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# Stochastic Gradient Descent in NPIV estimation

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## 1 Problem setup

### 1.1 Basic definitions

Fix a probability space  $(\Omega, \mathcal{A}, \mathbb{P})$ . Given  $X \in L^2(\Omega, \mathcal{A}, \mathbb{P}; \mathcal{X} \subseteq \mathbf{R}^p)$ , we define

$$L^2(X) \triangleq \{h : \mathcal{X} \rightarrow \mathbf{R} : \mathbb{E}[h(X)^2] < \infty\},$$

that is,  $L^2(X) = L^2(\mathcal{X}, \mathcal{B}(\mathcal{X}), \nu_X)$ , where we denote by  $\nu_X$  the distribution of the r.v.  $X$  and by  $\mathcal{B}(\mathcal{X})$  the Borel  $\sigma$ -algebra in  $\mathcal{X}$ . This is a Hilbert space equipped with the inner product  $\langle h, g \rangle_{L^2(X)} = \mathbb{E}[h(X)g(X)]$ . The regression problem we are interested in has the form

$$Y = h^*(X) + \varepsilon, \tag{1}$$

where  $h^* \in L^2(X)$  and  $\varepsilon$  is an square-integrable r.v. such that  $\mathbb{E}[\varepsilon | X] \neq 0$ . We assume there exists  $Z \in L^2(\Omega, \mathcal{A}, \mathbb{P}; \mathcal{Z} \subseteq \mathbf{R}^q)$  such that

- i)  $Z$  influences  $X$ , that is,  $\nu_{X|Z}(\cdot | Z) \neq \nu_X(\cdot)$ ;
- ii)  $Z$  and  $\varepsilon$  are uncorrelated, that is,  $\mathbb{E}[\varepsilon | Z] = 0$ .

The space  $L^2(Z) = L^2(\mathcal{Z}, \mathcal{B}(\mathcal{Z}), \nu_Z)$  is defined accordingly. This variable is called the *instrumental variable*. The problem consists of estimating  $h^*$  based on independent joint samples from  $X, Z$  and  $Y$ .

Conditioning (1) in  $Z$ , we find

$$\mathbb{E}[Y | Z] = \mathbb{E}[h^*(X) | Z]. \tag{2}$$

This motivates us to introduce the operator  $\mathcal{P} : L^2(X) \rightarrow L^2(Z)$  defined by

$$\mathcal{P}[h](z) \triangleq \mathbb{E}[h(X) | Z = z].$$

Clearly  $\mathcal{P}$  is linear and, using Jensen's inequality, one may prove that it's bounded. It's also interesting to notice that its adjoint  $\mathcal{P}^* : L^2(Z) \rightarrow L^2(X)$  satisfies

$$\mathcal{P}^*[g](x) = \mathbb{E}[g(Z) | X = x]. \tag{3}$$

Define  $r_0 : \mathcal{Z} \rightarrow \mathbf{R}$  by  $r_0(Z) = \mathbb{E}[Y | Z]$ . Again by Jensen's inequality, we have  $r_0 \in L^2(Z)$ , and thus we can rewrite (2) as

$$\mathcal{P}[h^*] = r_0. \tag{4}$$

Hence, (1) can be formulated as an inverse problem, where we wish to invert the operator  $\mathcal{P}$ .

### 1.2 Risk measure

Let  $\ell : \mathbf{R} \times \mathbf{R} \rightarrow \mathbf{R}$  be a pointwise loss function, which, with respect to its second argument, is convex and differentiable. We use the symbol  $\partial_2$  to denote a derivative with respect to the second

Discuss the other implication, that if  $h$  satisfies  $\mathcal{P}[h] = r_0$ , then  $h = h^*$ . This is false, but the reason can be connected to the strength of the instrument  $Z$ .

24 argument. The example to keep in mind is the quadratic loss function  $\ell(y, y') = \frac{1}{2}(y - y')^2$ . Given  
 25  $h \in L^2(X)$ , we define the *populational risk* associated with it to be

$$\mathcal{R}(h) \triangleq \mathbb{E}[\ell(r_0(Z), \mathcal{P}[h](Z))].$$

26 We would like to solve

$$\inf_{h \in \mathcal{F}} \mathcal{R}(h),$$

27 where  $\mathcal{F} \subseteq L^2(X)$  is a bounded, closed, convex set such that  $h^* \in \mathcal{F}$ . We also assume that  
 28  $D \triangleq \text{diam } \mathcal{F} < \infty$  and that  $0 \in \mathcal{F}$ , so that  $\|h\| \leq D$  if  $h \in \mathcal{F}$ . A possible choice for the set  $\mathcal{F}$  is

Assumption

$$\mathcal{F} = \{h \in L^2(X) : \|h\|_\infty \leq A\},$$

29 where  $A > 0$  is a constant chosen *a priori*. This set is obviously closed, convex and bounded in the  
 30  $L^2(X)$  norm. Furthermore, the projection operator  $\pi_{\mathcal{F}}$  is very easy to compute, as  $\pi_{\mathcal{F}}[h]$  is obtained  
 31 by cropping  $h$  inside  $[-A, A]$ . More formally,

$$\pi_{\mathcal{F}}[h] = h^+ \wedge A - h^- \wedge A.$$

32 We now state all the assumptions needed about the function  $\ell$ :

33 **Assumption 1** (Regularity of  $\ell$ ).

- 34 1. The function  $\ell : \mathbf{R} \times \mathbf{R} \rightarrow \mathbf{R}$  is convex and  $C^2$  with respect to its second argument;
- 35 2. The function  $\ell$  has Lipschitz first derivative with respect to the second argument, i.e., there  
 36 exists  $L \geq 0$  such that, for all  $y, y', u, u' \in \mathbf{R}$  we have

$$|\partial_2 \ell(y, y') - \partial_2 \ell(u, u')| \leq L(|y - u| + |y' - u'|).$$

37

38 Some useful facts which follow immediately from these assumptions are:

39 **Proposition 1.** Under Assumption 1 we have:

- 40 1. Setting  $C_0 = |\partial_2 \ell(0, 0)|$  we have

$$|\partial_2 \ell(y, y')| \leq C_0 + L(|y| + |y'|)$$

41 for all  $y, y' \in \mathbf{R}$ ;

- 42 2. The map  $f \mapsto \partial_2 \ell(r_0(\cdot), f(\cdot))$  from  $L^2(Z)$  to  $L^2(Z)$  is well-defined and  $L$ -Lipschitz.
- 43 3. The second derivative with respect to the second argument is bounded:  $|\partial_2^2 \ell(y, y')| \leq L$  for  
 44 all  $y, y' \in \mathbf{R}$ ;

45 *Proof.*

- 46 1. Write  $\partial_2 \ell(y, y') = \partial_2 \ell(y, y') - \partial_2 \ell(0, 0) + \partial_2 \ell(0, 0)$  and apply the triangle inequality as  
 47 well as Assumption 1.2.

- 48 2. From the previous item we know this map is well-defined. If  $f$  and  $g$  belong to  $L^2(Z)$ , we  
 49 have

$$\begin{aligned} \|\partial_2 \ell(r_0(\cdot), f(\cdot)) - \partial_2 \ell(r_0(\cdot), g(\cdot))\|_{L^2(Z)}^2 &= \mathbb{E} \left[ |\partial_2 \ell(r_0(Z), f(Z)) - \partial_2 \ell(r_0(Z), g(Z))|^2 \right] \\ &\leq L^2 \mathbb{E} \left[ |f(Z) - g(Z)|^2 \right] \\ &= L^2 \|f - g\|_{L^2(Z)}^2. \end{aligned}$$

- 50 3. Follows from the definition of derivative and Assumption 1.2.

51

□

## 52 2 Gradient computation

53 We'd like to compute  $\nabla \mathcal{R}(h)$  for  $h \in L^2(X)$ . We start by computing the directional derivative of  $\mathcal{R}$   
 54 at  $h$  in the direction  $f$ , denoted by  $D\mathcal{R}[h](f)$ :

$$\begin{aligned}
 D\mathcal{R}[h](f) &= \lim_{\delta \rightarrow 0} \frac{1}{\delta} [\mathcal{R}(h + \delta f) - \mathcal{R}(h)] \\
 &= \lim_{\delta \rightarrow 0} \frac{1}{\delta} \mathbb{E} [\ell(r_0(Z), \mathcal{P}[h + \delta f](Z)) - \ell(r_0(Z), \mathcal{P}[h](Z))] \\
 &= \lim_{\delta \rightarrow 0} \frac{1}{\delta} \mathbb{E} [\ell(r_0(Z), \mathcal{P}[h](Z) + \delta \mathcal{P}[f](Z)) - \ell(r_0(Z), \mathcal{P}[h](Z))] \\
 &= \lim_{\delta \rightarrow 0} \frac{1}{\delta} \mathbb{E} \left[ \delta \partial_2 \ell(r_0(Z), \mathcal{P}[h](Z)) \cdot \mathcal{P}[f](Z) \right. \\
 &\quad \left. + \frac{\delta^2}{2} \partial_2^2 \ell(r_0(Z), \mathcal{P}[h + \theta f](Z)) \cdot \mathcal{P}[f](Z)^2 \right] \\
 &= \mathbb{E} [\partial_2 \ell(r_0(Z), \mathcal{P}[h](Z)) \cdot \mathcal{P}[f](Z)] \\
 &\quad + \lim_{\delta \rightarrow 0} \mathbb{E} \left[ \frac{\delta}{2} \partial_2^2 \ell(r_0(Z), \mathcal{P}[h + \theta f](Z)) \cdot \mathcal{P}[f](Z)^2 \right] \\
 &= \mathbb{E} [\partial_2 \ell(r_0(Z), \mathcal{P}[h](Z)) \cdot \mathcal{P}[f](Z)],
 \end{aligned}$$

55 where  $\theta \in \mathbf{R}$  is due to Taylor's formula. The last step is then due to Proposition 1.3.

56 We can in fact expand the calculation a bit more, as follows:

$$\begin{aligned}
 D\mathcal{R}[h](f) &= \mathbb{E} [\partial_2 \ell(r_0(Z), \mathcal{P}[h](Z)) \cdot \mathcal{P}[f](Z)] \\
 &= \langle \partial_2 \ell(r_0(\cdot), \mathcal{P}[h](\cdot)), \mathcal{P}[f] \rangle_{L^2(Z)} \\
 &= \langle \mathcal{P}^* [\partial_2 \ell(r_0(Z), \mathcal{P}[h](\cdot))], f \rangle_{L^2(X)}.
 \end{aligned}$$

57 This shows that  $\mathcal{R}$  is Gateux-differentiable, with Gateux derivative at  $h$  given by

$$D\mathcal{R}[h] = \mathcal{P}^* [\partial_2 \ell(r_0(\cdot), \mathcal{P}[h](\cdot))].$$

58 By Proposition 1.2 we have that  $h \mapsto D\mathcal{R}[h]$  is a continuous mapping from  $L^2(X)$  to  $L^2(X)$ , which  
 59 implies that  $\mathcal{R}$  is also Fréchet-differentiable, and both derivatives coincide. Therefore,

$$\nabla \mathcal{R}(h) = \mathcal{P}^* [\partial_2 \ell(r_0(\cdot), \mathcal{P}[h](\cdot))].$$

Cite a reference for this.

## 60 3 Estimating the gradient

61 We have found that

$$\nabla \mathcal{R}(h)(x) = \mathcal{P}^* [\partial_2 \ell(r_0(\cdot), \mathcal{P}[h](\cdot))](x) = \mathbb{E} [\partial_2 \ell(r_0(Z), \mathcal{P}[h](Z)) \mid X = x].$$

62 This turns out to be hard to estimate in practice, as we have two nested conditional expectation  
 63 operators. Our objective in this section is to write  $\nabla \mathcal{R}(h)(x) = \mathbb{E} [\Phi(x, Z) \partial_2 \ell(r_0(Z), \mathcal{P}[h](Z))]$ ,  
 64 for some suitable kernel  $\Phi$ . Then, for a given sample of  $Z$ , the function  $\Phi(\cdot, Z) \partial_2 \ell(r_0(Z), \mathcal{P}[h](Z))$   
 65 acts as an stochastic estimate for  $\nabla \mathcal{R}(h)$ . To ease the notation, define  $\Psi_h(z) \triangleq \partial_2 \ell(r_0(z), \mathcal{P}[h](z))$ .  
 66 Assuming that  $X$  and  $Z$  have a joint distribution which is absolutely continuous with respect to  
 67 Lebesgue measure in  $\mathbf{R}^{p+q}$ , we can write

Assumption

$$\begin{aligned}
 \nabla \mathcal{R}(h)(x) &= \mathbb{E} [\Psi_h(Z) \mid X = x] \\
 &= \int_{\mathbb{Z}} p(z \mid x) \Psi_h(z) \, dz \\
 &= \int_{\mathbb{Z}} p(z) \frac{p(z \mid x)}{p(z)} \Psi_h(z) \, dz \\
 &= \mathbb{E} \left[ \frac{p(Z \mid x)}{p(Z)} \Psi_h(Z) \right].
 \end{aligned}$$

68 Thus, we must take

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

69 With this choice, setting  $u_h(x) = \Phi(x, Z)\Psi_h(Z)$ , we clearly have  $\mathbb{E}[u_h(x)] = \nabla \mathcal{R}(h)(x)$ .

70 An obvious obstacle for this approach is that we don't know how to analytically compute  $\Phi$ ,  $r_0$  nor  $\mathcal{P}$ ,  
 71 se we will proceed with estimators  $\hat{\Phi}$ ,  $\hat{r}_0$  and  $\hat{\mathcal{P}}$ . In what follows, we will remain agnostic to the exact  
 72 form taken by these estimators and will present the algorithm assuming we know how to compute  
 73 them. Later, we will show how the individual convergence rates of these three pieces come together  
 74 to determine the convergence rate of our method.

75 We state here all the assumptions which we need from these estimators to bound the excess risk:

76 **Assumption 2.**

- 77 1.  $\hat{r}_0 \in L^2(Z)$ ;
- 78 2.  $\hat{\mathcal{P}} : L^2(X) \rightarrow L^2(Z)$  is a bounded linear operator;
- 79 3. Letting  $\mathcal{W} = \mathcal{X} \times \mathcal{Z}$ , we have

$$\|\hat{\Phi}\|_{\infty} \triangleq \sup_{\mathbf{w} \in \mathcal{W}} |\Phi(\mathbf{w})| < \infty.$$

## 80 4 Algorithm

81 Having an estimator of the gradient, we can construct Functional GD algorithm for estimating  $h^*$ .

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### Algorithm 1: SGD-NPIV

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**input :** Datasets  $\mathcal{D}_{r_0}$ ,  $\mathcal{D}_{\Phi}$  and  $\mathcal{D}_{\mathcal{P}}$  for estimating  $r_0$ ,  $\Phi$  and  $\mathcal{P}$ , respectively. Samples  
 $\{(z_m)\}_{m=1}^M$  for the gradient descent loop. Discretization  $\{\mathbf{x}_k\}_{k=1}^K$  of  $\mathcal{X}$  which contains  
 the observed values of  $X$ . Sequence of learning rates  $(\alpha_m)_{m=1}^M$ .

**output :**  $\hat{h}$

82 Compute  $\hat{r}_0$ ,  $\hat{\Phi}$ ,  $\hat{\mathcal{P}}$  using  $\mathcal{D}_{r_0}$ ,  $\mathcal{D}_{\Phi}$ ,  $\mathcal{D}_{\mathcal{P}}$ , respectively ;  
**for**  $1 \leq m \leq M$  **do**  
     Set  $u_m = \hat{\Phi}(\cdot, z_m) \partial_2 \ell(\hat{r}_0(z_m), \hat{\mathcal{P}}[\hat{h}_{m-1}](z_m))$  ;  
     Set  $\hat{h}_m(\mathbf{x}_k) = \pi_{\mathcal{F}}[\hat{h}_{m-1} - \alpha_m u_m](\mathbf{x}_k)$  for  $1 \leq k \leq K$  ;  
**end**  
 Set  $\hat{h} = \frac{1}{M} \sum_{m=1}^M \hat{h}_m$  ;

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## 83 5 Proof of convergence

84 To lighten the notation, the symbols  $\|\cdot\|$  and  $\langle \cdot, \cdot \rangle$ , when written without a subscript to specify which  
 85 space they refer to, will act as the norm and inner product, respectively, of  $L^2(X)$ .

86 **Lemma 1.** In the procedure of Algorithm 1 we have  $u_m \in L^2(X)$  for all  $1 \leq m \leq M$  and,  
 87 furthermore,

$$\mathbb{E}_{\mathbf{z}_{1:M}}[\|u_m\|^2] \leq \rho(\hat{\Phi}, \hat{r}_0, \hat{\mathcal{P}}),$$

88 where

$$\rho(\hat{\Phi}, \hat{r}_0, \hat{\mathcal{P}}) = 3\|\hat{\Phi}\|_{\infty}^2 \left( C_0^2 + L^2 \|\hat{r}_0\|_{L^2(Z)}^2 + L^2 D^2 \|\hat{\mathcal{P}}\|_{\text{op}}^2 \right).$$

Must discuss why  $u_h \in L^2(X)$ .

Must we? Since we end up not using  $u_h$ , but an approximation which we know is in  $L^2(X)$ .

Discuss everything we don't know and must estimate.

Comment on exactly what is needed to estimate each unknown (samples from which r.v.'s).

Discuss necessity of discretizing  $\mathcal{X}$ .

89 *Proof.* By Assumption 2 we have:

$$\begin{aligned}
\|u_m\|_{L^2(X)}^2 &= \left\| \widehat{\Phi}(\cdot, \mathbf{z}_m) \partial_2 \ell \left( \widehat{r}_0(\mathbf{z}_m), \widehat{\mathcal{P}}[\widehat{h}_{m-1}](\mathbf{z}_m) \right) \right\|_{L^2(X)}^2 \\
&= \mathbb{E}_X \left[ \left| \widehat{\Phi}(X, \mathbf{z}_m) \partial_2 \ell \left( \widehat{r}_0(\mathbf{z}_m), \widehat{\mathcal{P}}[\widehat{h}_{m-1}](\mathbf{z}_m) \right) \right|^2 \right] \\
&\leq \partial_2 \ell \left( \widehat{r}_0(\mathbf{z}_m), \widehat{\mathcal{P}}[\widehat{h}_{m-1}](\mathbf{z}_m) \right)^2 \left\| \widehat{\Phi} \right\|_{\infty}^2 \\
&< \infty.
\end{aligned} \tag{5}$$

90 Hence,  $u_m \in L^2(X)$  for all  $m$ . This computation and Proposition 1.1 then imply

$$\begin{aligned}
\mathbb{E}_{\mathbf{z}_{1:M}} \left[ \|u_m\|^2 \right] &\leq 3 \left\| \widehat{\Phi} \right\|_{\infty}^2 \left( C_0^2 + L^2 \left( \|\widehat{r}_0\|_{L^2(Z)}^2 + \left\| \widehat{\mathcal{P}}[\widehat{h}_{m-1}] \right\|_{L^2(Z)}^2 \right) \right) \\
&\leq 3 \left\| \widehat{\Phi} \right\|_{\infty}^2 \left( C_0^2 + L^2 \left( \|\widehat{r}_0\|_{L^2(Z)}^2 + \left\| \widehat{\mathcal{P}} \right\|_{\text{op}}^2 \left\| \widehat{h}_{m-1} \right\|^2 \right) \right) \\
&\leq 3 \left\| \widehat{\Phi} \right\|_{\infty}^2 \left( C_0^2 + L^2 \left( \|\widehat{r}_0\|_{L^2(Z)}^2 + D^2 \left\| \widehat{\mathcal{P}} \right\|_{\text{op}}^2 \right) \right) \\
&= 3 \left\| \widehat{\Phi} \right\|_{\infty}^2 \left( C_0^2 + L^2 \|\widehat{r}_0\|_{L^2(Z)}^2 + L^2 D^2 \left\| \widehat{\mathcal{P}} \right\|_{\text{op}}^2 \right) \triangleq \rho \left( \widehat{\Phi}, \widehat{r}_0, \widehat{\mathcal{P}} \right). \quad \square
\end{aligned}$$

91 **Lemma 2.** In the procedure of Algorithm 1 we have

$$\left\| \mathbb{E}_{\mathbf{z}_m} \left[ \nabla \mathcal{R}(\widehat{h}_{m-1}) - u_m \right] \right\| \leq \kappa \left( \widehat{\Phi} \right) \left( \left\| \Phi - \widehat{\Phi} \right\|_{L^2(\nu_X \otimes \nu_Z)}^2 + \|r_0 - \widehat{r}_0\|_{L^2(Z)}^2 + \left\| \mathcal{P} - \widehat{\mathcal{P}} \right\|_{\text{op}}^2 \right)^{\frac{1}{2}},$$

Comment on how this is the step that is different from the other article, since in the simpler scenario, this difference would vanish.

92 where

$$\kappa^2 \left( \widehat{\Phi} \right) \triangleq 2 \max \left\{ 3(C_0^2 + L^2 \mathbb{E}[Y^2] + L^2 D^2), 2L^2 \left\| \widehat{\Phi} \right\|_{\infty}^2, 2L^2 D^2 \left\| \widehat{\Phi} \right\|_{\infty}^2 \right\}.$$

93 *Proof.* To ease the notation, we define

$$\begin{aligned}
\Psi_m(Z) &\triangleq \partial_2 \ell(r_0(Z), \mathcal{P}[\widehat{h}_{m-1}](Z)), \\
\widehat{\Psi}_m(Z) &\triangleq \partial_2 \ell(\widehat{r}_0(Z), \widehat{\mathcal{P}}[\widehat{h}_{m-1}](Z)).
\end{aligned}$$

94 Let's expand the definition of  $\|\cdot\|$ :

$$\begin{aligned}
\left\| \mathbb{E}_{\mathbf{z}_m} \left[ \nabla \mathcal{R}(\widehat{h}_{m-1}) - u_m \right] \right\| &= \mathbb{E}_X \left[ \mathbb{E}_{\mathbf{z}_m} \left[ \nabla \mathcal{R}(\widehat{h}_{m-1})(X) - u_m(X) \right]^2 \right]^{\frac{1}{2}} \\
&= \mathbb{E}_X \left[ \left( \nabla \mathcal{R}(\widehat{h}_{m-1})(X) - \mathbb{E}_{\mathbf{z}_m} [u_m(X)] \right)^2 \right]^{\frac{1}{2}} \\
&= \mathbb{E}_X \left[ \left( \mathbb{E}_Z [\Phi(X, Z) \Psi_m(Z)] - \mathbb{E}_{\mathbf{z}_m} [\widehat{\Phi}(X, \mathbf{z}_m) \widehat{\Psi}_m(\mathbf{z}_m)] \right)^2 \right]^{\frac{1}{2}} \\
&= \mathbb{E}_X \left[ \left( \mathbb{E}_Z [\Phi(X, Z) \Psi_m(Z) - \widehat{\Phi}(X, Z) \widehat{\Psi}_m(Z)] \right)^2 \right]^{\frac{1}{2}},
\end{aligned}$$

95 Now we add and subtract  $\widehat{\Phi}(X, Z)\Psi_m(Z)$ , so that

$$\begin{aligned}
& \mathbb{E}_X \left[ \left( \mathbb{E}_Z \left[ \Phi(X, Z)\Psi_m(Z) - \widehat{\Phi}(X, Z)\widehat{\Psi}_m(Z) \right] \right)^2 \right]^{\frac{1}{2}} \\
&= \mathbb{E}_X \left[ \left( \mathbb{E}_Z \left[ \Psi_m(Z) \left( \Phi(X, Z) - \widehat{\Phi}(X, Z) \right) + \widehat{\Phi}(X, Z) \left( \Psi_m(Z) - \widehat{\Psi}_m(Z) \right) \right] \right)^2 \right]^{\frac{1}{2}} \\
&\leq \mathbb{E}_X \left[ \left( \left\| \Psi_m \right\|_{L^2(Z)} \left\| \Phi(X, \cdot) - \widehat{\Phi}(X, \cdot) \right\|_{L^2(Z)} + \left\| \widehat{\Phi}(X, \cdot) \right\|_{L^2(Z)} \left\| \Psi_m - \widehat{\Psi}_m \right\|_{L^2(Z)} \right)^2 \right]^{\frac{1}{2}} \\
&\leq \sqrt{2} \mathbb{E}_X \left[ \left\| \Psi_m \right\|_{L^2(Z)}^2 \left\| \Phi(X, \cdot) - \widehat{\Phi}(X, \cdot) \right\|_{L^2(Z)}^2 + \left\| \widehat{\Phi}(X, \cdot) \right\|_{L^2(Z)}^2 \left\| \Psi_m - \widehat{\Psi}_m \right\|_{L^2(Z)}^2 \right]^{\frac{1}{2}} \\
&= \sqrt{2} \left( \left\| \Psi_m \right\|_{L^2(Z)}^2 \left\| \Phi - \widehat{\Phi} \right\|_{L^2(\nu_X \otimes \nu_Z)}^2 + \left\| \widehat{\Phi} \right\|_{L^2(\nu_X \otimes \nu_Z)}^2 \left\| \Psi_m - \widehat{\Psi}_m \right\|_{L^2(Z)}^2 \right)^{\frac{1}{2}},
\end{aligned}$$

96 where

$$\left\| \Phi \right\|_{L^2(\nu_X \otimes \nu_Z)}^2 = \int_{\mathcal{X} \times \mathcal{Z}} \Phi(x, z)^2 p(x) p(z) \, dx dz$$

97 is the norm with respect to the independent coupling of the distributions of  $X$  and  $Z$ . By Proposition  
98 1.1 we have

$$\begin{aligned}
\left\| \Psi_m \right\|_{L^2(Z)}^2 &= \mathbb{E}_Z \left[ \partial_2 \ell(r_0(Z), \mathcal{P}[\widehat{h}_{m-1}](Z))^2 \right] \\
&\leq \mathbb{E}_Z \left[ \left( C_0 + L \left( |r_0(Z)| + \left| \mathcal{P}[\widehat{h}_{m-1}](Z) \right| \right) \right)^2 \right] \\
&\leq 3 \left( C_0^2 + L^2 \|r_0\|_{L^2(Z)}^2 + L^2 \left\| \mathcal{P}[\widehat{h}_{m-1}] \right\|_{L^2(Z)}^2 \right) \\
&\leq 3 (C_0^2 + L^2 \mathbb{E}[Y^2] + L^2 D^2).
\end{aligned}$$

99 It is also clear that, by Assumption 2,

$$\left\| \widehat{\Phi} \right\|_{L^2(\nu_X \otimes \nu_Z)}^2 \leq \left\| \widehat{\Phi} \right\|_{\infty}^2.$$

100 Finally, by Assumption 1.2 we also have

$$\begin{aligned}
\left\| \Psi_m - \widehat{\Psi}_m \right\|_{L^2(Z)}^2 &= \mathbb{E}_Z \left[ \left( \partial_2 \ell(r_0(Z), \mathcal{P}[\widehat{h}_{m-1}](Z)) - \partial_2 \ell(\widehat{r}_0(Z), \widehat{\mathcal{P}}[\widehat{h}_{m-1}](Z)) \right)^2 \right] \\
&\leq 2L^2 \left( \|r_0 - \widehat{r}_0\|_{L^2(Z)}^2 + \left\| (\mathcal{P} - \widehat{\mathcal{P}})[\widehat{h}_{m-1}] \right\|_{L^2(Z)}^2 \right) \\
&\leq 2L^2 \left( \|r_0 - \widehat{r}_0\|_{L^2(Z)}^2 + D^2 \left\| \mathcal{P} - \widehat{\mathcal{P}} \right\|_{\text{op}}^2 \right).
\end{aligned}$$

101 To combine all terms, we first define

$$\kappa^2(\widehat{\Phi}) \triangleq 2 \max \left\{ 3(C_0^2 + L^2 \mathbb{E}[Y^2] + L^2 D^2), 2L^2 \left\| \widehat{\Phi} \right\|_{\infty}^2, 2L^2 D^2 \left\| \widehat{\Phi} \right\|_{\infty}^2 \right\}.$$

102 Then, it's easy to see that

$$\left\| \mathbb{E}_{\mathbf{z}_m} \left[ \nabla \mathcal{R}(\widehat{h}_{m-1}) - u_m \right] \right\| \leq \kappa(\widehat{\Phi}) \left( \left\| \Phi - \widehat{\Phi} \right\|_{L^2(\nu_X \otimes \nu_Z)}^2 + \|r_0 - \widehat{r}_0\|_{L^2(Z)}^2 + \left\| \mathcal{P} - \widehat{\mathcal{P}} \right\|_{\text{op}}^2 \right)^{\frac{1}{2}},$$

103 as we wanted to show.  $\square$

104 **Theorem 1.** Assume that  $\widehat{h}_0, \dots, \widehat{h}_{M-1}$  are generated according to Algorithm 1. If we let  $\widehat{h} =$   
105  $\sum_{m=1}^M \widehat{h}_{m-1}$ , the following excess risk bound holds:

$$\begin{aligned}
\mathbb{E}_{\mathbf{z}_{1:M}} \left[ \mathcal{R}(\widehat{h}) - \mathcal{R}(h^*) \right] &\leq \frac{D^2}{2M\alpha_m} + \xi(\widehat{\Phi}, \widehat{r}_0, \widehat{\mathcal{P}}) \frac{1}{M} \sum_{m=1}^M \alpha_m \\
&\quad + \tau(\widehat{\Phi}) \left( \left\| \Phi - \widehat{\Phi} \right\|_{L^2(\nu_X \otimes \nu_Z)}^2 + \|r_0 - \widehat{r}_0\|_{L^2(Z)}^2 + \left\| \mathcal{P} - \widehat{\mathcal{P}} \right\|_{\text{op}}^2 \right)^{\frac{1}{2}},
\end{aligned}$$

106 where

$$\begin{aligned}\xi(\hat{\Phi}, \hat{r}_0, \hat{\mathcal{P}}) &= \frac{3}{2} \|\hat{\Phi}\|_\infty^2 \left( C_0^2 + L^2 \|\hat{r}_0\|_{L^2(Z)}^2 + L^2 D^2 \|\hat{\mathcal{P}}\|_{\text{op}}^2 \right), \\ \tau(\hat{\Phi}) &= 2D \max \left\{ 3(C_0^2 + L^2 \mathbb{E}[Y^2] + L^2 D^2), 2L^2 \|\hat{\Phi}\|_\infty^2, 2L^2 D^2 \|\hat{\Phi}\|_\infty^2 \right\}, \\ \|\hat{\Phi} - \hat{\Phi}\|_{L^2(\nu_X) \otimes \nu_Z}^2 &= \int_{\mathcal{X} \times \mathcal{Z}} (\Phi - \hat{\Phi})^2(x, z) p(x) p(z) dx dz.\end{aligned}$$

107 *Proof.* We start by checking that  $\mathcal{R}$  is convex in  $\mathcal{F}$ : if  $h, g \in \mathcal{F}$  and  $\lambda \in [0, 1]$ , then

$$\begin{aligned}\mathcal{R}(\lambda h + (1 - \lambda)g) &= \mathbb{E}[\ell(r_0(Z), \mathcal{P}[\lambda h + (1 - \lambda)g](Z))] \\ &= \mathbb{E}[\ell(r_0(Z), \lambda \mathcal{P}[h](Z) + (1 - \lambda)\mathcal{P}[g](Z))] \\ &\leq \lambda \mathbb{E}[\ell(r_0(Z), \mathcal{P}[h](Z))] + (1 - \lambda) \mathbb{E}[\ell(r_0(Z), \mathcal{P}[g](Z))] \\ &= \lambda \mathcal{R}(h) + (1 - \lambda) \mathcal{R}(g).\end{aligned}$$

108 By the Algorithm 1 procedure, we have

$$\begin{aligned}\frac{1}{2} \|\hat{h}_m - h^*\|^2 &= \frac{1}{2} \left\| \pi_{\mathcal{F}} [\hat{h}_{m-1} - \alpha_m u_m] - h^* \right\|^2 \\ &\leq \frac{1}{2} \|\hat{h}_{m-1} - \alpha_m u_m - h^*\|^2 \\ &= \frac{1}{2} \|\hat{h}_{m-1} - h^*\|^2 - \alpha_m \langle u_m, \hat{h}_{m-1} - h^* \rangle + \frac{\alpha_m^2}{2} \|u_m\|^2.\end{aligned}$$

109 After adding and subtracting  $\alpha_m \langle \nabla \mathcal{R}(\hat{h}_{m-1}), \hat{h}_{m-1} - h^* \rangle$ , we are left with

$$\frac{1}{2} \|\hat{h}_{m-1} - h^*\|^2 - \alpha_m \langle u_m - \nabla \mathcal{R}(\hat{h}_{m-1}), \hat{h}_{m-1} - h^* \rangle + \frac{\alpha_m^2}{2} \|u_m\|^2 - \alpha_m \langle \nabla \mathcal{R}(\hat{h}_{m-1}), \hat{h}_{m-1} - h^* \rangle.$$

110 Applying the basic convexity inequality on the last term give us, in total,

$$\begin{aligned}\frac{1}{2} \|\hat{h}_m - h^*\|^2 &\leq \frac{1}{2} \|\hat{h}_{m-1} - h^*\|^2 - \alpha_m \langle u_m - \nabla \mathcal{R}(\hat{h}_{m-1}), \hat{h}_{m-1} - h^* \rangle \\ &\quad + \frac{\alpha_m^2}{2} \|u_m\|^2 - \alpha_m (\mathcal{R}(\hat{h}_{m-1}) - \mathcal{R}(h^*)).\end{aligned}$$

111 Rearranging terms, we get

$$\begin{aligned}\mathcal{R}(\hat{h}_{m-1}) - \mathcal{R}(h^*) &\leq \frac{1}{2\alpha_m} \left( \|\hat{h}_{m-1} - h^*\|^2 - \|\hat{h}_m - h^*\|^2 \right) \\ &\quad + \frac{\alpha_m}{2} \|u_m\|^2 - \langle u_m - \nabla \mathcal{R}(\hat{h}_{m-1}), \hat{h}_{m-1} - h^* \rangle.\end{aligned}$$

112 Finally, summing over  $1 \leq m \leq M$  leads to

$$\begin{aligned}\sum_{n=1}^M [\mathcal{R}(\hat{h}_{m-1}) - \mathcal{R}(h^*)] &\leq \sum_{m=1}^M \frac{1}{2\alpha_m} \left( \|\hat{h}_{m-1} - h^*\|^2 - \|\hat{h}_m - h^*\|^2 \right) \\ &\quad + \sum_{m=1}^M \frac{\alpha_m}{2} \|u_m\|^2 \\ &\quad + \sum_{m=1}^M \langle \nabla \mathcal{R}(\hat{h}_{m-1}) - u_m, \hat{h}_{m-1} - h^* \rangle.\end{aligned} \tag{6}$$

113 The next step is to take the average of both sides with respect to  $\mathbf{z}_{1:M}$ , taking advantage of the  
114 independence between  $\mathbf{z}_{1:M}$  and  $\mathcal{D}_{r_0, \Phi, \mathcal{P}}$ . Each summation in the RHS is then bounded separately.

115 The first summation admits a deterministic bound: By assumption, we have  $\text{diam } \mathcal{F} = D < \infty$ .  
 116 Hence

$$\begin{aligned} \sum_{m=1}^M \frac{1}{2\alpha_m} \left( \|\hat{h}_{m-1} - h^*\|^2 - \|\hat{h}_m - h^*\|^2 \right) &= \sum_{m=2}^M \left( \frac{1}{2\alpha_m} - \frac{1}{2\alpha_{m-1}} \right) \|\hat{h}_{m-1} - h^*\|^2 \\ &\quad + \frac{1}{2\alpha_1} \|\hat{h}_0 - h^*\|^2 - \frac{1}{2\alpha_M} \|\hat{h}_M - h^*\|^2 \\ &\leq \sum_{m=2}^M \left( \frac{1}{2\alpha_m} - \frac{1}{2\alpha_{m-1}} \right) D^2 + \frac{1}{2\alpha_1} D^2 \\ &= \frac{D^2}{2\alpha_M}. \end{aligned} \quad (7)$$

117 The second summation can be bounded with the aid of Lemma 1:

$$\mathbb{E}_{\mathbf{z}_{1:M}} \left[ \sum_{m=1}^M \frac{\alpha_m}{2} \|u_m\|^2 \right] = \frac{\mathbb{E}_{\mathbf{z}_{1:M}} [\|u_m\|^2]}{2} \sum_{m=1}^M \alpha_m \leq \frac{\rho(\hat{\Phi}, \hat{r}_0, \hat{\mathcal{P}})}{2} \sum_{m=1}^M \alpha_m. \quad (8)$$

118 Finally, the third summation can be bounded using Lemma 2. Let  $\mathbb{E}_{\mathbf{z}_{-m}}$  denote the expectation with  
 119 respect to  $\mathbf{z}_1, \dots, \mathbf{z}_{m-1}, \mathbf{z}_{m+1}, \dots, \mathbf{z}_M$  and notice that

$$\begin{aligned} \mathbb{E}_{\mathbf{z}_{1:M}} [\langle \nabla \mathcal{R}(\hat{h}_{m-1}) - u_m, \hat{h}_{m-1} - h^* \rangle] &= \mathbb{E}_{\mathbf{z}_{-m}} [\mathbb{E}_{\mathbf{z}_m} [\langle \nabla \mathcal{R}(\hat{h}_{m-1}) - u_m, \hat{h}_{m-1} - h^* \rangle]] \\ &= \mathbb{E}_{\mathbf{z}_{-m}} [\langle \mathbb{E}_{\mathbf{z}_m} [\nabla \mathcal{R}(\hat{h}_{m-1}) - u_m], \hat{h}_{m-1} - h^* \rangle] \\ &= \mathbb{E}_{\mathbf{z}_{-m}} [\| \mathbb{E}_{\mathbf{z}_m} [\nabla \mathcal{R}(\hat{h}_{m-1}) - u_m] \| \| \hat{h}_{m-1} - h^* \|] \\ &\leq D \mathbb{E}_{\mathbf{z}_{-m}} [\| \mathbb{E}_{\mathbf{z}_m} [\nabla \mathcal{R}(\hat{h}_{m-1}) - u_m] \|]. \end{aligned}$$

120 Then, applying Lemma 2 and setting  $\tau \triangleq D\kappa$  we get

$$\begin{aligned} \mathbb{E}_{\mathbf{z}_{1:M}} [\langle \nabla \mathcal{R}(\hat{h}_{m-1}) - u_m, \hat{h}_{m-1} - h^* \rangle] \\ \leq \tau(\hat{\Phi}) \left( \|\Phi - \hat{\Phi}\|_{L^2(\nu_X \otimes \nu_Z)}^2 + \|r_0 - \hat{r}_0\|_{L^2(Z)}^2 + \|\mathcal{P} - \hat{\mathcal{P}}\|_{\text{op}}^2 \right)^{\frac{1}{2}}. \end{aligned} \quad (9)$$

121 All that is left to do is to apply equations (6), (7), (8) and (9) along with a basic convexity inequality.

122 Let  $\hat{h} \triangleq \frac{1}{M} \sum_{m=1}^M \hat{h}_{m-1}$  and  $\xi \triangleq \rho/2$ . Then:

$$\begin{aligned} \mathbb{E}_{\mathbf{z}_{1:M}} [\mathcal{R}(\hat{h}) - \mathcal{R}(h^*)] \\ \leq \frac{1}{M} \sum_{m=1}^M \mathbb{E}_{\mathbf{z}_{1:M}} [\mathcal{R}(\hat{h}_m) - \mathcal{R}(h^*)] \\ \leq \frac{D^2}{2M\alpha_m} + \xi(\hat{\Phi}, \hat{r}_0, \hat{\mathcal{P}}) \frac{1}{M} \sum_{m=1}^M \alpha_m \\ + \tau(\hat{\Phi}) \left( \|\Phi - \hat{\Phi}\|_{L^2(\nu_X \otimes \nu_Z)}^2 + \|r_0 - \hat{r}_0\|_{L^2(Z)}^2 + \|\mathcal{P} - \hat{\mathcal{P}}\|_{\text{op}}^2 \right)^{\frac{1}{2}}. \quad \square \end{aligned}$$

123 What's left to do:

124 • Use some estimate on  $\|\mathcal{P} - \hat{\mathcal{P}}\|_{\text{op}}$  (Adapt notation and setup in the KIV paper).

125 Conclusion (20/08/2023): We might need the extra hypothesis that  $\text{Im}(\text{id}_{L^2(X)} - \iota_X \iota_X^*) \subseteq$   
 126  $\ker \mathcal{P}$ , where  $\iota_X : \mathcal{H}_X \rightarrow L^2(X)$  is the inclusion operator, whose adjoint is given by

$$\iota_X^*(f) = (x \mapsto \mathbb{E}_X[f(X)k_X(X, x)]),$$



127 with  $k_X : \mathbb{X} \times \mathbb{X} \rightarrow \mathbf{R}$  being the kernel associated with  $\mathcal{H}_X$ . Then  $\mathcal{P} = \mathcal{P} \circ \iota_X \iota_X^*$   
128 and we can directly apply the result on KIV's paper, since  $\mathcal{P} \circ i_X$  can be seen as the  
129 restriction of  $\mathcal{P}$  to  $\mathcal{H}_X$ . We then also need the further hypothesis that  $\text{Im}(\mathcal{P} \circ \iota_X) \subseteq \mathcal{H}_Z$ , or  
130 something like this (because, rigorously speaking,  $\mathcal{P}f$  is an equivalence class of functions,  
131 so in what way can we say that this equivalence class is "in  $\mathcal{H}_Z$ "?). This hypothesis is  
132 implicitly made in the KIV paper, when they say that  $E : \mathcal{H}_X \rightarrow \mathcal{H}_Z$  without providing  
133 any assumptions on  $\mathcal{H}_X$  and  $\mathcal{H}_Z$ , other than saying that they are RKHS. Who can guarantee  
134 that  $(z \mapsto \mathbb{E}[f(X) \mid Z = z]) \in \mathcal{H}_Z$  for every  $f \in \mathcal{H}_X$ ?

- 135 • Find way to estimate  $r_0$  which gives estimate on  $\|r_0 - \hat{r}_0\|_{L^2(Z)}$ . Maybe use the same  
136 estimation technique we have for  $\mathcal{P}$  as an operator from  $L^2(Y) \rightarrow L^2(Z)$  applied to the  
137 identity and employ the same bound?

138 For the rest of the paper:

- 139 • Create section which describes, in detail, how we are estimating  $\Phi$ ,  $\mathcal{P}$  and  $r_0$ , lists all the  
140 references, states the main convergence theorems and lists all of the assumptions that are  
141 being made.
- 142 • Adapt the algorithm section to use the KIV first stage, which directly estimates  $\mathcal{P}$ .
- 143 • Find better letter for either the number of iterations or the upper bound for the set  $\mathcal{F}$ . Right  
144 now, both are being denoted by the letter  $M$ .