Debiasing and functional derivatives

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June 2, 2023

Outline

- Understand the efficient influence curve as the derivative of our target parameter
- Investigate the bias-variance trade-off with infinite-dimensional nuisance parameters
- See how the derivative interpretation can help us understand targeted/debiased estimation strategies

High-level perspective on a statistical problem

Example (the average treatment effect)

Given i.i.d. data $O_i = (X_i, A_i, Y_i) \in \mathbb{R}^d \times \{0,1\} \times \mathbb{R}$, estimate

$$\mathbb{E}_P[f(1,W) - f(0,W)], \quad \text{with} \quad f(a,x) = \mathbb{E}_P[Y \mid A = a, X = x],$$

assuming $P(A = 1 \mid X = x) \in [\varepsilon, 1-\varepsilon]$ for all x for some fixed $\varepsilon > 0$.

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- Ψ the target parameter of interest
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The targeted learning philosophy tells us that any statistical estimation problem is essentially characterized by

$$\begin{aligned} \Psi &= \mathbb{E}_P\left[f(1,W) - f(0,W)\right] \\ \mathcal{P} &= \text{all distributions } P \text{ such that } P(A = 1 \mid X = x) \in [\varepsilon, 1-\varepsilon] \end{aligned}$$

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What can we say about

- the statistical problem $(\Psi, \mathcal{P})$?
- estimators of $\Psi(P)$ based on data generated by some $P \in \mathcal{P}$?

General approach – understand the derivative of Ψ

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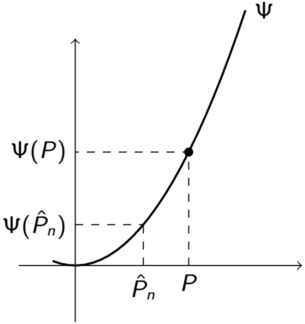

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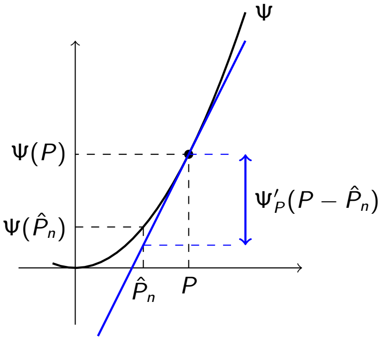

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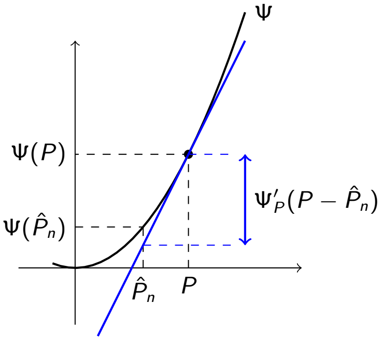

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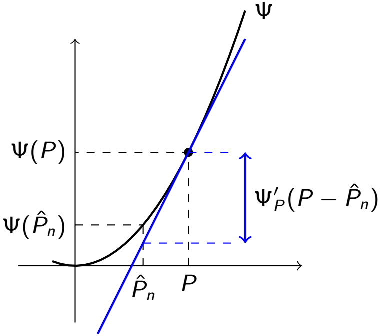

- The derivative provides a local approximation of the map Ψ around P
- We can think of estimation of P as approaching P with our estimator $\hat{P}_n$
- Thus, asymptotically, the derivative could give us a good idea about the behavior of $\Psi(\hat{P}_n)$

Geometric perspective

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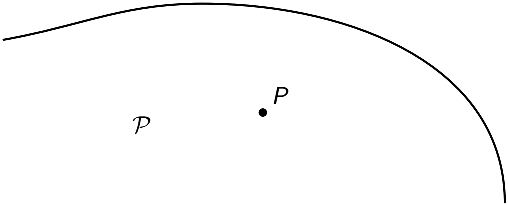

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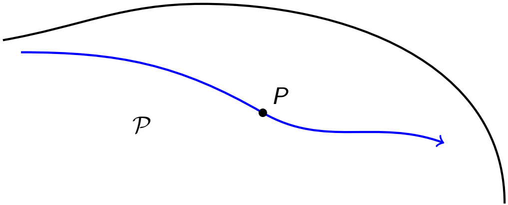

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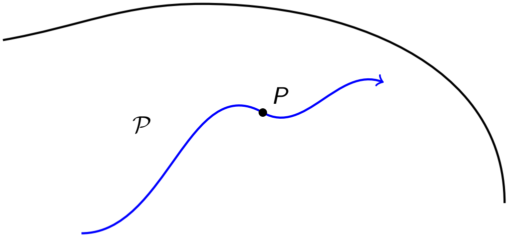

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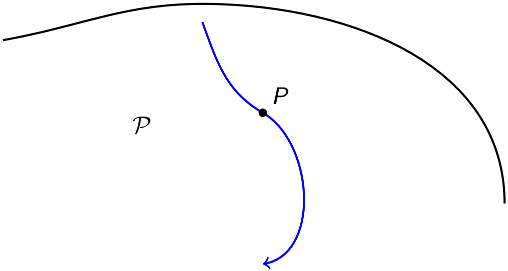

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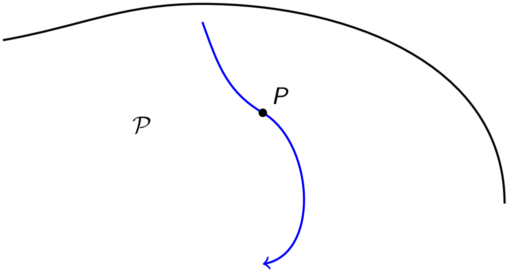

Using finite-dimensional submodels we know how to talk about the *likelihood* and the *score function* of such models. The tangent space is the collection of all score functions,

$$\dot{\mathcal{P}}_P = \overline{\mathrm{span}}\{\dot{\ell}_0\}, \quad \text{where} \quad \dot{\ell}_0 = \frac{\partial}{\partial t}\Big|_{t=0} \log(p_t), \quad P_t = p_t \cdot \mu.$$

Gradients

One can show that $\dot{\mathcal{P}}_P \subset \mathcal{L}_0^2(P) = \{f \in \mathcal{L}^2(P) : P[f] = 0\}$, where $\mathcal{L}^2(P)$ is the Hilbert space of P-square integrable functions with inner product $\langle f, g \rangle_P = P[fg] = \mathbb{E}_P\,[f(O)g(O)]$.

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A *gradient* is a function $g \in \mathcal{L}_0^2(P)$ such that

$$\frac{\partial}{\partial t}\bigg|_{t=0} \Psi(P_t) = \langle g, \dot{\ell}_0 \rangle_P, \quad \text{for all submodels } \{P_t\} \text{ with score } \dot{\ell}_0.$$

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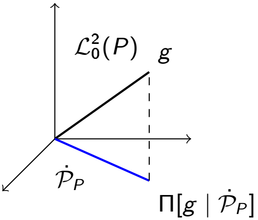
The canonical gradient can be found as the projection of any gradient onto the tangent space,

$$\varphi_P = \Pi[g \mid \dot{\mathcal{P}}_P].$$



Derivative and the chain rule

If $t \mapsto P_t \in \mathbb{R}^k$ and $\Psi \colon \mathbb{R}^k \to \mathbb{R}$, the chain rule tells us that

$$(\Psi \circ P)'(t) = (\Psi'(P_t))^T P_t' = \left\langle \Psi'(P_t), P_t' \right\rangle .$$

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Define the canonical gradient as a function such that the chain rule holds

$$\Updownarrow$$

Define a suitable type of derivative and then prove that the chain rule holds

Submodels and information bounds

For a one-dimensional submodel $\{P_t\}$ the Cramér-Rao bound states

$$\mathrm{Var}[\hat{\Psi}_n] \geq \frac{\left(\frac{\partial}{\partial t}\Big|_{t=0} \Psi(P_t)\right)^2}{P[\dot{\ell}_0^2]} =: V(\{P_t\}, \Psi),$$

for any (suitably regular) estimator $\hat{\Psi}_n$. The *information bound* for the finite-dimensional model $\{P_t\}$ is $\mathcal{I}(\{P_t\}, \Psi) = V(\{P_t\}, \Psi)^{-1}$.

The information bound for the full model $\mathcal{P}$ is

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$\mathcal{I}(\mathcal{P}, \Psi)^{-1} = P[\varphi_P^2]$, where φ_P is the canonical gradient.

Influence functions and RAL estimators

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

$$\hat{\Psi}_n - \Psi = \mathbb{P}_n[\mathrm{IF}(\cdot, P)] + o_P(n^{-1/2}).$$

In particular, the asymptotic variance of $\hat{\Psi}_n$ is $P[\mathrm{IF}(\cdot, P)^2]$.

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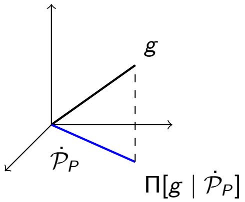
This implies that a RAL estimator with φ_P as influence function will be *efficient* – it has lowest possible asymptotic variance among all RAL estimators.



Summary so far

- The geometric perspective is useful because it allows us to talk about how difficult a statistical problem is through the information bound.
- The differential perspective is useful because it provides us with a completely description of the asymptotic behavior of any (RAL) estimator.
- It even suggests a strategy for constructing efficient estimators.

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- It even suggests a strategy for constructing efficient estimators.

$\rightarrow$ We move on to talk a bit more about estimation, in particular ...

Estimating low-dimensional target parameters using estimators of infinite-dimensional nuisance parameters

The naïve plug-in strategy

Often we can write

$$\Psi(P) = \tilde{\Psi}(Q(P)),$$

for some nuisance parameter Q.

Natural strategy: Estimate Q with $\hat{Q}_n$ and use $\hat{\Psi}_n = \tilde{\Psi}(\hat{Q}_n)$.

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so here $Q = (f, \mu)$. This suggests using

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

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When $Q \in \mathbb{R}^k$ then, under regularity conditions, we have

- if $\hat{Q}_n$ is asymptotically linear so is $\tilde{\Psi}(\hat{Q}_n)$
- if $\hat{Q}_n$ is efficient so is $\tilde{\Psi}(\hat{Q}_n)$

Infinite-dimensional nuisance parameter

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Example (Kernel density plug-in)

Consider the problem of estimating

$$\Psi(P) = P(X \leq x), \quad \text{for some fixed} \quad x \in \mathbb{R}.$$

We assume that P has a Lebesgue density and write

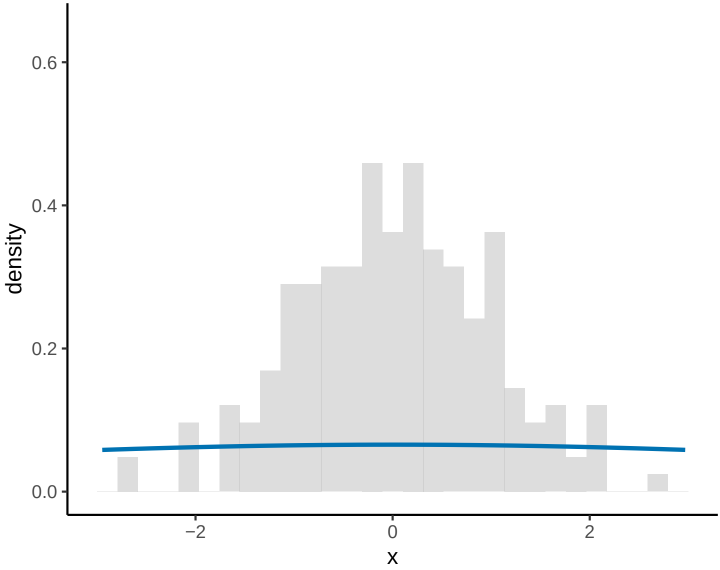
$$\Psi(P) = \tilde{\Psi}(f) := \int_{-\infty}^{x} f(z)\,\mathrm{d}z.$$

We decide to estimate Ψ by first estimating the density f with a kernel-based density estimator $\hat{f}_h$. We then obtain an estimator of Ψ as

$$\hat{\Psi}_n = \tilde{\Psi}(\hat{f}_h) = \int_{-\infty}^{x} \hat{f}_h(z)\,\mathrm{d}z.$$

Kernel estimator and bandwidth

small h large



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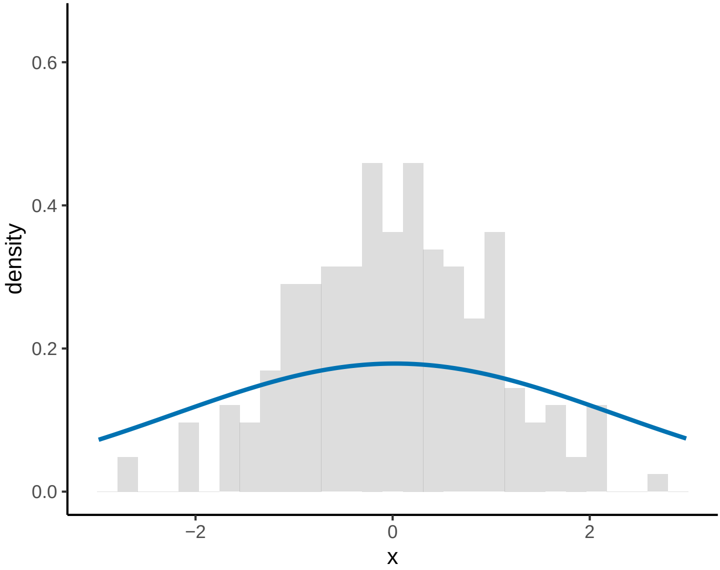

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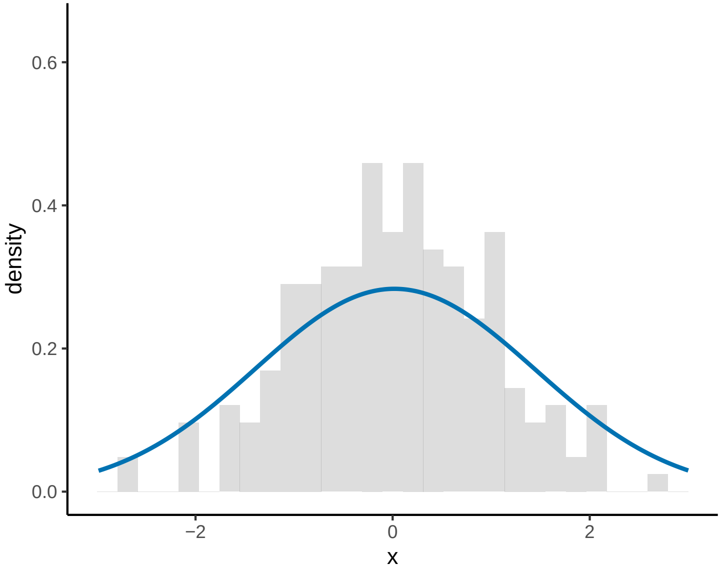

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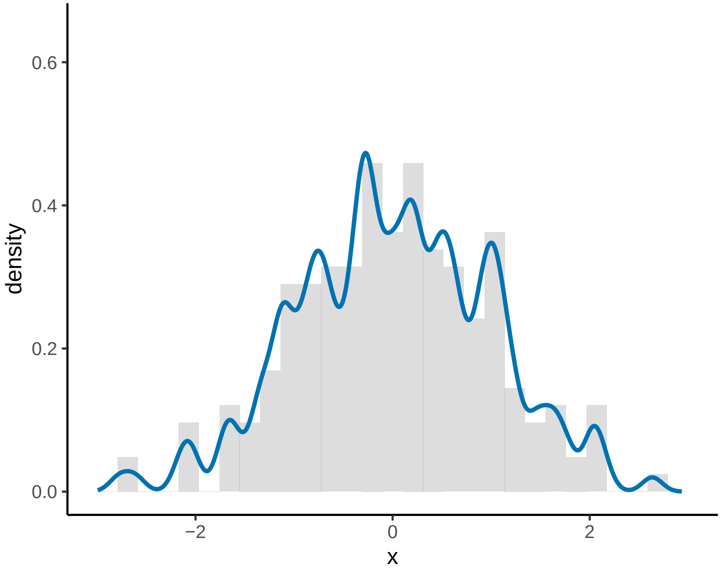

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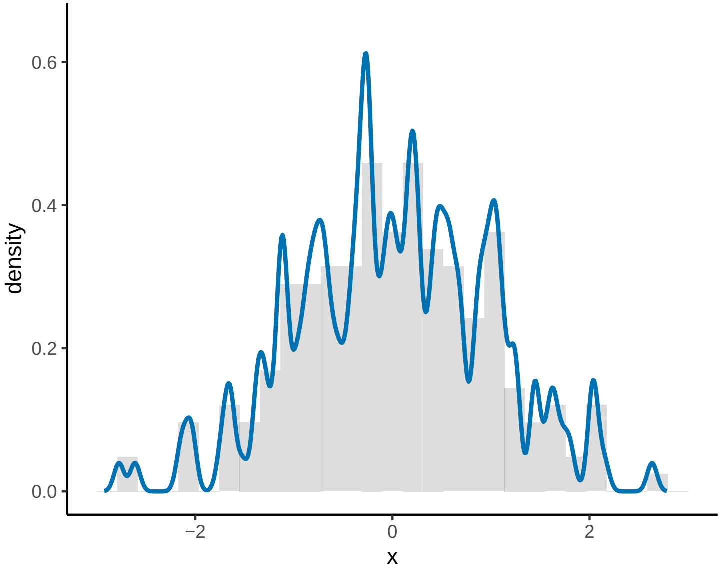
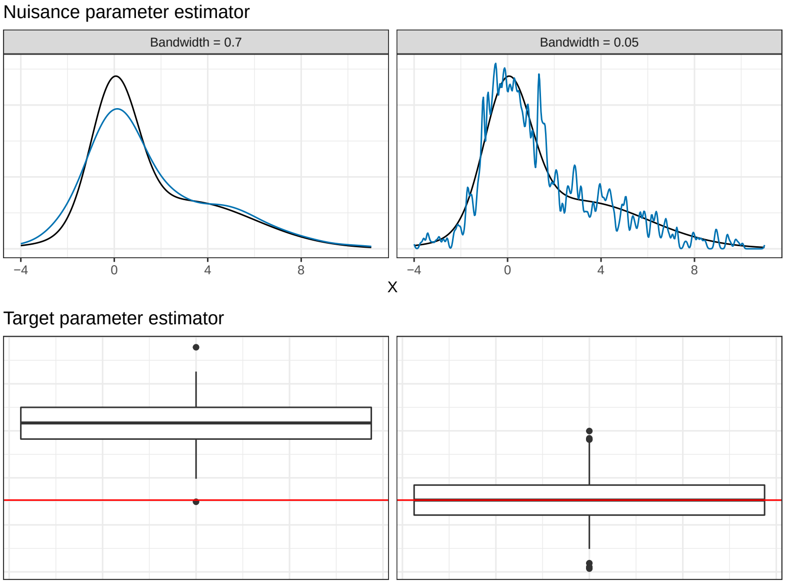
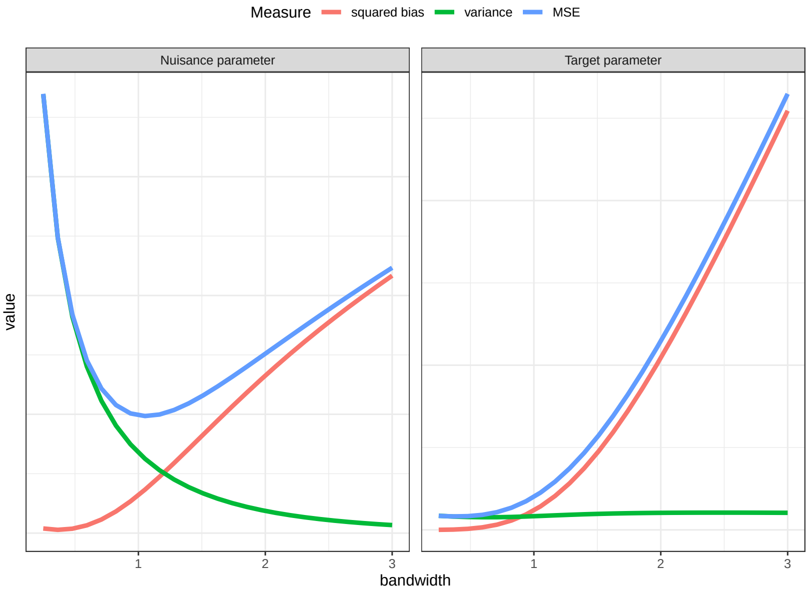


How does this work?



Exercise

Conclusion from the exercise – bias-variance trade-off



Decomposition

For a general problem, we can write

$$n^{1/2}\left(\Psi(\hat{P}_n) - \Psi(P)\right) = n^{1/2}\left(\Psi(\hat{P}_n) - \Psi(P)\right) + \mathbb{G}_n[\varphi_P - \varphi_{\hat{P}_n}] + o_P(1),$$

where $\mathbb{G}_n := n^{1/2}(\mathbb{P}_n - P)$ is the empirical process and φ the canonical gradient, when $\varphi_{\hat{P}_n} \xrightarrow{P} \varphi_P$. Informally, imagine that $\mathbb{G}_n$ and $\hat{P}_n$ are independent; then

$$\mathbb{G}_n[\varphi_P - \varphi_{\hat{P}_n}] \sim \mathcal{N}\left(0, P\left[\left(\varphi_{\hat{P}_n} - \varphi_P\right)^2\right]\right) \rightsquigarrow 0.$$

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Thus

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One-step $\hat{\Psi}_n^* = \Psi(\hat{P}_n) + \mathbb{P}_n[\varphi_{\hat{P}_n}]$

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where $\mathbb{G}_n := n^{1/2}(\mathbb{P}_n - P)$ is the empirical process and φ the canonical gradient, when $\varphi_{\hat{P}_n} \xrightarrow{P} \varphi_P$. Informally, imagine that $\mathbb{G}_n$ and $\hat{P}_n$ are independent; then

$$\mathbb{G}_n[\varphi_P - \varphi_{\hat{P}_n}] \sim \mathcal{N}\left(0, P\left[\left(\varphi_{\hat{P}_n} - \varphi_P\right)^2\right]\right) \rightsquigarrow 0.$$

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TMLE $\Psi(\hat{P}_n^*)$ with $\hat{P}_n^*$ such that $n^{1/2}\mathbb{P}_n[\varphi_{\hat{P}_n^*}] = o_P(1)$

Decomposition

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The remainder term vanishes if only $\hat{P}_n = P + o_P(n^{-1/4})$!

Functional Taylor expansion

For $f \to \mathbb{R} \to \mathbb{R}$ differentiable at $a \in \mathbb{R}$ we have

$$f(x) = f(a) + f'(a)(x - a) + \mathrm{Rem}(a, x)$$

with $\mathrm{Rem}(a, x) = o(|x - a|)$ – when f is smooth enough the remainder is of second order, i.e., $\mathrm{Rem}(a, x) = o((x - a)^2)$.

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$$\begin{aligned} \Psi(P) &= \Psi(\hat{P}_n) + \langle \varphi_{\hat{P}_n}, p - \hat{p}_n \rangle_\mu + \mathrm{Rem}(\hat{P}_n, P) \\ &= \Psi(\hat{P}_n) + P[\varphi_{\hat{P}_n}] - \hat{P}_n[\varphi_{\hat{P}_n}] + \mathrm{Rem}(\hat{P}_n, P) \\ &= \Psi(\hat{P}_n) + P[\varphi_{\hat{P}_n}] + \mathrm{Rem}(\hat{P}_n, P) \end{aligned}$$

$$\implies \quad |\mathrm{Rem}(\hat{P}_n, P)| = \left| \Psi(\hat{P}_n) - \Psi(P) + P[\varphi_{\hat{P}_n}] \right|$$

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So if Ψ is smooth enough we would expect

$$\begin{aligned} \mathrm{Rem}(\hat{P}_n, P) &= o_P(\|\hat{P}_n - P\|^2) \\ \implies n^{1/2} \left(\Psi(\hat{P}_n) - \Psi(P) + P[\varphi_{\hat{P}_n}] \right) &= o_P(1) \quad \text{if} \quad \hat{P}_n = P + o_P(n^{-1/4}). \end{aligned}$$

Summary so far

- Targeted or "debiased" learning essentially works by calculating and correcting the first order asymptotic bias due to estimation of an (infinite-dimensional) nuisance parameter.
- This is done using a functional Taylor expansion.
- The canonical gradient is an important tool in this regard, because it is the derivative of the map $\Psi \colon \mathcal{P} \to \mathbb{R}$.
- The targeting/debiasing step is important when working with flexible, data-adaptive estimators of infinite-dimensional nuisance parameters (as we saw in the exercise)

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The non-parametric case is important because it implies that that all RAL estimators are efficient and asymptotically equivalent.

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Changing assumptions does not *always* imply changing the information bound.

- Smoothness- or shape-constraints often does not change $\dot{\mathcal{P}}_P$
- Independence assumptions can change $\dot{\mathcal{P}}_P$ without changing φ_P

This type of information have no effect asymptotically – but it might still be relevant to incorporate to improve finite sample performance.

Strategy for finding (candidate for) the canonical gradient

We can find a candidate for the canonical gradient in a nonparametric model by calculating the directional derivative of Ψ in the direction of the Dirac measure δ_{O_i}.[1]

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For any $h \in \mathbb{R}_+$, define the sub-model $P_\varepsilon^h := P + \varepsilon K_{O_i}^h$, where $K_{O_i}^h \to \delta_{O_i}$, $h \to 0$. The score function of this model is

$$\frac{\partial}{\partial \varepsilon}\Big|_{\varepsilon=0} \log(\mathrm{d}P + \varepsilon\, \mathrm{d}K_{O_i}^h) = \frac{\mathrm{d}K_{O_i}^h}{\mathrm{d}P}.$$

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Using the property of a gradient we have

$$\frac{\partial}{\partial \varepsilon}\Big|_{\varepsilon=0} \Psi(P_\varepsilon^h) = \left\langle \varphi_P, \frac{\mathrm{d}K_{O_i}^h}{\mathrm{d}P} \right\rangle_P = \int \varphi_P(o) \frac{\mathrm{d}K_{O_i}^h(o)}{\mathrm{d}P(o)}\, \mathrm{d}P(o) = \int \varphi_P(o)\, \mathrm{d}K_{O_i}^h(o).$$

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

$$\frac{\partial}{\partial \varepsilon}\Big|_{\varepsilon=0} \Psi(P + \varepsilon \delta_{O_i}) = \lim_{h \to 0} \frac{\partial}{\partial \varepsilon}\Big|_{\varepsilon=0} \Psi(P_\varepsilon^h) = \lim_{h \to 0} \int \varphi_P(o)\, \mathrm{d}K_{O_i}^h(o) = \varphi_P(O_i).$$

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Example – estimating the mean

Consider the parameter

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Let O_i be a fixed point and consider

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Taking the derivative with respect to ε we get

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Thus $\tilde{\varphi}_P(o) = o$ is a candidate – to make it integrate to 0 we can use

$$\varphi_P(o) = \tilde{\varphi}_P(o) - \int \tilde{\varphi}_P \,\mathrm{d}P(o) = o - \Psi(P).$$

Exercise

References

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H. Ichimura and W. K. Newey. The influence function of semiparametric estimators. *arXiv preprint arXiv:1508.01378*, 2015.