Lecture 4: Bias-variance trade-off with infinite-dimensional nuisance parameters

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Outline

A statistical estimation problem

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$$\mathbb{E}_{\mathrm{P}} \left[f_P(1, X) - f_P(0, X) \right],$$

with $f_P(a, x) := \mathbb{E}_{\mathrm{P}} \left[Y \mid A = a, X = x \right]$. The target parameter is

$$\Psi(\mathrm{P}) = \mathbb{E}_{\mathrm{P}} \left[f_{\mathrm{P}}(1, X) - f_{\mathrm{P}}(0, X) \right].$$

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$$\Psi(P) = \tilde{\Psi}(f, \mu) := \int_{\mathbb{R}^p} [f(1, x) - f(0, x)] \, \mathrm{d}\mu(x),$$

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where μ is the marginal distribution of X. The nuisance parameters are f and μ. This immediately suggests the target estimator

$$\hat{\psi}_n^{\text{g-formula}} = \Psi(\hat{f}_n, \hat{\mu}_X).$$

For instance, if we use $\hat{\mu}_X = \hat{\mathbb{P}}_n$ we have

$$\hat{\psi}_n^{\text{g-formula}} = \tilde{\Psi}(\hat{f}_n, \hat{\mathbb{P}}_n) = \frac{1}{n} \sum_{i=1}^{n} \left\{ \hat{f}_n(1, X_i) - \hat{f}_n(0, X_i) \right\}.$$

Hence we just have to select a nuisance estimator $\hat{f}_n$.

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We will demonstrate this with the following a toy example.

Toy example: Integrated kernel density

$\mathcal{P}$ consist all probability measures with continuous Lebesgue-density (this is an infinite-dimensional space). We want to estimate $F_P(x) = P(X \leq x)$ for unknown $P \in \mathcal{P}$.

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$$\hat{f}_n(x) = \hat{\mathbb{P}}_n[k_h(X, x)] = \frac{1}{n}\sum_{i=1}^{n} k_h(X_i, x),$$

to estimate the density f, where $h \in \mathbb{R}_+$ is the bandwidth (a tuning parameter).

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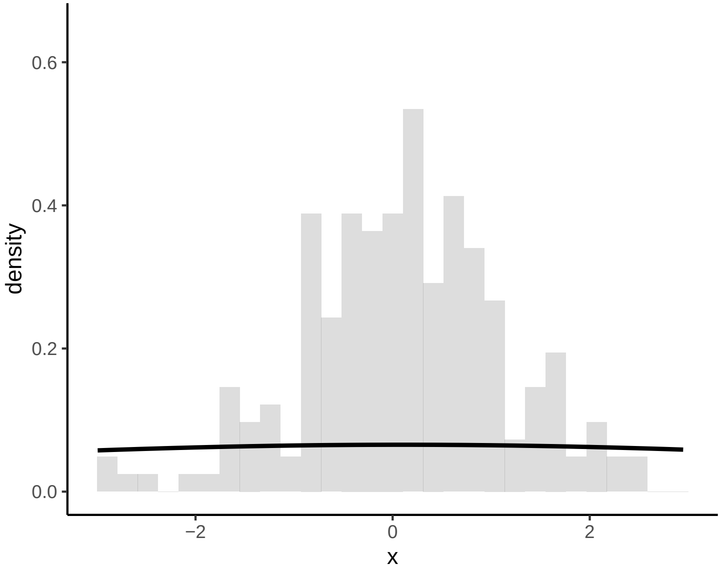
Visualize kernel estimator

small h large



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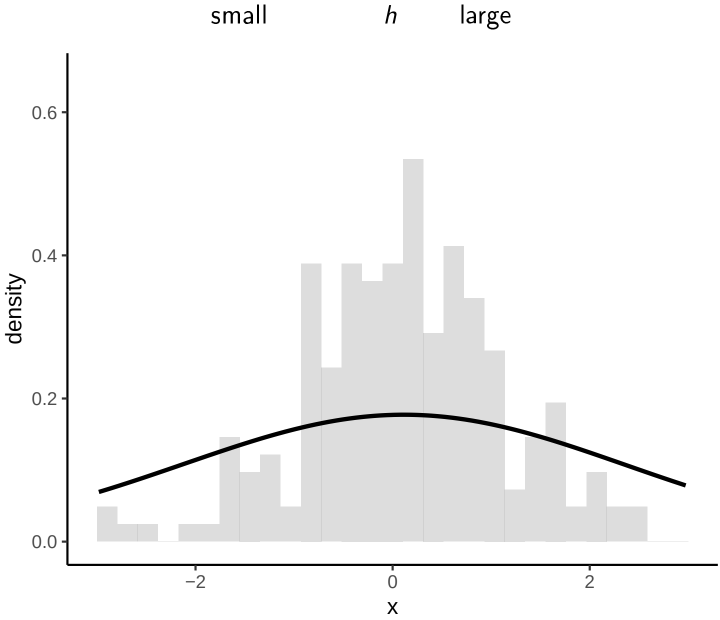

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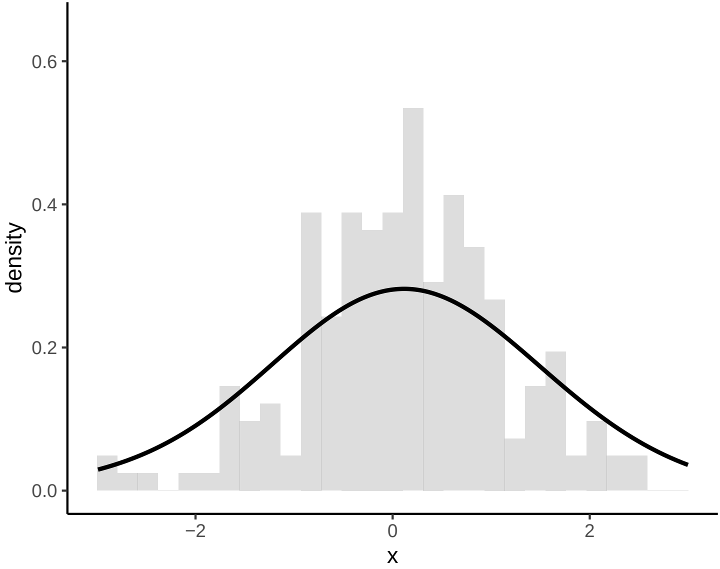

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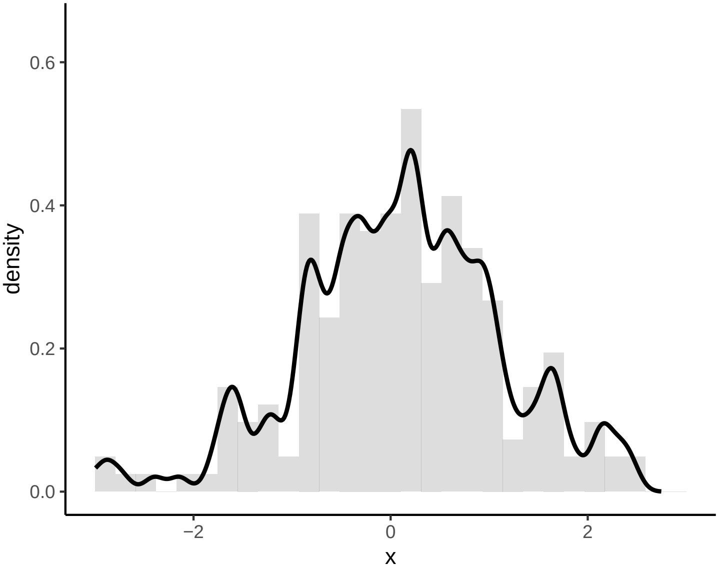

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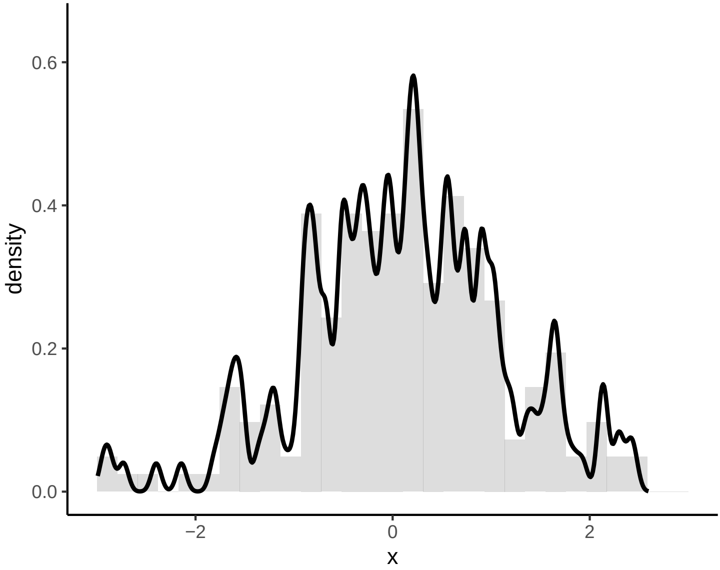

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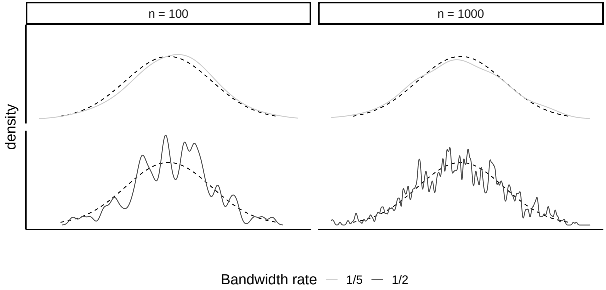

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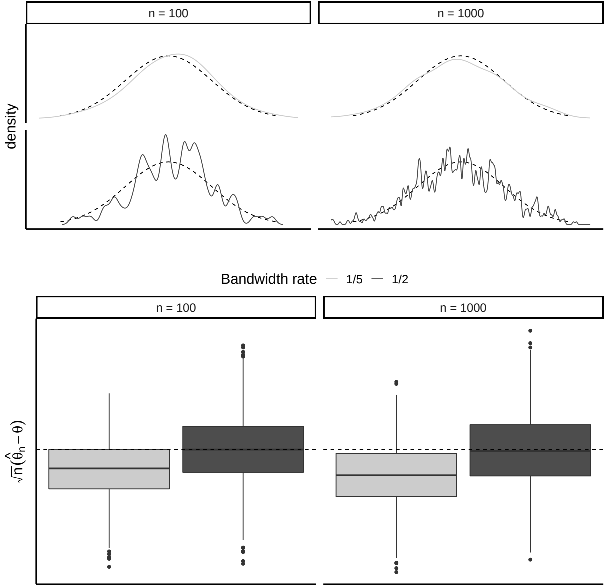

What happened?

The bias-variance trade-off for the nuisance parameter f is

$$\mathrm{MSE}(\hat{f}_n) = C_1 h^4 + C_2(nh)^{-1} + \mathcal{O}(h^2) + \mathcal{O}(n^{-1}),$$

where $n \to \infty$ and $h \to 0$. This implies that the optimal value for the bandwidth h is $h \asymp n^{-1/5}$ [van der Vaart, 2000, chp. 24].

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For the target parameter $\int_{-\infty}^{x} f(z)\,\mathrm{d}\lambda(z)$ the bias-variance "trade-off" becomes

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Using $h = 0$ can be interpreted as just using the empirical distribution function $\hat{F}_n$, i.e.,

$$\int_{-\infty}^{x} \hat{f}_n(z)\,\mathrm{d}z = \hat{\mathbb{P}}_n\left[\int_{-\infty}^{x} k_h(X_i, z)\,\mathrm{d}z\right] \longrightarrow \hat{\mathbb{P}}_n[\mathbb{1}(X_i \leq x)] =: \hat{F}_n(x).$$

The bias-variance tradeoff revisited

Consider a statistical estimation problem $(\mathcal{P}, \Psi)$ for which we can write $\Psi(\mathrm{P}) = \tilde{\Psi}(\mathrm{P}, \nu) = \mathrm{P}[\varphi(O, \nu)]$.

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$$\begin{aligned}
\sqrt{n}\left(\hat{\theta}_n - \theta\right) &= \sqrt{n}\left(\tilde{\Psi}(\hat{\mathbb{P}}_n, \hat{\nu}_n) - \tilde{\Psi}(\mathrm{P}, \nu)\right) \\
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with $\mathbb{G}_n := \sqrt{n}(\hat{\mathbb{P}}_n - \mathrm{P})$ the empirical process.

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$\tilde{\Psi}(\mathrm{P}, \hat{\nu}_n) - \tilde{\Psi}(\mathrm{P}, \nu)$ is bias $\rightarrow$ This is what ruined the naive plug-in strategy!

Finite- versus infinite-dimensional nuisance parameters

This phenomena only occurs when there are infinite-dimensional nuisance parameters (e.g., smooth functions, shape-constrained densities, etc.) – or more precisely, when we do not have parametric ($n^{-1/2}$) rate of convergence for the nuisance parameter estimator.

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$$\sqrt{n}(\hat{\nu}_n - \nu) \rightsquigarrow \mathcal{N}(0, \sigma^2)$$

then, by the delta method, also

$$\sqrt{n}(\Psi(\hat{\nu}_n) - \Psi(\nu)) \rightsquigarrow \mathcal{N}(0, \dot{\Psi}\sigma^2).$$

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When ν is infinite-dimensional this no longer holds $\rightarrow$ we have to do something different.

Functional derivatives (brief digression)

Functional derivatives and von Mises expansions are useful for analyzing and handling the issues we have encountered [Serfling, 1980].

Defining a functional derivative

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A linear approximation $\dot{\Psi}_P$ of the map Ψ at $P \in \mathcal{P}$, i.e.,

$$\left\| \Psi(P + \varepsilon_n g_n) - \Psi(P) - \dot{\Psi}_P(\varepsilon_n g_n) \right\| = \mathcal{O}(\varepsilon_n),$$

when $\varepsilon_n \to 0$.

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- Which norm on $\mathcal{P}$ should we use?
- Is there a natural space $\mathcal{M}$ in which to embed $\mathcal{P}$?

Gâteaux and Hadamard differentiability

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A stronger type is *Hadamard differentiability* which demands that the linear approximation is valid along any converging sequence $g_n \to g$. A Hadamard differentiable map is also called *compactly differentiable*, because this requirement is equivalent to a uniformly valid linear approximation over compact subsets [Reeds, 1976]. This makes Hadamard differentiability well-suited for statistical problems [Gill et al., 1989, van der Vaart, 2000].

If Ψ is Hadamard differentiability, Ψ is also Gâteaux differentiability, and in that case the Hadamard and Gâteaux derivative are identical.

The efficient influence function

(bag to the statistical estimation problem)

Hadamard differentiability and the canonical gradient

The "gradient" of $\Psi \colon \mathcal{P} \to \mathbb{R}$ is called the *canonical gradient* or *efficient influence function* of a statistical estimation problem $(\mathcal{P}, \Psi)$, and it is a fundamental object for semi-parametric efficiency theory – we will see why in a moment. More formally we define (following Bickel et al. [1993]):

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Definition (Tangent space)

The *tangent space* $\dot{\mathcal{P}}_P$ for the model $\mathcal{P}$ at $P \in \mathcal{P}$ is the (closed linear span of the) collection of (Hadamard) derivatives $\dot{P}_\varepsilon$ for all one-dimensional parametric submodel $P_\varepsilon \subset \mathcal{P}$ with $P_0 = P$.

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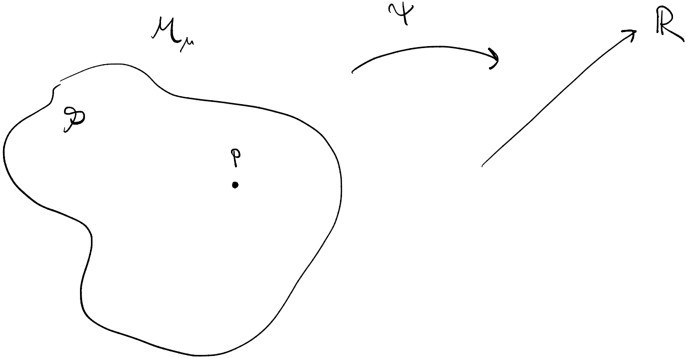
[1] This just means that the Ψ and $\dot{\Psi}_P$ need only be defined on the subsets $\mathcal{P} \subset \mathcal{M}$ and $\dot{\mathcal{P}}_P \subset \mathcal{M}$, respectively.

Visualization

Think of the gradient of a function defined on manifold (e.g., a surface).



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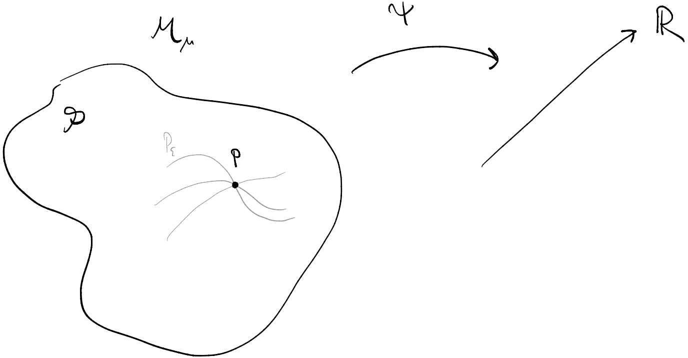

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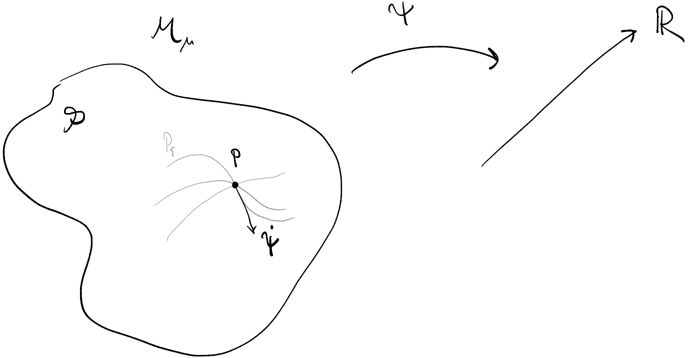

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By Riesz' representation theorem, and the (Hadamard) chain rule, this implies that the canonical gradient (efficient influence function) $\dot{\Psi}_P$ can be identified with an element $\varphi_P \in \dot{\mathcal{P}}_P \subset \mathcal{L}_0^2(P)$ such that

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holds for any differentiable submodel P_ε with score function $\dot{\ell}_0$, where $= \langle \varphi_P, \dot{\ell}_0 \rangle_{\mathrm{P}} = \int \varphi_P(o)\dot{\ell}_0(o)\, \mathrm{d}P(o)$.

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In the important special case of a *fully non-parametric model* $\mathcal{P}$, $\dot{\mathcal{P}}_P = \mathcal{L}_0^2(P)$ and thus (2) alone uniquely identifies the function φ_P.

Efficient estimation and the canonical gradient

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Definition (RAL estimators)

An estimator $\hat{\theta}_n$ of the parameter $\theta = \Psi(P)$ under the model $\mathcal{P}$, is called *asymptotically linear* with *influence function* $\mathrm{IF}(\cdot, P) \in \mathcal{L}^2_{\mathrm{P}}$, if $P[\mathrm{IF}(O, P)] = 0$ for all $P \in \mathcal{P}$, and

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Information bound

The *information bound* for estimating Ψ in the model $\mathcal{P}$ is

$$\mathcal{I}(\mathcal{P}, \Psi) := \inf_{P_\varepsilon} \{\mathcal{I}(P_\varepsilon, \Psi)\}, \quad \text{with} \quad \mathcal{I}(P_\varepsilon, \Psi) := \frac{P[\dot{\ell}_0^2]}{(\partial_0 \Psi(P_\varepsilon))^2}.$$

It holds that $\mathcal{I}(\mathcal{P}, \Psi)^{-1} = P[\varphi^2]$.

Debiasing and the canonical gradient

Recall the statistical estimation problem $\Psi(P) = \tilde{\Psi}(P, \nu) = P[\varphi(O, \nu)]$ and the decomposition

$$\sqrt{n}(\hat{\theta}_n - \theta) = \mathbb{G}_n[\varphi(O, \hat{\nu}_n)] + \sqrt{n}\left\{\tilde{\Psi}(P, \hat{\nu}_n) - \tilde{\Psi}(P, \nu)\right\}.$$

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[2] This property is referred to as *Neyman orthogonality*, and is a central component of "debiased machine learning"; see Chernozhukov et al. [2018] for details.

Summary

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- Instead we should aim at constructing estimators that have the canonical gradient (efficient influence function) as their influence function.
- This provides estimators with a bias-variance trade-off that is optimized for the *target parameter* instead of the nuisance parameter, because such estimators are *efficient* and have *vanishing first order bias*, asymptotically.

Exercises

How do we find the efficient influence function for a statistical estimation problem?

Introduction: Finding the canonical gradient for a given Ψ

We can (informally and heuristically[3]) find a candidate for the efficient influence function by calculating the Gâteaux derivative of Ψ at δ_O, where δ_O is the Dirac measure in the point O:

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Letting $h \to 0$, we get a candidate for the efficient influence function:

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[4] One should then verify that the found the candidate φ_P fulfills (2) for *all* parametric sub-model. In addition, if we impose restrictions on $\mathcal{P}$ such that $\dot{\mathcal{P}}_P$ is a proper subset of $\mathcal{L}_0^2(P)$ we also need to check that $\varphi_P \in \dot{\mathcal{P}}_P$.

Exercise 1 – efficient influence function of the toy example

Find a candidate for the efficient influence function by calculating the Gâteaux derivative of Ψ at δ_X for $\Psi(P) = F_P(x)$ where

$$F_P(x) = P(X \leq x) = \int_{-\infty}^{x} \mathrm{d}P(z)$$

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$$f(1,x) = \int_{\mathcal{Y}} y \frac{P(\mathrm{d}y, 1, x)}{\int_{\mathcal{Y}} P(\mathrm{d}y, 1, x)},$$

Exercise 2 – first step

Express $\Psi(P) = \int_{\mathcal{X}} f(1,x)\mu_P(\mathrm{d}x)$ explicitly as a functional of P: We can write

$$\mu_P(x) = \sum_{a=0}^{1} \int_{\mathcal{Y}} P(\mathrm{d}y, a, x),$$

and

$$f(1,x) = \int_{\mathcal{Y}} y \frac{P(\mathrm{d}y, 1, x)}{\int_{\mathcal{Y}} P(\mathrm{d}y, 1, x)},$$

so

$$\Psi(P_\varepsilon) = \int_{\mathcal{X}} \left\{ \frac{\int_{\mathcal{Y}} y \, P_\varepsilon(\mathrm{d}y, 1, x)}{\int_{\mathcal{Y}} P_\varepsilon(\mathrm{d}y, 1, x)} \left(\sum_{a=0}^{1} \int_{\mathcal{Y}} P_\varepsilon(\mathrm{d}y, a, \mathrm{d}x) \right) \right\}.$$

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