
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 $X \in L^2(\Omega; \mathbb{X} \subseteq \mathbf{R}^p)$, we define

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

that is, $L^2(X) = L^2(\mathbb{X}, \mathcal{B}(\mathbb{X}), \mathbb{P}_X)^1$, 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

$$Y = h^*(X) + \varepsilon, \quad (1)$$

where $h^* \in L^2(X)$ and ε is an integrable r.v. such that $\mathbb{E}[\varepsilon | X] \neq 0$. We assume there exists $Z \in L^2(\Omega; \mathbb{Z} \subseteq \mathbf{R}^q)$ such that $Z \not\perp X$, Z influences Y only through X and $\mathbb{E}[\varepsilon | Z] = 0$. 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

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

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

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

Clearly \mathcal{T} is linear and, using Jensen's inequality, one may prove that it's bounded. It's also interesting to notice that its adjoint $\mathcal{T}^* : L^2(Z) \rightarrow L^2(X)$ satisfies

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

Define $r_0 : \mathbb{Z} \rightarrow \mathbf{R}$ 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

$$\mathcal{T}[h^*] = r_0. \quad (4)$$

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

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 ∂_2 to denote a derivative with respect to the second argument. The example to keep in mind is the quadratic loss function $\ell(y, y') = (y - y')^2$. Given $h \in L^2(X)$, we define the *populational risk* associated with it to be

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

We would like to solve

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

where $\mathcal{F} \subseteq L^2(X)$ is a closed, convex set such that $h^* \in \mathcal{F}$.

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

Assumption

¹We denote by \mathbb{P}_X the distribution of the r.v. X and by $\mathcal{B}(\mathbb{X})$ the Borel σ -algebra in \mathbb{X} .

24 2 Gradient computation

25 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}
 26 at h in the direction f , denoted by $D\mathcal{R}[h](f)$:

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

27 where $\theta \in \mathbf{R}$ is due to Taylor's formula and can be assumed to be inside a fixed interval $(-\theta_0, \theta_0)$,
 28 with θ_0 arbitrarily small. We have assumed at the last step that there exists $\theta_0 > 0$ such that

$$\sup_{|\theta| < \theta_0} \mathbb{E} [\partial_2^2 \ell(r_0(Z), \mathcal{T}[h + \theta f](Z)) \mathcal{T}[f](Z)^2] < \infty.$$

29 This is a mild integrability condition which can be shown to hold in the quadratic case.

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

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

31 where we are assuming that $\partial_2 \ell(r_0(\cdot), \mathcal{T}[h](\cdot)) \in L^2(Z)$. This shows that \mathcal{R} is Gateux-differentiable,
 32 with Gateux derivative at h given by

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

33 If we assume² that $h \mapsto D\mathcal{R}[h]$ is a continuous mapping from $L^2(Z)$ to $L^2(Z)$, then \mathcal{R} is also
 34 Fréchet-differentiable, and both derivatives coincide. Therefore, under this assumption, which we
 35 henceforth make, $\nabla \mathcal{R}(h) = \mathcal{T}^* [\partial_2 \ell(r_0(\cdot), \mathcal{T}[h](\cdot))]$.

36 3 Unbiased estimator of the gradient

37 We have found that

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

38 This turns out to be hard to estimate in practice, as we have two nested conditional expectation
 39 operators. Our objective in this section is to find a random element $u_h \in L^2(X)$ such that $\mathbb{E}[u_h(x)] =$
 40 $\nabla \mathcal{R}(h)(x)$, so we can replace $\nabla \mathcal{R}(h)(x)$ by $u_h(x)$ in a gradient descent algorithm, obtaining a
 41 stochastic version which will be easier to compute.

42 Our strategy to obtain u_h will be to write $\nabla \mathcal{R}(h)(x) = \mathbb{E} [\Phi(x, Z) \partial_2 \ell(r_0(Z), \mathcal{T}[h](Z))]$, for some
 43 suitable kernel Φ . To ease the notation, define $\xi_h(z) \triangleq \partial_2 \ell(r_0(z), \mathcal{T}[h](z))$. Assuming that X and

²It is if ℓ is quadratic.

44 Z have a joint distribution which is absolutely continuous with respect to Lebesgue measure in \mathbf{R}^{p+q} ,
 45 we can write

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

46 Thus, we must take

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

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

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

48 4 Algorithm

49 Having an unbiased estimator of the gradient, we can construct an SGD algorithm for estimating h^* .

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 \mathbb{X} .

Algorithm 1: SGD-NPIV

input : Datasets $\mathcal{D}_{r_0} = \{(y_i, z_i)\} \stackrel{\text{iid}}{\sim} \mathbb{P}_{YZ}$, $\mathcal{D}_{\Phi} = \{(\mathbf{x}_i, z_i)\} \stackrel{\text{iid}}{\sim} \mathbb{P}_{XZ}$,
 $\mathcal{D}_{\mathcal{T}} = \{(\mathbf{x}_i, z_i)\} \stackrel{\text{iid}}{\sim} \mathbb{P}_{XZ}$, discretization $\{\mathbf{x}_k\}_{k=1}^K$ of \mathbb{X} which contains the observed
 values of X , sequence of learning rates $(\alpha_m)_{m=1}^M$.

output : $\{\hat{h}(\mathbf{x}_k)\}_{k=1}^K$

Compute $\{\hat{r}_0(z_m; \mathcal{D}_{r_0})\}_{m=1}^M$;

50 Compute $\hat{\Phi}(\mathbf{x}, z; \mathcal{D}_{\Phi})$;

for $1 \leq m \leq M$ **do**

 Compute $\mathcal{T}[\hat{h}_{m-1}](z_m; \mathcal{D}_{\mathcal{T}})$;

 Set $u_m(\mathbf{x}_k) = \hat{\Phi}(\mathbf{x}_k, z_m) \partial_2 \ell \left(\hat{r}_0(z_m, \mathcal{D}_{r_0}), \mathcal{T}[\hat{h}_{m-1}](z_m; \mathcal{D}_{\mathcal{T}}) \right)$ for $1 \leq k \leq K$;

 Set $\hat{h}_m(\mathbf{x}_k) = \hat{h}_{m-1}(\mathbf{x}_k) - \alpha_m u_m(\mathbf{x}_k)$ for $1 \leq k \leq K$;

end

Set $\hat{h} = \frac{1}{M} \sum_{m=1}^M \hat{h}_m$;

51 An option we have is to project onto the closed, convex, bounded set \mathcal{F} after applying the stochastic
 52 gradient, that is, constructing the new estimate as

Should we do this?

$$\hat{h}_m = P_{\mathcal{F}} \left[\hat{h}_{m-1} - \alpha_m u_m \right].$$

53 From what I can see, this would require minor changes to the proof and would justify the assumption
 54 that $\hat{h}_m \in \mathcal{F}$ for all m .

55 A possible choice for the set \mathcal{F} is

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

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

$$P_{\mathcal{F}}[h] = h^+ \wedge M - h^- \wedge M.$$

59 5 Proof of convergence

60 The first problem is proving our sequence of estimates is, in fact, contained in $L^2(X)$. This amounts
 61 to proving $u_m \in L^2(X)$ for every m . It's not even immediate why $u_h(x) = \Phi(x, Z)\xi_h(Z)$ (the
 62 unbiased gradient when we know r_0, Φ and \mathcal{T}) belongs to $L^2(X)$

We'll need to bound the norm of u_m by a constant later in the proof.

63 After doing this, we check that \mathcal{R} is convex in \mathcal{F} : if $h, g \in \mathcal{F}$ and $\lambda \in [0, 1]$, then

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

64 To lighten the notation, the symbols $\|\cdot\|$ and $\langle \cdot, \cdot \rangle$, when written without a subscript to specify which
 65 space they refer to, will act as the norm and inner product, respectively, of $L^2(X)$. By the Algorithm
 66 1 procedure, we have

$$\begin{aligned}\frac{1}{2} \|\hat{h}_m - h^*\|^2 &= \frac{1}{2} \|\hat{h}_{m-1} - \alpha_m u_m - h^*\|^2 \\ &= \frac{1}{2} \|\hat{h}_{m-1} - h^*\|^2 - \alpha_m \langle u_m, \hat{h}_{m-1} - h^* \rangle + \frac{\alpha_m^2}{2} \|u_m\|^2.\end{aligned}$$

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

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

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

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

69 Rearranging terms, we get

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

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

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

71 We then treat each of the three terms in the RHS of the inequality above separately:

72 **First term** By assumption, we have $\text{diam } \mathcal{F} = D < \infty$. Hence

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

73 **Second term** We are fixing the offline data $\mathcal{D}_{\Phi, \mathcal{T}, r_0}$ and averaging with respect to the other samples
 74 of the instrumental variable. Therefore, what we wish to compute is

$$\begin{aligned}\mathbb{E}_{\mathbf{z}_{1:M}} \left[\|u_m\|^2 \mid \mathcal{D}_{\Phi, \mathcal{T}, r_0} \right] &= \mathbb{E}_{\mathbf{z}_{1:m}} \left[\mathbb{E}_X \left[\widehat{\Phi}(X, \mathbf{z}_m)^2 \partial_2 \ell \left(\widehat{r}_0(\mathbf{z}_m), \widehat{\mathcal{T}}[\widehat{h}_{m-1}](\mathbf{z}_m) \right)^2 \mid \mathcal{D}_{\Phi, \mathcal{T}, r_0} \right] \right. \\ &= \mathbb{E}_X \left[\mathbb{E}_{\mathbf{z}_{1:m}} \left[\widehat{\Phi}(X, \mathbf{z}_m)^2 \partial_2 \ell \left(\widehat{r}_0(\mathbf{z}_m), \widehat{\mathcal{T}}[\widehat{h}_{m-1}](\mathbf{z}_m) \right)^2 \mid \mathcal{D}_{\Phi, \mathcal{T}, r_0} \right] \right].\end{aligned}$$

75 Since $\mathbf{z}_{1:m}$ is independent from $\mathcal{D}_{\Phi, \mathcal{T}, r_0}$, this is equal to

$$\mathbb{E}_X \left[\mathbb{E}_{\mathbf{z}_{1:m}} \left[\widehat{\Phi}(X, \mathbf{z}_m)^2 \partial_2 \ell \left(\widehat{r}_0(\mathbf{z}_m), \widehat{\mathcal{T}}[\widehat{h}_{m-1}](\mathbf{z}_m) \right)^2 \right] \right].$$

76 Reversing back the expectations, we get

$$\begin{aligned}\mathbb{E}_{\mathbf{z}_{1:m}} \left[\mathbb{E}_X \left[\widehat{\Phi}(X, \mathbf{z}_m)^2 \partial_2 \ell \left(\widehat{r}_0(\mathbf{z}_m), \widehat{\mathcal{T}}[\widehat{h}_{m-1}](\mathbf{z}_m) \right)^2 \right] \right] \\ = \mathbb{E}_{\mathbf{z}_{1:m}} \left[\mathbb{E}_X \left[\widehat{\Phi}(X, \mathbf{z}_m)^2 \right] \partial_2 \ell \left(\widehat{r}_0(\mathbf{z}_m), \widehat{\mathcal{T}}[\widehat{h}_{m-1}](\mathbf{z}_m) \right)^2 \right].\end{aligned}$$

77 Now we use Assumption 14.5.1 in [1], which states that

$$\sup_{\mathbf{w} \in \mathbb{W}} k(\mathbf{w}, \mathbf{w}) \leq 1,$$

78 where $\mathbb{W} = \mathbb{X} \times \mathbb{Z}$, $\mathbf{w} = (\mathbf{x}, \mathbf{z})$ and $k : \mathbb{W} \times \mathbb{W} \rightarrow \mathbf{R}$ is the kernel corresponding to the RKHS used
 79 to estimate Φ , which we denote by $\mathcal{R}_{\mathbb{W}}$. This assumption implies

$$\begin{aligned}\widehat{\Phi}(\mathbf{w}) &= \langle \widehat{\Phi}, k(\mathbf{w}, \cdot) \rangle_{\mathcal{R}_{\mathbb{W}}} \leq \left\| \widehat{\Phi} \right\|_{\mathcal{R}_{\mathbb{W}}} \|k(\mathbf{w}, \cdot)\|_{\mathcal{R}_{\mathbb{W}}} = \left\| \widehat{\Phi} \right\|_{\mathcal{R}_{\mathbb{W}}} \sqrt{\langle k(\mathbf{w}, \cdot), k(\mathbf{w}, \cdot) \rangle} = \\ &= \left\| \widehat{\Phi} \right\|_{\mathcal{R}_{\mathbb{W}}} \sqrt{k(\mathbf{w}, \mathbf{w})} \leq \left\| \widehat{\Phi} \right\|_{\mathcal{R}_{\mathbb{W}}}\end{aligned}$$

80 for all $\mathbf{w} \in \mathbb{W}$. Therefore,

$$\begin{aligned}\mathbb{E}_{\mathbf{z}_{1:m}} \left[\mathbb{E}_X \left[\widehat{\Phi}(X, \mathbf{z}_m)^2 \right] \partial_2 \ell \left(\widehat{r}_0(\mathbf{z}_m), \widehat{\mathcal{T}}[\widehat{h}_{m-1}](\mathbf{z}_m) \right)^2 \right] \\ \leq \mathbb{E}_{\mathbf{z}_{1:m}} \left[\mathbb{E}_X \left[\left\| \widehat{\Phi} \right\|_{\mathcal{R}_{\mathbb{W}}}^2 \right] \partial_2 \ell \left(\widehat{r}_0(\mathbf{z}_m), \widehat{\mathcal{T}}[\widehat{h}_{m-1}](\mathbf{z}_m) \right)^2 \right] \\ = \left\| \widehat{\Phi} \right\|_{\mathcal{R}_{\mathbb{W}}}^2 \mathbb{E}_{\mathbf{z}_{1:m}} \left[\partial_2 \ell \left(\widehat{r}_0(\mathbf{z}_m), \widehat{\mathcal{T}}[\widehat{h}_{m-1}](\mathbf{z}_m) \right)^2 \right].\end{aligned}$$

81 To bound the expectation, we assume the loss is quadratic and then

Assumption

$$\begin{aligned}\mathbb{E}_{\mathbf{z}_{1:m}} \left[\left(\widehat{\mathcal{T}}[\widehat{h}_{m-1}](\mathbf{z}_m) - \widehat{r}_0(\mathbf{z}_m) \right)^2 \right] \\ = \mathbb{E}_{\mathbf{z}_{1:m}} \left[\left(\left(\widehat{\mathcal{T}}[\widehat{h}_{m-1}](\mathbf{z}_m) - \mathcal{T}[\widehat{h}_{m-1}](\mathbf{z}_m) \right) + (r_0(\mathbf{z}_m) - \widehat{r}_0(\mathbf{z}_m)) \right. \right. \\ \left. \left. + \left(\mathcal{T}[\widehat{h}_{m-1}](\mathbf{z}_m) - r_0(\mathbf{z}_m) \right) \right)^2 \right] \\ \leq 3 \mathbb{E}_{\mathbf{z}_{1:m}} \left[\left(\widehat{\mathcal{T}}[\widehat{h}_{m-1}](\mathbf{z}_m) - \mathcal{T}[\widehat{h}_{m-1}](\mathbf{z}_m) \right)^2 + (r_0(\mathbf{z}_m) - \widehat{r}_0(\mathbf{z}_m))^2 \right. \\ \left. + \left(\mathcal{T}[\widehat{h}_{m-1}](\mathbf{z}_m) - r_0(\mathbf{z}_m) \right)^2 \right] \\ = 3 \left\{ \mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\left\| (\widehat{\mathcal{T}} - \mathcal{T})[\widehat{h}_{m-1}] \right\|_{L^2(\mathbb{Z})}^2 \right] + \mathbb{E}_{\mathbf{z}_{1:m}} \left[\|r_0 - \widehat{r}_0\|_{L^2(\mathbb{Z})}^2 \right] \right. \\ \left. + \mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\left\| \mathcal{T}[\widehat{h}_{m-1}] - r_0 \right\|_{L^2(\mathbb{Z})}^2 \right] \right\}.\end{aligned}$$

82 We treat each part of this expression separately. Firstly,

$$\left\| (\widehat{\mathcal{T}} - \mathcal{T})[\widehat{h}_{m-1}] \right\|_{L^2(\mathbb{Z})}^2 \leq \left\| \widehat{\mathcal{T}} - \mathcal{T} \right\|_{\text{op}}^2 \left\| \widehat{h}_{m-1} \right\|_{L^2(\mathbb{X})}^2 \leq M^2 \left\| \widehat{\mathcal{T}} - \mathcal{T} \right\|_{\text{op}}^2.$$

83 We leave the second part as $\|r_0 - \widehat{r}_0\|_{L^2(\mathbb{Z})}^2$. Finally, for the third part, we have

$$\begin{aligned} \left\| \mathcal{T}[\widehat{h}_{m-1}] - r_0 \right\|_{L^2(\mathbb{Z})}^2 &= \mathbb{E}_Z \left[\left(\mathcal{T}[\widehat{h}_{m-1}](Z) - r_0(Z) \right)^2 \right] \\ &= \mathbb{E}_Z \left[\left(\mathbb{E} \left[\widehat{h}_{m-1}(X) - Y \mid Z \right] \right)^2 \right] \\ &\leq \mathbb{E}_{(X,Y)} \left[\left(\widehat{h}_{m-1}(X) - Y \right)^2 \right] \\ &\leq 2 \left(\mathbb{E}_X \left[\widehat{h}_{m-1}(X)^2 \right] + \mathbb{E} \left[Y^2 \right] \right) \\ &= 2 \left(\left\| \widehat{h}_{m-1} \right\|_{L^2(\mathbb{X})}^2 + \mathbb{E} \left[Y^2 \right] \right) \\ &\leq 2 \left(M^2 + \mathbb{E} \left[Y^2 \right] \right). \end{aligned}$$

84 Putting everything together, what we conclude is

$$\mathbb{E}_{\mathbf{z}_{1:m}} \left[\|u_m\|_{L^2(\mathbb{X})}^2 \mid \mathcal{D}_{\Phi, \mathcal{T}, r_0} \right] \leq 3 \left\| \widehat{\Phi} \right\|_{\mathcal{R}_W}^2 \left(M^2 \left\| \widehat{\mathcal{T}} - \mathcal{T} \right\|_{\text{op}}^2 + \|r_0 - \widehat{r}_0\|_{L^2(\mathbb{Z})}^2 + 2 \left(M^2 + \mathbb{E}[Y^2] \right) \right).$$

85 We still have to use convergence results for $\widehat{\mathcal{T}}$ and \widehat{r}_0 to finish this bound. It doesn't need to be good,
 86 we only need to bound this by something which remains bounded as $|\mathcal{D}_{\Phi, \mathcal{T}, r_0}|$ and the number of
 87 iterations grow. Another idea is to simply say that this whole thing is $\mathcal{O}_p(1)$, that is, almost surely
 88 finite, and rely on the (fast enough) decay of the learning rate to achieve convergence.

89 Third term

90 Our goal is to open up the inner product and make explicit the estimation errors of our model's
 91 different components, like we did before. Here, we define $\Psi_m(Z) \triangleq \partial_2 \ell(r_0(Z), \mathcal{T}[\widehat{h}_{m-1}](Z))$. The
 92 hat version $\widehat{\Psi}_m$ is defined accordingly, replacing r_0 and \mathcal{T} by their estimators.

$$\begin{aligned} \mathbb{E}_{\mathbf{z}_{1:m}} \left[\langle \nabla \mathcal{R}(\widehat{h}_{m-1}) - u_m, \widehat{h}_{m-1} - h^* \rangle \mid \mathcal{D}_{\Phi, \mathcal{T}, r_0} \right] &= \mathbb{E}_{\mathbf{z}_{1:m}} \left[\langle \nabla \mathcal{R}(\widehat{h}_{m-1}) - u_m, \widehat{h}_{m-1} - h^* \rangle \right] && (\mathbf{z}_{1:m} \perp\!\!\!\perp \mathcal{D}_{\Phi, \mathcal{T}, r_0}) \\ &= \mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\mathbb{E}_{\mathbf{z}_m} \left[\langle \nabla \mathcal{R}(\widehat{h}_{m-1}) - u_m, \widehat{h}_{m-1} - h^* \rangle \right] \right] && (\mathbf{z}_m \perp\!\!\!\perp \mathbf{z}_{1:m-1}) \\ &= \mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\langle \nabla \mathcal{R}(\widehat{h}_{m-1}) - \mathbb{E}_{\mathbf{z}_m} [u_m], \widehat{h}_{m-1} - h^* \rangle \right] \\ &\leq \mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\left\| \nabla \mathcal{R}(\widehat{h}_{m-1}) - \mathbb{E}_{\mathbf{z}_m} [u_m] \right\| \left\| \widehat{h}_{m-1} - h^* \right\| \right] \\ &\leq D \mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\left\| \nabla \mathcal{R}(\widehat{h}_{m-1}) - \mathbb{E}_{\mathbf{z}_m} [u_m] \right\| \right] && (\text{diam } \mathcal{F} = D) \\ &\leq D \mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\mathbb{E}_X \left[\left(\nabla \mathcal{R}(\widehat{h}_{m-1})(X) - \mathbb{E}_{\mathbf{z}_m} [u_m] \right)^2 \right] \right]^{\frac{1}{2}} && (\text{Jensen}) \\ &= D \mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\mathbb{E}_X \left[\left(\mathbb{E}_Z [\Phi(X, Z) \Psi_m(Z)] \right. \right. \right. \\ &\quad \left. \left. \left. - \mathbb{E}_{\mathbf{z}_m} \left[\widehat{\Phi}(X, \mathbf{z}_m) \widehat{\Psi}_m(\mathbf{z}_m) \right] \right)^2 \right] \right]^{\frac{1}{2}} \\ &= D \mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\mathbb{E}_X \left[\mathbb{E}_Z \left[\Phi(X, Z) \Psi_m(Z) - \widehat{\Phi}(X, Z) \widehat{\Psi}_m(Z) \right]^2 \right] \right]^{\frac{1}{2}} && (Z \stackrel{\text{iid}}{\sim} \mathbf{z}_m) \end{aligned}$$

$$\begin{aligned}
&= D\mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\mathbb{E}_X \left[\mathbb{E}_Z \left[\Psi_m(Z) \left(\Phi(X, Z) - \widehat{\Phi}(X, Z) \right) \right. \right. \right. \\
&\quad \left. \left. \left. + \widehat{\Phi}(X, Z) \left(\Psi_m(Z) - \widehat{\Psi}_m(Z) \right) \right]^2 \right] \right] \right]^{\frac{1}{2}} \\
&\leq D\mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\mathbb{E}_X \left[\left(\|\Psi_m\|_{L^2(Z)} \left\| \Phi(X, \cdot) - \widehat{\Phi}(X, \cdot) \right\|_{L^2(Z)} \right. \right. \right. \\
&\quad \left. \left. \left. + \left\| \widehat{\Phi}(X, \cdot) \right\|_{L^2(Z)} \left\| \Psi_m - \widehat{\Psi}_m \right\|_{L^2(Z)} \right)^2 \right] \right] \right]^{\frac{1}{2}} \\
&\leq \sqrt{2}D\mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\mathbb{E}_X \left[\|\Psi_m\|_{L^2(Z)}^2 \left\| \Phi(X, \cdot) - \widehat{\Phi}(X, \cdot) \right\|_{L^2(Z)}^2 \right. \right. \\
&\quad \left. \left. + \left\| \widehat{\Phi}(X, \cdot) \right\|_{L^2(Z)}^2 \left\| \Psi_m - \widehat{\Psi}_m \right\|_{L^2(Z)}^2 \right] \right] \right]^{\frac{1}{2}} \\
&= \sqrt{2}D \left(\mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\|\Psi_m\|_{L^2(Z)}^2 \mathbb{E}_X \left[\left\| \Phi(X, \cdot) - \widehat{\Phi}(X, \cdot) \right\|_{L^2(Z)}^2 \right] \right. \right. \\
&\quad \left. \left. + \mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\left\| \Psi_m - \widehat{\Psi}_m \right\|_{L^2(Z)}^2 \mathbb{E}_X \left[\left\| \widehat{\Phi}(X, \cdot) \right\|_{L^2(Z)}^2 \right] \right] \right] \right)^{\frac{1}{2}} \\
&= \sqrt{2}D \left(\mathbb{E}_X \left[\left\| \Phi(X, \cdot) - \widehat{\Phi}(X, \cdot) \right\|_{L^2(Z)}^2 \right] \mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\|\Psi_m\|_{L^2(Z)}^2 \right] \right. \\
&\quad \left. + \mathbb{E}_X \left[\left\| \widehat{\Phi}(X, \cdot) \right\|_{L^2(Z)}^2 \right] \mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\left\| \Psi_m - \widehat{\Psi}_m \right\|_{L^2(Z)}^2 \right] \right)^{\frac{1}{2}} \\
&=: \sqrt{2}D(A + B)^{\frac{1}{2}}.
\end{aligned}$$

93 We proceed to analyze each term separately:

94 • To bound A , first notice that

$$\mathbb{E}_X \left[\left\| \Phi(X, \cdot) - \widehat{\Phi}(X, \cdot) \right\|_{L^2(Z)}^2 \right] = \mathbb{E}_X \left[\mathbb{E}_Z \left[\left(\Phi(X, Z) - \widehat{\Phi}(X, Z) \right)^2 \right] \right] = \left\| \Phi - \widehat{\Phi} \right\|_{L^2(X \otimes Z)}^2,$$

95 where $L^2(X \otimes Z)$ is the space of square integrable functions with respect to the measure
96 induced by independent copies of X and Z . If we estimate $\widehat{\Phi}$ using the uLSIF algorithm de-
97 scribed in [1], under some regularity conditions, and decreasing the regularization parameter
98 according to a specific rate, we have the following estimate:

Create section describ-
ing how we are esti-
mating each term.

$$\left\| \Phi - \widehat{\Phi} \right\|_{L^2(X \otimes Z)}^2 = \mathcal{O}_p \left(\left(\frac{\log |\mathcal{D}_\Phi|}{|\mathcal{D}_\Phi|} \right)^{\frac{2}{2+\gamma}} \right).$$

99 Furthermore, we can bound $\|\Psi_m\|_{L^2(Z)}^2$ as follows:

$$\begin{aligned}
\|\Phi_m\|_{L^2(Z)}^2 &= \left\| r_0 - \mathcal{T}[\widehat{h}_{m-1}] \right\|_{L^2(Z)}^2 \\
&\leq 2 \left(\|r_0\|_{L^2(Z)}^2 + \left\| \mathcal{T}[\widehat{h}_{m-1}] \right\|_{L^2(Z)}^2 \right) \\
&\leq 2 \left(\mathbb{E}[Y^2] + \|\mathcal{T}\|_{\text{op}}^2 \left\| \widehat{h}_{m-1} \right\|_{L^2(Z)}^2 \right) \\
&\leq 2 \left(\mathbb{E}[Y^2] + M^2 \right) \quad (\|\mathcal{T}\|_{\text{op}} \leq 1).
\end{aligned}$$

100

In total, what we have is

$$\begin{aligned}
A &= \mathbb{E}_X \left[\left\| \Phi(X, \cdot) - \hat{\Phi}(X, \cdot) \right\|_{L^2(Z)}^2 \right] \mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\|\Psi_m\|_{L^2(Z)}^2 \right] \\
&\leq \left\| \Phi - \hat{\Phi} \right\|_{L^2(Z)}^2 \cdot 2(\mathbb{E}[Y^2] + M^2) \\
&= \mathcal{O}_p \left(\left(\frac{\log |\mathcal{D}_\Phi|}{|\mathcal{D}_\Phi|} \right)^{\frac{2}{2+\gamma}} \right).
\end{aligned}$$

101

- To bound B , notice that, by Assumption 14.15 of [1], we have

$$\mathbb{E}_X \left[\left\| \hat{\Phi}(X, \cdot) \right\|_{L^2(Z)}^2 \right] = \mathbb{E}_X \left[\mathbb{E}_Z \left[\hat{\Phi}(X, Z)^2 \right] \right] \leq \left\| \hat{\Phi} \right\|_{\mathcal{R}_W}^2.$$

102

We still need to bound this norm somehow.

103

Furthermore, we also have

$$\begin{aligned}
\left\| \Psi_m - \hat{\Psi}_m \right\|_{L^2(Z)}^2 &= \left\| \left(\mathcal{T}[\hat{h}_{m-1}] - r_0 \right) - \left(\hat{\mathcal{T}}[\hat{h}_{m-1}] - \hat{r}_0 \right) \right\|_{L^2(Z)}^2 \\
&= \left\| \left(\mathcal{T}[\hat{h}_{m-1}] - \hat{\mathcal{T}}[\hat{h}_{m-1}] \right) - (r_0 - \hat{r}_0) \right\|_{L^2(Z)}^2 \\
&\leq 2 \left(\left\| \mathcal{T}[\hat{h}_{m-1}] - \hat{\mathcal{T}}[\hat{h}_{m-1}] \right\|_{L^2(Z)}^2 + \|r_0 - \hat{r}_0\|_{L^2(Z)}^2 \right) \\
&\leq 2 \left(\left\| \mathcal{T} - \hat{\mathcal{T}} \right\|_{\text{op}}^2 \left\| \hat{h}_{m-1} \right\|_{L^2(Z)}^2 + \|r_0 - \hat{r}_0\|_{L^2(Z)}^2 \right) \\
&\leq 2 \left(M^2 \left\| \mathcal{T} - \hat{\mathcal{T}} \right\|_{\text{op}}^2 + \|r_0 - \hat{r}_0\|_{L^2(Z)}^2 \right).
\end{aligned}$$

104

Therefore,

$$\begin{aligned}
B &= \mathbb{E}_X \left[\left\| \hat{\Phi}(X, \cdot) \right\|_{L^2(Z)}^2 \right] \mathbb{E}_{\mathbf{z}_{1:m-1}} \left[\left\| \Psi_m - \hat{\Psi}_m \right\|_{L^2(Z)}^2 \right] \\
&\leq \left\| \hat{\Phi} \right\|_{\mathcal{R}_W}^2 \mathbb{E}_{\mathbf{z}_{1:m-1}} \left[2 \left(M^2 \left\| \mathcal{T} - \hat{\mathcal{T}} \right\|_{\text{op}}^2 + \|r_0 - \hat{r}_0\|_{L^2(Z)}^2 \right) \right] \\
&= 2 \left\| \hat{\Phi} \right\|_{\mathcal{R}_W}^2 \left(M^2 \left\| \mathcal{T} - \hat{\mathcal{T}} \right\|_{\text{op}}^2 + \|r_0 - \hat{r}_0\|_{L^2(Z)}^2 \right).
\end{aligned}$$

105 What's left to do:

106

- Bound $\left\| \hat{\Phi} \right\|_{\mathcal{R}_W}$. (May not be strictly necessary. This is finite, and since it multiplies something which is \mathcal{O}_p of something which goes to zero, we may not need to further bound it.)

107

108

109

- Use some estimate on $\left\| \mathcal{T} - \hat{\mathcal{T}} \right\|_{\text{op}}$ (Adapt notation and setup in the KIV paper)

110

111

112

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

113

For the rest of the paper:

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119

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

120 **References**

- 121 [1] Masashi Sugiyama, Taiji Suzuki, and Takafumi Kanamori. *Density Ratio Estimation in Machine*
122 *Learning*. Cambridge University Press, 2012. DOI: 10.1017/CB09781139035613.