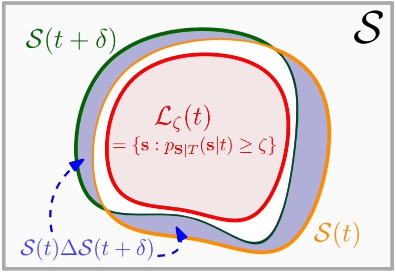
Support shrinking approach



Level set approach



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

and define

$$p_\zeta(\boldsymbol{s}|t) = \frac{p_{S|T}(\boldsymbol{s}|t) \cdot \mathbb{1}_{\{\boldsymbol{s} \in \mathcal{S}(t) \ominus \zeta\}}}{\int_{\mathcal{S}(t)\ominus\zeta} p_{S|T}(\boldsymbol{s}_1|t)\, d\boldsymbol{s}_1}.$$

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

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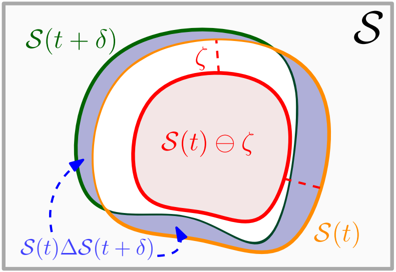

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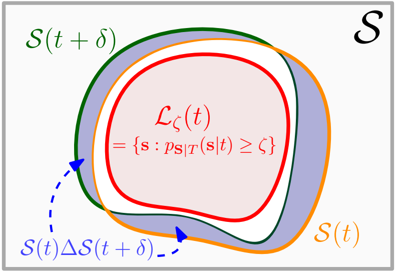

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Remark: Practically, the level set approach is recommended, because we only need to choose $\zeta > 0$.

Bias-Corrected IPW and DR Estimators of $\theta(t)$

- **Bias-Corrected IPW Estimator:**

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

where

- $\widehat{p}(t, \boldsymbol{s}), \widehat{p}_{\zeta}(\boldsymbol{s}|t)$ are estimators of $p(t, \boldsymbol{s}), p_{\zeta}(\boldsymbol{s}|t)$.
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- **Bias-Corrected DR Estimator:**

$$\begin{aligned}
&\widehat{\theta}_{\mathrm{C,DR}}(t) \\
&= \underbrace{\frac{1}{nh^2} \sum_{i=1}^{n} \frac{\left(\frac{T_i - t}{h}\right) K\left(\frac{T_i - t}{h}\right) \widehat{p}_\zeta(\boldsymbol{S}_i|t)}{\kappa_2 \cdot \widehat{p}(T_i, \boldsymbol{S}_i)} \left[Y_i - \widehat{\mu}(t, \boldsymbol{S}_i) - (T_i - t) \cdot \widehat{\beta}(t, \boldsymbol{S}_i)\right]}_{\text{IPW component}} \\
&\quad + \underbrace{\int \widehat{\beta}(t, \boldsymbol{s}) \cdot \widehat{p}_\zeta(\boldsymbol{s}|t)\, d\boldsymbol{s}}_{\text{RA component}}.
\end{aligned}$$

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* $\{(Y_i, T_i, \boldsymbol{S}_i)\}_{i=1}^n$;
2. $\sqrt{nh^3}\, ||\widehat{p}_\zeta(\boldsymbol{S}|t) - \bar{p}_\zeta(\boldsymbol{S}|t)||_{L_2} = o_P(1)$, *where* $\widehat{p}_\zeta(\boldsymbol{s}|t) \xrightarrow{P} \bar{p}_\zeta(\boldsymbol{s}|t)$;
3. *at least one of the model specification conditions hold:*
    - $\widehat{p}(t,\boldsymbol{s}) \xrightarrow{P} \bar{p}(t,\boldsymbol{s}) = p(t,\boldsymbol{s})$ *(joint density model),*
    - $\widehat{\mu}(t,\boldsymbol{s}) \xrightarrow{P} \bar{\mu}(t,\boldsymbol{s}) = \mu(t,\boldsymbol{s})$ *and* $\widehat{\beta}(t,\boldsymbol{s}) \xrightarrow{P} \bar{\beta}(t,\boldsymbol{s}) = \beta(t,\boldsymbol{s})$ *(outcome model);*
4. $$\sup_{|u-t|\le h} ||\widehat{p}(u,\boldsymbol{S}) - p(u,\boldsymbol{S})||_{L_2} \left[||\widehat{\mu}(t,\boldsymbol{S}) - \mu(t,\boldsymbol{S})||_{L_2} + h \left|\left| \widehat{\beta}(t,\boldsymbol{S}) - \beta(t,\boldsymbol{S}) \right|\right|_{L_2} \right] = o_P\left(\frac{1}{\sqrt{nh}}\right)$$

we prove that

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

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we prove that

- $$\sqrt{nh^3}\left[\widehat{\theta}_{\mathrm{C,DR}}(t) - \theta(t)\right] = \frac{1}{\sqrt{n}}\sum_{i=1}^n \phi_{C,h,t}\left(Y_i, T_i, \boldsymbol{S}_i; \bar{\mu}, \bar{\beta}, \bar{p}_{T|\boldsymbol{S}}\right) + o_P(1).$$
- $$\sqrt{nh^3}\left[\widehat{\theta}_{\mathrm{C,DR}}(t) - \theta(t) - h^2 B_{C,\theta}(t)\right] \xrightarrow{d} \mathcal{N}\left(0, V_{C,\theta}(t)\right).$$

Statistical Inference on $\theta(t)$ Without Positivity

Asymptotically valid inference on $\theta(t) = \frac{d}{dt}\mathbb{E}\left[Y(t)\right]$ can be done via

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

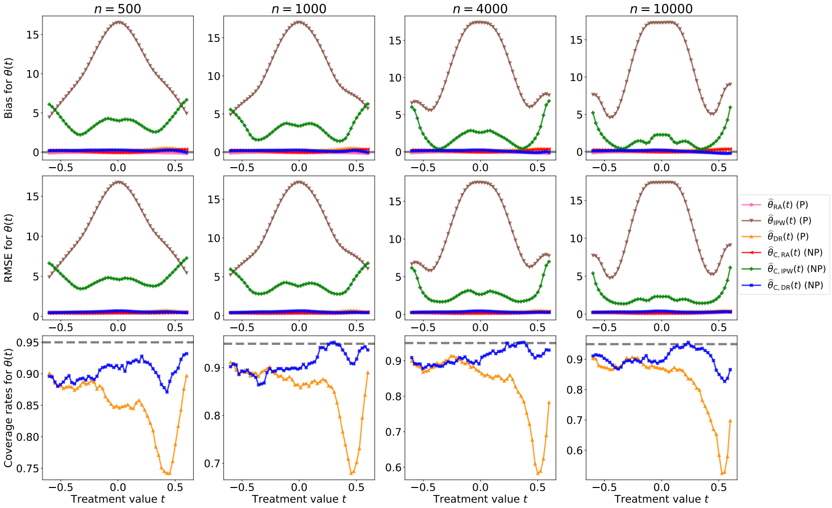
1. We estimate $V_{C,\theta}(t) = \mathbb{E}\left[\phi^2_{C,h,t}\left(Y, T, \boldsymbol{S}; \bar{\mu}, \bar{\beta}, \bar{p}, \bar{p}_\zeta\right)\right]$ with

   $$\phi_{C,h,t}\left(Y, T, \boldsymbol{S}; \bar{\mu}, \bar{\beta}, \bar{p}, \bar{p}_\zeta\right) = \frac{\left(\frac{T-t}{h}\right) K\left(\frac{T-t}{h}\right) \cdot \bar{p}_\zeta(\boldsymbol{S}|t)}{\sqrt{h} \cdot \kappa_2 \cdot \bar{p}(T, \boldsymbol{S})} \cdot \left[Y - \bar{\mu}(t, \boldsymbol{S}) - (T-t) \cdot \bar{\beta}(t, \boldsymbol{S})\right]$$

   by $\widehat{V}_{C,\theta}(t) = \frac{1}{n}\sum_{i=1}^{n} \phi^2_{C,h,t}\left(Y, T, \boldsymbol{S}; \widehat{\mu}, \widehat{\beta}, \widehat{p}, \widehat{p}_\zeta\right)$.
2. $\widehat{\mu}, \widehat{\beta}, \widehat{p}, \widehat{p}_\zeta$ can be estimated via sample-splitting or cross-fitting.
3. We choose an implicit undersmoothing bandwidth $h = O\left(n^{-\frac{1}{5}}\right)$ to neglect the bias $h^2 B_{C,\theta}(t)$.

Simulations Without Positivity

$$Y = T^3 + T^2 + 10S + \epsilon, \quad T = \sin(\pi S) + E, \quad S \sim \text{Unif}[-1,1],\ E \sim \text{Unif}[-0.3, 0.3].$$



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

A Case Study Under Positivity

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

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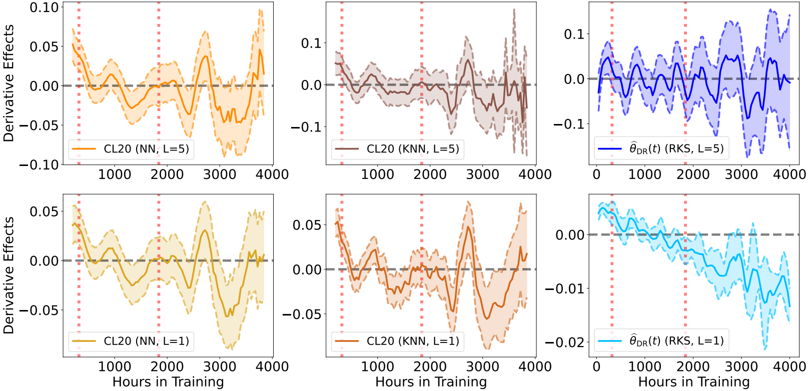

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Causal Inference Meets Geometric Data Analysis
(https://uwgeometry.github.io/)!

Open Questions and Future Work

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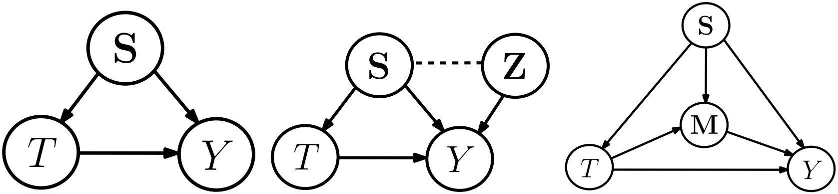
3. **Derivative Estimation in Other Causal Contexts:** Can we generalize our derivative estimators to other causal estimands:
   - instantaneous causal effect $\frac{d}{dt}\mathbb{E}\left[Y(t)|\boldsymbol{S}=\boldsymbol{s}\right]$ (Stolzenberg, 1980);
   - direct and indirect effects in mediation analysis (Huber et al., 2020)?



Thank you!

More details can be found in

[1] Y. Zhang, Y.-C. Chen, and A. Giessing. Nonparametric Inference on Dose-Response Curves Without the Positivity Condition. *arXiv preprint*, 2024. https://arxiv.org/abs/2405.09003.

[2] 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
hhttps://github.com/zhangyk8/npDRDeriv.

Python Package: npDoseResponse.

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Detailed Regularity Assumptions

Assumption (Differentiability of the conditional mean outcome function)

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

1. $\mu(t, \boldsymbol{s})$ *is at least four times continuously differentiable with respect to* t.
2. $\mu(t, \boldsymbol{s})$ *and all of its partial derivatives are uniformly bounded on* $\mathcal{T} \times \mathcal{S}$.

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

Assumption (Differentiability of the density functions)

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

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

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

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

Assumption (Smoothness condition on $\mathcal{S}(t)$)

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

1. **Self-Normalized Estimators Under Positivity:**

$$\widehat{\theta}_{\mathrm{IPW}}^{\mathrm{norm}}(t) = \frac{\widehat{\theta}_{\mathrm{IPW}}(t)}{\frac{1}{nh}\sum_{j=1}^{n} \frac{K\left(\frac{T_j-t}{h}\right)}{\widehat{p}_{T|S}(T_j|\mathbf{S}_j)}} = \frac{\sum_{i=1}^{n} \frac{Y_i\left(\frac{T_i-t}{h}\right)K\left(\frac{T_i-t}{h}\right)}{\widehat{p}_{T|S}(T_i|\mathbf{S}_i)}}{\kappa_2 h \sum_{j=1}^{n} \frac{K\left(\frac{T_j-t}{h}\right)}{\widehat{p}_{T|S}(T_j|\mathbf{S}_j)}},$$

and

$$\widehat{\theta}_{\mathrm{DR}}^{\mathrm{norm}}(t) = \frac{\sum_{i=1}^{n} \frac{\left[Y_i-\widehat{\mu}(t,\mathbf{S}_i)-(T_i-t)\cdot\widehat{\beta}(t,\mathbf{S}_i)\right]\left(\frac{T_i-t}{h}\right)K\left(\frac{T_i-t}{h}\right)}{\widehat{p}_{T|S}(T_i|\mathbf{S}_i)}}{\kappa_2 h \sum_{j=1}^{n} \frac{K\left(\frac{T_j-t}{h}\right)}{\widehat{p}_{T|S}(T_j|\mathbf{S}_j)}} + \frac{1}{n}\sum_{i=1}^{n} \widehat{\beta}(t,\mathbf{S}_i).$$

2. **Self-Normalized Estimators Without Positivity:**

$$\widehat{\theta}_{\text{C,IPW}}^{\text{norm}}(t) = \frac{\widehat{\theta}_{\text{C,IPW}}(t)}{\frac{1}{nh}\sum_{j=1}^{n} \frac{K\left(\frac{T_j-t}{h}\right)\cdot \widehat{p}_{\zeta}(\boldsymbol{S}_j|t)}{\widehat{p}(T_j,\boldsymbol{S}_j)}} = \frac{\sum_{i=1}^{n} \frac{Y_i\left(\frac{T_i-t}{h}\right)K\left(\frac{T_i-t}{h}\right)\cdot \widehat{p}_{\zeta}(\boldsymbol{S}_i|t)}{\widehat{p}(T_i,\boldsymbol{S}_i)}}{\kappa_2 h \sum_{j=1}^{n} \frac{K\left(\frac{T_j-t}{h}\right)\cdot \widehat{p}_{\zeta}(\boldsymbol{S}_j|t)}{\widehat{p}(T_j,\boldsymbol{S}_j)}},$$

and

$$\widehat{\theta}_{\text{C,DR}}^{\text{norm}}(t) = \frac{\sum_{i=1}^{n} \frac{\left[Y_i-\widehat{\mu}(t,\boldsymbol{S}_i)-(T_i-t)\cdot\widehat{\beta}(t,\boldsymbol{S}_i)\right]\left(\frac{T_i-t}{h}\right)K\left(\frac{T_i-t}{h}\right)\cdot \widehat{p}_{\zeta}(\boldsymbol{S}_i|t)}{\widehat{p}(T_i,\boldsymbol{S}_i)}}{\kappa_2 h \sum_{j=1}^{n} \frac{K\left(\frac{T_j-t}{h}\right)\cdot \widehat{p}_{\zeta}(\boldsymbol{S}_j|t)}{\widehat{p}(T_j,\boldsymbol{S}_j)}} + \int \widehat{\beta}(t,\boldsymbol{s})\cdot \widehat{p}_{\zeta}(\boldsymbol{s}|t)\,d\boldsymbol{s}.$$

Simulations Under the Positivity Condition

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

$$Y = 1.2\,T + T^2 + TS_1 + 1.2\,\boldsymbol{\xi}^T\boldsymbol{S} + \epsilon\sqrt{0.5 + F_{\mathcal{N}(0,1)}(S_1)}, \quad \epsilon \sim \mathcal{N}(0,1),$$

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

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 Under the Positivity Condition

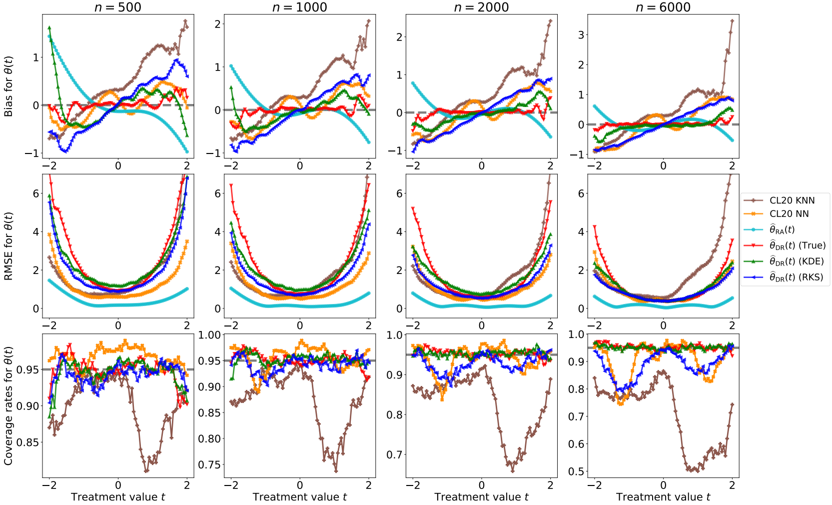

Figure: Comparisons between our proposed estimators and the finite-difference approaches by Colangelo and Lee (2020) ("CL20") under positivity and with 5-fold cross-fitting across various sample sizes.

Simulations Under the Positivity Condition

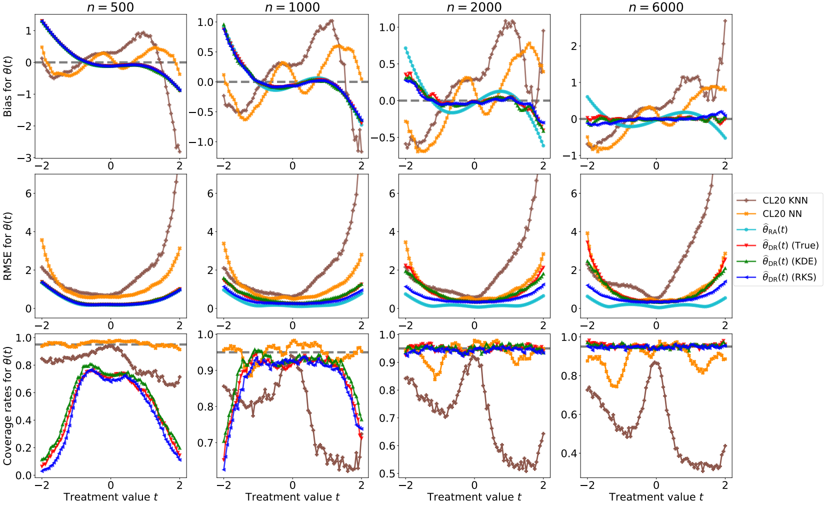

Figure: Comparisons between our proposed estimators and the finite-difference approaches by Colangelo and Lee (2020) ("CL20") under positivity and **without cross-fitting** across various sample sizes.