# NPIV estimation through functional SGD

Student: Caio Lins Advisor: Yuri Saporito

EMAp - FGV

August 21, 2023



# Summary

### **NPIV** estimation

Our approach

Where we are at

Next steps

► Consider a generic regression problem:

$$Y = h^*(X) + \varepsilon$$

where  $\mathbb{E}[\varepsilon] = 0$  and we wish to estimate  $h^*$ .

► Consider a generic regression problem:

$$Y=h^{\star}(X)+\varepsilon,$$

where  $\mathbb{E}[\varepsilon] = 0$  and we wish to estimate  $h^*$ .

▶ What happens if  $\varepsilon \not\perp \!\!\! \perp X$ ? That is,  $\mathbb{E}[\varepsilon \mid X] \neq 0$ ?

► Consider a generic regression problem:

$$Y=h^{\star}(X)+\varepsilon,$$

where  $\mathbb{E}[\varepsilon] = 0$  and we wish to estimate  $h^*$ .

- ▶ What happens if  $\varepsilon \not\perp \!\!\! \perp X$ ? That is,  $\mathbb{E}[\varepsilon \mid X] \neq 0$ ?
- ▶ Minimizing  $\mathbb{E}[(Y h(X))^2]$  over h gives biased results.

Consider a generic regression problem:

$$Y=h^{\star}(X)+\varepsilon,$$

where  $\mathbb{E}[\varepsilon] = 0$  and we wish to estimate  $h^*$ .

- ▶ What happens if  $\varepsilon \not\perp \!\!\! \perp X$ ? That is,  $\mathbb{E}[\varepsilon \mid X] \neq 0$ ?
- ▶ Minimizing  $\mathbb{E}[(Y h(X))^2]$  over h gives biased results.

$$Y = \underbrace{h^{\star}(X) + \mathbb{E}[\varepsilon \mid X]}_{= f(X) \text{ for some } f} + (\varepsilon - \mathbb{E}[\varepsilon \mid X]).$$

Consider a generic regression problem:

$$Y=h^{\star}(X)+\varepsilon,$$

where  $\mathbb{E}[\varepsilon] = 0$  and we wish to estimate  $h^*$ .

- ▶ What happens if  $\varepsilon \not\perp \!\!\! \perp X$ ? That is,  $\mathbb{E}[\varepsilon \mid X] \neq 0$ ?
- ▶ Minimizing  $\mathbb{E}[(Y h(X))^2]$  over h gives biased results.

$$Y = \underbrace{h^{\star}(X) + \mathbb{E}[\varepsilon \mid X]}_{= f(X) \text{ for some } f} + (\varepsilon - \mathbb{E}[\varepsilon \mid X]).$$

▶ We end up estimating f instead of  $h^*$ !

▶ Suppose we have access to a variable Z such that

- ▶ Suppose we have access to a variable Z such that
  - 1.  $Z \not\perp \!\!\! \perp X$ , i.e.,  $\mathbb{E}[X \mid Z]$  is not constant,

- ▶ Suppose we have access to a variable Z such that
  - 1.  $Z \not\perp\!\!\!\perp X$ , i.e.,  $\mathbb{E}[X \mid Z]$  is not constant,
  - 2. Z affects Y only through X,

- ▶ Suppose we have access to a variable Z such that
  - 1.  $Z \not\perp \!\!\! \perp X$ , i.e.,  $\mathbb{E}[X \mid Z]$  is not constant,
  - 2. Z affects Y only through X,
  - 3.  $\varepsilon \perp \!\!\! \perp Z$ , i.e.,  $\mathbb{E}[\varepsilon \mid Z] = 0$ .

- ▶ Suppose we have access to a variable Z such that
  - 1.  $Z \not\perp \!\!\! \perp X$ , i.e.,  $\mathbb{E}[X \mid Z]$  is not constant,
  - 2. Z affects Y only through X,
  - 3.  $\varepsilon \perp \!\!\! \perp Z$ , i.e.,  $\mathbb{E}[\varepsilon \mid Z] = 0$ .

Z is called an instrumental variable.

- ▶ Suppose we have access to a variable Z such that
  - 1.  $Z \not\perp \!\!\! \perp X$ , i.e.,  $\mathbb{E}[X \mid Z]$  is not constant,
  - 2. Z affects Y only through X,
  - 3.  $\varepsilon \perp \!\!\! \perp Z$ , i.e.,  $\mathbb{E}[\varepsilon \mid Z] = 0$ .

Z is called an instrumental variable.

▶ How does it help us?

► Structural equation:

$$Y = h^{\star}(X) + \varepsilon,$$

where  $\mathbb{E}[\varepsilon \mid Z] = 0$ .

► Structural equation:

$$Y=h^{\star}(X)+\varepsilon,$$

where  $\mathbb{E}[\varepsilon \mid Z] = 0$ .

► Consider minimizing  $\mathcal{R}(h) = \mathbb{E}\left[\left(\mathbb{E}[Y - h(X) \mid Z]\right)^2\right]$  over h.

► Structural equation:

$$Y=h^{\star}(X)+\varepsilon,$$

where  $\mathbb{E}[\varepsilon \mid Z] = 0$ .

- ▶ Consider minimizing  $\mathcal{R}(h) = \mathbb{E}\left[\left(\mathbb{E}[Y h(X) \mid Z]\right)^2\right]$  over h.
- Since

$$\mathbb{E}[Y \mid Z] = \mathbb{E}[h^{\star}(X) + \varepsilon \mid Z] = \mathbb{E}[h^{\star}(X) \mid Z],$$

► Structural equation:

$$Y = h^*(X) + \varepsilon,$$

where  $\mathbb{E}[\varepsilon \mid Z] = 0$ .

- ► Consider minimizing  $\mathcal{R}(h) = \mathbb{E}\left[\left(\mathbb{E}[Y h(X) \mid Z]\right)^2\right]$  over h.
- Since

$$\mathbb{E}[Y \mid Z] = \mathbb{E}[h^*(X) + \varepsilon \mid Z] = \mathbb{E}[h^*(X) \mid Z],$$

We have

$$\mathcal{R}(h) = \mathbb{E}\left[\left(\mathbb{E}\left[(h^*-h)(X)\mid Z\right]\right)^2\right].$$

► Structural equation:

$$Y = h^*(X) + \varepsilon,$$

where  $\mathbb{E}[\varepsilon \mid Z] = 0$ .

- ▶ Consider minimizing  $\mathcal{R}(h) = \mathbb{E}\left[\left(\mathbb{E}[Y h(X) \mid Z]\right)^2\right]$  over h.
- Since

$$\mathbb{E}[Y \mid Z] = \mathbb{E}[h^{\star}(X) + \varepsilon \mid Z] = \mathbb{E}[h^{\star}(X) \mid Z],$$

We have

$$\mathcal{R}(h) = \mathbb{E}\left[\left(\mathbb{E}\left[\left(h^{\star} - h\right)(X) \mid Z\right]\right)^{2}\right].$$

 $\mathbb{P}(h) = 0 \iff \mathbb{E}[(h^* - h)(X) \mid Z] = 0 \iff \mathbb{E}[h^*(X) \mid Z] = \mathbb{E}[h(X) \mid Z].$ 

Structural equation:

$$Y = h^*(X) + \varepsilon,$$

where  $\mathbb{E}[\varepsilon \mid Z] = 0$ .

- ▶ Consider minimizing  $\mathcal{R}(h) = \mathbb{E}\left[\left(\mathbb{E}[Y h(X) \mid Z]\right)^2\right]$  over h.
- Since

$$\mathbb{E}[Y \mid Z] = \mathbb{E}[h^{\star}(X) + \varepsilon \mid Z] = \mathbb{E}[h^{\star}(X) \mid Z],$$

We have

$$\mathcal{R}(h) = \mathbb{E}\left[\left(\mathbb{E}\left[(h^{\star} - h)(X) \mid Z\right]\right)^{2}\right].$$

- $\mathbb{P}(h) = 0 \iff \mathbb{E}[(h^* h)(X) \mid Z] = 0 \iff \mathbb{E}[h^*(X) \mid Z] = \mathbb{E}[h(X) \mid Z].$
- ▶ Still does *not* imply  $h = h^*$ , but reduces bias if Z is a good instrument.

$$\underbrace{\mathsf{Grades}}_{Y} = h^{\star} \underbrace{\left( \underbrace{\mathsf{Attends} \ \mathsf{tutoring} \ \mathsf{sessions?}}_{X} \right) + \varepsilon}.$$

$$\underbrace{\mathsf{Grades}}_{Y} = h^{\star} \underbrace{\left( \underbrace{\mathsf{Attends} \ \mathsf{tutoring} \ \mathsf{sessions?}}_{X} \right) + \varepsilon}.$$

▶ Natural ability is a confounding variable: maybe only people who struggle a lot go to tutoring sessions.

$$\underbrace{\mathsf{Grades}}_{Y} = h^{\star} \underbrace{\left( \mathsf{Attends} \ \mathsf{tutoring} \ \mathsf{sessions?} \right)}_{X} + \varepsilon.$$

- ▶ Natural ability is a confounding variable: maybe only people who struggle a lot go to tutoring sessions.
- ightharpoonup Z = Lives close to school?

$$\underbrace{\mathsf{Grades}}_{Y} = h^{\star} \underbrace{\left( \mathsf{Attends} \ \mathsf{tutoring} \ \mathsf{sessions?} \right)}_{X} + \varepsilon.$$

- ▶ Natural ability is a confounding variable: maybe only people who struggle a lot go to tutoring sessions.
- ightharpoonup Z = Lives close to school?
  - 1. *Z* ⊥ *X*,
  - 2. Z affects Y only through X,
  - 3.  $\varepsilon \perp \!\!\! \perp Z$ .

$$\underbrace{\mathsf{Grades}}_{Y} = \mathit{h}^{\star} \underbrace{\left( \mathsf{Attends} \ \mathsf{tutoring} \ \mathsf{sessions?} \right)}_{X} + \varepsilon.$$

- ▶ Natural ability is a confounding variable: maybe only people who struggle a lot go to tutoring sessions.
- ightharpoonup Z = Lives close to school?
  - 1. *Z* ⊥ *X*,
  - 2. Z affects Y only through X, (Kind of)
  - 3.  $\varepsilon \perp \!\!\! \perp Z$ .

#### **NPIV** estimation

▶ Stands for "Nonparametric Instrumental Variable estimation".

#### **NPIV** estimation

- ▶ Stands for "Nonparametric Instrumental Variable estimation".
- ▶ No assumptions on some parametric form for  $h^*$ .

# Summary

Our approach

► We have

$$Y = h^{\star}(X) + \varepsilon,$$

where  $\mathbb{E}[\varepsilon \mid Z] = 0$ , and want to estimate  $h^*$ .

We have

$$Y = h^{\star}(X) + \varepsilon,$$

where  $\mathbb{E}[\varepsilon \mid Z] = 0$ , and want to estimate  $h^*$ .

Equivalently,

$$r_0(Z) = \mathcal{T}[h^*](Z),$$

with

We have

$$Y = h^{\star}(X) + \varepsilon,$$

where  $\mathbb{E}[\varepsilon \mid Z] = 0$ , and want to estimate  $h^*$ .

Equivalently,

$$r_0(Z) = \mathcal{T}[h^*](Z),$$

with

- $r_0(Z) = \mathbb{E}[Y \mid Z],$
- $\mathcal{T}[h](Z) = \mathbb{E}[h(X) \mid Z].$

We have

$$Y = h^{\star}(X) + \varepsilon,$$

where  $\mathbb{E}[\varepsilon \mid Z] = 0$ , and want to estimate  $h^*$ .

Equivalently,

$$r_0(Z) = \mathcal{T}[h^*](Z),$$

with

- $r_0(Z) = \mathbb{E}[Y \mid Z],$
- $\mathcal{T}[h](Z) = \mathbb{E}[h(X) \mid Z].$
- ► Risk measure:

$$\mathcal{R}(h) = \mathbb{E}\left[\frac{1}{2}\left(\mathbb{E}\left[Y - h(X) \mid Z\right]\right)^2\right] = \mathbb{E}\left[\frac{1}{2}\left(r_0(Z) - \mathcal{T}[h](Z)\right)^2\right].$$

▶ It turns out that  $\nabla \mathcal{R}(h)(X) = \mathcal{T}^*[\mathcal{T}[h] - r_0](X)$ .

- ▶ It turns out that  $\nabla \mathcal{R}(h)(X) = \mathcal{T}^*[\mathcal{T}[h] r_0](X)$ .
- Immediate idea:

$$\begin{cases} h_0 \equiv 0, \\ h_t \leftarrow h_{t-1} - \alpha_t \nabla \mathcal{R}(h_{t-1}) & \text{for t } \geq 1. \end{cases}$$

▶ Problem: We don't observe  $r_0$  neither know how to compute  $\mathcal{T}^*$  nor  $\mathcal{T}$ .

Problem: We don't observe  $r_0$  neither know how to compute  $\mathcal{T}^*$  nor  $\mathcal{T}$ . We only have access to joint independent samples from X, Y and Z.

- Problem: We don't observe  $r_0$  neither know how to compute  $\mathcal{T}^*$  nor  $\mathcal{T}$ . We only have access to joint independent samples from X, Y and Z.
- Solution 1: "No problem, we estimate everything!" ...doable, but horrible, since  $\mathcal{T}^*[\mathcal{T}[h] r_0]$  involves plugin estimates into other estimates. Goodbye theoretical guarantees.

► Solution 2: Notice that

$$\nabla \mathcal{R}(h)(X) = \mathbb{E}_{Z} \left[ \Phi(X, Z) (\mathcal{T}[h](Z) - r_0(Z)) \right],$$

where 
$$\Phi(x, z) = \frac{p(x, z)}{p(x)p(z)}$$
.

► Solution 2: Notice that

$$\nabla \mathcal{R}(h)(X) = \mathbb{E}_{Z} \left[ \Phi(X, Z) (\mathcal{T}[h](Z) - r_0(Z)) \right],$$

where 
$$\Phi(x,z) = \frac{p(x,z)}{p(x)p(z)}$$
.

► Second idea: *Now* we estimate everything:

$$\begin{cases} h_0 \equiv 0, \\ h_t \leftarrow \widehat{\Phi}(\cdot, Z_i) \left(\widehat{\mathcal{T}[h_{t-1}]}(Z_i) - \widehat{r_0}(Z_i)\right). \end{cases}$$

► Solution 2: Notice that

$$\nabla \mathcal{R}(h)(X) = \mathbb{E}_{Z} \left[ \Phi(X, Z) (\mathcal{T}[h](Z) - r_0(Z)) \right],$$

where 
$$\Phi(x,z) = \frac{p(x,z)}{p(x)p(z)}$$
.

Second idea: Now we estimate everything:

$$\begin{cases} h_0 \equiv 0, \\ h_t \leftarrow \widehat{\Phi}(\cdot, Z_i) \left(\widehat{\mathcal{T}[h_{t-1}]}(Z_i) - \widehat{r_0}(Z_i)\right). \end{cases}$$

...Not pretty, but manageable, since we no longer have iterated conditional expectations

► Solution 2: Notice that

$$\nabla \mathcal{R}(h)(X) = \mathbb{E}_{Z} \left[ \Phi(X, Z) (\mathcal{T}[h](Z) - r_0(Z)) \right],$$

where 
$$\Phi(x, z) = \frac{p(x, z)}{p(x)p(z)}$$
.

Second idea: Now we estimate everything:

$$\begin{cases} h_0 \equiv 0, \\ h_t \leftarrow \widehat{\Phi}(\cdot, Z_i) \left(\widehat{\mathcal{T}[h_{t-1}]}(Z_i) - \widehat{r_0}(Z_i)\right). \end{cases}$$

► ...Not pretty, but manageable, since we no longer have iterated conditional expectations (but must estimate ratio of densities).

## Summary

NPIV estimatio

Our approach

Where we are at

# Prototype

#### Prototype gave reasonable results

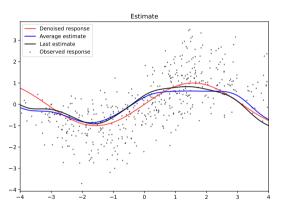


Figure: In red we have  $h^* = \sin$ , in black we have  $h_N$  and in blue,  $\frac{1}{N} \sum_{t=1}^{N} h_N$ .

## Theoretical properties

► Still working on convergence guarantees.

## Theoretical properties

- ► Still working on convergence guarantees.
- $\blacktriangleright$  This is helping us find better ways to estimate  $\Phi$  and  $\mathcal{T}$  (mainly RKHS methods).

## Summary

NPIV estimation

Our approach

Where we are at

# Next steps

Finalize convergence guarantees.

- Finalize convergence guarantees.
- ▶ Implement modifications which the theory points to.

- Finalize convergence guarantees.
- ▶ Implement modifications which the theory points to.
- Benchmark against current methods.

#### References

- [1] Yuri R. Fonseca and Yuri F. Saporito. Statistical Learning and Inverse Problems: A Stochastic Gradient Approach. 2022. arXiv: 2209.14967 [stat.ML].
- [2] Whitney K. Newey and James L. Powell. "Instrumental Variable Estimation of Nonparametric Models". In: Econometrica 71.5 (2003), pp. 1565–1578. ISSN: 00129682, 14680262. URL: http://www.jstor.org/stable/1555512 (visited on 07/03/2023).

Thank You!