Stochastic Gradient Descent in NPIV estimation

Anonymous Author(s)
Affiliation
Address
email

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

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

that is, $L^2(X) = L^2(\mathcal{X}, \mathcal{B}(\mathcal{X}), \nu_X)$[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

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

where $h^\star \in L^2(X)$ and ε is an square-integrable r.v. such that $\mathbb{E}[\varepsilon \mid X] \neq 0$. 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, $\nu_{X|Z}(\cdot \mid Z) \neq \nu_X(\cdot)$;

ii) Z influences Y only through Z;

iii) Z and ε are uncorrelated, that is, $\mathbb{E}[\varepsilon \mid Z] = 0$.

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

Conditioning (1) in Z, we find

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

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

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

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 $\mathcal{P}^* : L^2(Z) \to L^2(X)$ satisfies

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

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

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

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

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

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

Submitted to 37th Conference on Neural Information Processing Systems (NeurIPS 2023). Do not distribute.

1.2 Risk measure

Let $\ell : \mathbf{R} \times \mathbf{R} \to \mathbf{R}$ 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 $\ell(y, y') = \frac{1}{2}(y - y')^2$. Given $h \in L^2(X)$, we define the *populational risk* associated with it to be

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

We would like to solve

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

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

We now state all the assumptions needed about the function ℓ for future reference:

Assumption 1 (Regularity of ℓ)**.**

1. *The function $\ell : \mathbf{R} \times \mathbf{R} \to \mathbf{R}$ is convex and C^2 with respect to its second argument;*
2. *There exists $\theta_0 > 0$ such that for all $f, g \in L^2(X)$*

$$\sup_{|\theta| < \theta_0} \mathbb{E}\left[\partial_2^2 \ell(r_0(Z), \mathcal{P}[g + \theta f](Z)) \cdot \mathcal{P}[f](Z)^2\right] < \infty; \tag{5}$$

Assumption 1.2 is a mild integrability condition which can be easily shown to hold in the quadratic case.

2 Gradient computation

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

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

where $\theta \in \mathbf{R}$ is due to Taylor's formula and can be assumed to be inside a fixed interval $(-\theta_0, \theta_0)$, Assumption
with θ_0 arbitrarily small. The last step is then due to Assumption 1.2.

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

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

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

Assumption

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

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

Assumption

Talk about which conditions ℓ can satisfy so that this is continuous.

3 Estimating the gradient

We have found that

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

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

Assumption

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

Thus, we must take

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

With this choice, setting $u_h(x) = \Phi(x, Z)\Psi_h(Z)$ we clearly have $\mathbb{E}[u_h(x)] = \nabla \mathcal{R}(h)(x)$. An obvious obstacle for this approach is that we don't know how to analytically compute Φ, r_0 nor $\mathcal{P}$, se we will proceed with estimators $\widehat{\Phi}, \widehat{r_0}$ and $\widehat{\mathcal{P}}$. In what follows, we remain agnostic to the exact form of these estimators and present the algorithm assuming we know how to compute them. Later, we'll show how the individual convergence rates of these three pieces come together to determine the convergence rate of our method.

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 $L^2(X)$.

4 Algorithm

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

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 $\mathcal{X}$.

[2] It is if ℓ is quadratic.

Algorithm 1: SGD-NPIV

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

output : $\left\{\widehat{h}(\boldsymbol{x}_k)\right\}_{k=1}^K$

Compute $\{\widehat{r_0}(\boldsymbol{z}_m; \mathcal{D}_{r_0})\}_{m=1}^M$;
Compute $\widehat{\Phi}(\boldsymbol{x}, \boldsymbol{z}; \mathcal{D}_\Phi)$;
for $1 \leq m \leq M$ **do**
  Compute $\widehat{\mathcal{P}}[\widehat{h}_{m-1}](\boldsymbol{z}_m; \mathcal{D}_\mathcal{P})$;
  Set $u_m(\boldsymbol{x}_k) = \widehat{\Phi}(\boldsymbol{x}_k, \boldsymbol{z}_m)\partial_2 \ell\left(\widehat{r_0}(\boldsymbol{z}_m, \mathcal{D}_{r_0}), \widehat{\mathcal{P}}[\widehat{h}_{m-1}](\boldsymbol{z}_m; \mathcal{D}_\mathcal{P})\right)$ for $1 \leq k \leq K$;
  Set $\widehat{h}_m(\boldsymbol{x}_k) = \widehat{h}_{m-1}(\boldsymbol{x}_k) - \alpha_m u_m(\boldsymbol{x}_k)$ for $1 \leq k \leq K$;
end
Set $\widehat{h} = \frac{1}{M}\sum_{m=1}^M \widehat{h}_m$;

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

Should we do this?

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

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

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

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

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

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

5 Proof of convergence

The first problem is proving our sequence of estimates is, in fact, contained in $L^2(X)$. This amounts 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 unbiased gradient when we know r_0, Φ and $\mathcal{P}$) belongs to $L^2(X)$

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

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

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

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

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

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

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

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

$$\frac{1}{2}\left\|\widehat{h}_m - h^\star\right\|^2 \leq \frac{1}{2}\left\|\widehat{h}_{m-1} - h^\star\right\|^2 - \alpha_m \langle u_m - \nabla\mathcal{R}(\widehat{h}_{m-1}), \widehat{h}_{m-1} - h^\star\rangle \\ + \frac{\alpha_m^2}{2}\|u_m\|^2 - \alpha_m(\mathcal{R}(\widehat{h}_{m-1}) - \mathcal{R}(h^\star)).$$

Rearranging terms, we get

$$\mathcal{R}(\widehat{h}_{m-1}) - \mathcal{R}(h^\star) \leq \frac{1}{2\alpha_m}\left(\left\|\widehat{h}_{m-1} - h^\star\right\|^2 - \left\|\widehat{h}_m - h^\star\right\|^2\right) \\ + \frac{\alpha_m}{2}\|u_m\|^2 - \langle u_m - \nabla\mathcal{R}(\widehat{h}_{m-1}), \widehat{h}_{m-1} - h^\star\rangle.$$

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

$$\sum_{n=1}^{M}\left[\mathcal{R}(\widehat{h}_{m-1}) - \mathcal{R}(h^\star)\right] \leq \sum_{m=1}^{M}\frac{1}{2\alpha_m}\left(\left\|\widehat{h}_{m-1} - h^\star\right\|^2 - \left\|\widehat{h}_m - h^\star\right\|^2\right) \\ + \sum_{m=1}^{M}\frac{\alpha_m}{2}\|u_m\|^2 \\ - \sum_{m=1}^{M}\langle u_m - \nabla\mathcal{R}(\widehat{h}_{m-1}), \widehat{h}_{m-1} - h^\star\rangle.$$

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

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

$$\sum_{m=1}^{M}\frac{1}{2\alpha_m}\left(\left\|\widehat{h}_{m-1} - h^\star\right\|^2 - \left\|\widehat{h}_m - h^\star\right\|^2\right) = \sum_{m=2}^{M}\left(\frac{1}{2\alpha_m} - \frac{1}{2\alpha_{m-1}}\right)\left\|\widehat{h}_{m-1} - h^\star\right\|^2 \\ + \frac{1}{2\alpha_1}\left\|\widehat{h}_0 - h^\star\right\|^2 - \frac{1}{2\alpha_M}\left\|\widehat{h}_M - h^\star\right\|^2 \\ \leq \sum_{m=2}^{M}\left(\frac{1}{2\alpha_m} - \frac{1}{2\alpha_{m-1}}\right)D^2 + \frac{1}{2\alpha_1}D^2 = \frac{D^2}{2\alpha_M}.$$

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

$$\mathbb{E}_{\boldsymbol{z}_{1:M}}\left[\|u_m\|^2 \mid \mathcal{D}_{\Phi,\mathcal{P},r_0}\right] = \mathbb{E}_{\boldsymbol{z}_{1:m}}\left[\mathbb{E}_X\left[\widehat{\Phi}(X,\boldsymbol{z}_m)^2\partial_2\ell\left(\widehat{r_0}(\boldsymbol{z}_m), \widehat{\mathcal{P}}[\widehat{h}_{m-1}](\boldsymbol{z}_m)\right)^2\right] \;\middle|\; \mathcal{D}_{\Phi,\mathcal{P},r_0}\right] \\ = \mathbb{E}_X\left[\mathbb{E}_{\boldsymbol{z}_{1:m}}\left[\widehat{\Phi}(X,\boldsymbol{z}_m)^2\partial_2\ell\left(\widehat{r_0}(\boldsymbol{z}_m), \widehat{\mathcal{P}}[\widehat{h}_{m-1}](\boldsymbol{z}_m)\right)^2 \;\middle|\; \mathcal{D}_{\Phi,\mathcal{P},r_0}\right]\right].$$

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

$$\mathbb{E}_X\left[\mathbb{E}_{\boldsymbol{z}_{1:m}}\left[\widehat{\Phi}(X,\boldsymbol{z}_m)^2\partial_2\ell\left(\widehat{r_0}(\boldsymbol{z}_m), \widehat{\mathcal{P}}[\widehat{h}_{m-1}](\boldsymbol{z}_m)\right)^2\right]\right].$$

Reversing back the expectations, we get

$$\mathbb{E}_{\boldsymbol{z}_{1:m}}\left[\mathbb{E}_X\left[\widehat{\Phi}(X,\boldsymbol{z}_m)^2\partial_2\ell\left(\widehat{r_0}(\boldsymbol{z}_m), \widehat{\mathcal{P}}[\widehat{h}_{m-1}](\boldsymbol{z}_m)\right)^2\right]\right] \\ = \mathbb{E}_{\boldsymbol{z}_{1:m}}\left[\mathbb{E}_X\left[\widehat{\Phi}(X,\boldsymbol{z}_m)^2\right]\partial_2\ell\left(\widehat{r_0}(\boldsymbol{z}_m), \widehat{\mathcal{P}}[\widehat{h}_{m-1}](\boldsymbol{z}_m)\right)^2\right].$$

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

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

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

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

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

$$\begin{aligned}&\mathbb{E}_{\boldsymbol{z}_{1:m}}\left[\mathbb{E}_X\left[\widehat{\Phi}(X, \boldsymbol{z}_m)^2\right] \partial_2 \ell\left(\widehat{r_0}(\boldsymbol{z}_m), \widehat{\mathcal{P}}[\widehat{h}_{m-1}](\boldsymbol{z}_m)\right)^2\right] \\ &\quad\leq \mathbb{E}_{\boldsymbol{z}_{1:m}}\left[\mathbb{E}_X\left[\left\|\widehat{\Phi}\right\|^2_{\mathcal{R}_{\mathbb{W}}}\right] \partial_2 \ell\left(\widehat{r_0}(\boldsymbol{z}_m), \widehat{\mathcal{P}}[\widehat{h}_{m-1}](\boldsymbol{z}_m)\right)^2\right] \\ &\quad= \left\|\widehat{\Phi}\right\|^2_{\mathcal{R}_{\mathbb{W}}} \mathbb{E}_{\boldsymbol{z}_{1:m}}\left[\partial_2 \ell\left(\widehat{r_0}(\boldsymbol{z}_m), \widehat{\mathcal{P}}[\widehat{h}_{m-1}](\boldsymbol{z}_m)\right)^2\right].\end{aligned}$$

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

$$\begin{aligned}&\mathbb{E}_{\boldsymbol{z}_{1:m}}\left[\left(\widehat{\mathcal{P}}[\widehat{h}_{m-1}](\boldsymbol{z}_m) - \widehat{r_0}(\boldsymbol{z}_m)\right)^2\right] \\ &\quad= \mathbb{E}_{\boldsymbol{z}_{1:m}}\Bigg[\Bigg(\left(\widehat{\mathcal{P}}[\widehat{h}_{m-1}](\boldsymbol{z}_m) - \mathcal{P}[\widehat{h}_{m-1}](\boldsymbol{z}_m)\right) + (r_0(\boldsymbol{z}_m) - \widehat{r_0}(\boldsymbol{z}_m)) \\ &\qquad\qquad + \left(\mathcal{P}[\widehat{h}_{m-1}](\boldsymbol{z}_m) - r_0(\boldsymbol{z}_m)\right)\Bigg)^2\Bigg] \\ &\quad\leq 3\mathbb{E}_{\boldsymbol{z}_{1:m}}\Bigg[\left(\widehat{\mathcal{P}}[\widehat{h}_{m-1}](\boldsymbol{z}_m) - \mathcal{P}[\widehat{h}_{m-1}](\boldsymbol{z}_m)\right)^2 + (r_0(\boldsymbol{z}_m) - \widehat{r_0}(\boldsymbol{z}_m))^2 \\ &\qquad\qquad + \left(\mathcal{P}[\widehat{h}_{m-1}](\boldsymbol{z}_m) - r_0(\boldsymbol{z}_m)\right)^2\Bigg] \\ &\quad= 3\Bigg\{\mathbb{E}_{\boldsymbol{z}_{1:m-1}}\left[\left\|(\widehat{\mathcal{P}} - \mathcal{P})[\widehat{h}_{m-1}]\right\|^2_{L^2(\mathbb{Z})}\right] + \mathbb{E}_{\boldsymbol{z}_{1:m}}\left[\|r_0 - \widehat{r_0}\|^2_{L^2(\mathbb{Z})}\right] \\ &\qquad\qquad + \mathbb{E}_{\boldsymbol{z}_{1:m-1}}\left[\left\|\mathcal{P}[\widehat{h}_{m-1}] - r_0\right\|^2_{L^2(\mathbb{Z})}\right]\Bigg\}.\end{aligned}$$

We treat each part of this expression separately. Firstly,

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

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

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

Putting everything together, what we conclude is

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

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

Third term

Our goal is to open up the inner product and make explicit the estimation errors of our model's different components, like we did before. Here, we define $\Psi_m(Z) \triangleq \partial_2 \ell(r_0(Z), \mathcal{P}[\widehat{h}_{m-1}](Z))$. The hat version $\widehat{\Psi}_m$ is defined accordingly, replacing r_0 and $\mathcal{P}$ by their estimators.

$$
\begin{aligned}
&\mathbb{E}_{\boldsymbol{z}_{1:m}}\left[\langle \nabla\mathcal{R}(\widehat{h}_{m-1}) - u_m, \widehat{h}_{m-1} - h^\star\rangle \mid \mathcal{D}_{\Phi,\mathcal{P},r_0}\right] \\
&\quad= \mathbb{E}_{\boldsymbol{z}_{1:m}}\left[\langle \nabla\mathcal{R}(\widehat{h}_{m-1}) - u_m, \widehat{h}_{m-1} - h^\star\rangle\right] && (\boldsymbol{z}_{1:m} \perp\!\!\!\perp \mathcal{D}_{\Phi,\mathcal{P},r_0}) \\
&\quad= \mathbb{E}_{\boldsymbol{z}_{1:m-1}}\left[\mathbb{E}_{\boldsymbol{z}_m}\left[\langle \nabla\mathcal{R}(\widehat{h}_{m-1}) - u_m, \widehat{h}_{m-1} - h^\star\rangle\right]\right] && (\boldsymbol{z}_m \perp\!\!\!\perp \boldsymbol{z}_{1:m-1}) \\
&\quad= \mathbb{E}_{\boldsymbol{z}_{1:m-1}}\left[\langle \nabla\mathcal{R}(\widehat{h}_{m-1}) - \mathbb{E}_{\boldsymbol{z}_m}[u_m], \widehat{h}_{m-1} - h^\star\rangle\right] \\
&\quad\leq \mathbb{E}_{\boldsymbol{z}_{1:m-1}}\left[\left\|\nabla\mathcal{R}(\widehat{h}_{m-1}) - \mathbb{E}_{\boldsymbol{z}_m}[u_m]\right\|\left\|\widehat{h}_{m-1} - h^\star\right\|\right] \\
&\quad\leq D\mathbb{E}_{\boldsymbol{z}_{1:m-1}}\left[\left\|\nabla\mathcal{R}(\widehat{h}_{m-1}) - \mathbb{E}_{\boldsymbol{z}_m}[u_m]\right\|\right] && (\operatorname{diam}\mathcal{F} = D) \\
&\quad\leq D\mathbb{E}_{\boldsymbol{z}_{1:m-1}}\left[\mathbb{E}_X\left[\left(\nabla\mathcal{R}(\widehat{h}_{m-1})(X) - \mathbb{E}_{\boldsymbol{z}_m}[u_m]\right)^2\right]\right]^{\frac{1}{2}} && (\text{Jensen}) \\
&\quad= D\mathbb{E}_{\boldsymbol{z}_{1:m-1}}\Bigg[\mathbb{E}_X\Bigg[\Big(\mathbb{E}_Z\left[\Phi(X,Z)\Psi_m(Z)\right] \\
&\qquad\qquad - \mathbb{E}_{\boldsymbol{z}_m}\left[\widehat{\Phi}(X,\boldsymbol{z}_m)\widehat{\Psi}_m(\boldsymbol{z}_m)\right]\Big)^2\Bigg]\Bigg]^{\frac{1}{2}} \\
&\quad= D\mathbb{E}_{\boldsymbol{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 \overset{\text{iid}}{\sim} \boldsymbol{z}_m) \\
&\quad= D\mathbb{E}_{\boldsymbol{z}_{1:m-1}}\Bigg[\mathbb{E}_X\Bigg[\mathbb{E}_Z\Big[\Psi_m(Z)\left(\Phi(X,Z) - \widehat{\Phi}(X,Z)\right) \\
&\qquad\qquad + \widehat{\Phi}(X,Z)\left(\Psi_m(Z) - \widehat{\Psi}_m(Z)\right)\Big]^2\Bigg]\Bigg]^{\frac{1}{2}} \\
&\quad\leq D\mathbb{E}_{\boldsymbol{z}_{1:m-1}}\Bigg[\mathbb{E}_X\Bigg[\Big(\|\Psi_m\|_{L^2(Z)}\left\|\Phi(X,\cdot) - \widehat{\Phi}(X,\cdot)\right\|_{L^2(Z)} \\
&\qquad\qquad + \left\|\widehat{\Phi}(X,\cdot)\right\|_{L^2(Z)}\left\|\Psi_m - \widehat{\Psi}_m\right\|_{L^2(Z)}\Big)^2\Bigg]\Bigg]^{\frac{1}{2}} \\
&\quad\leq \sqrt{2}D\mathbb{E}_{\boldsymbol{z}_{1:m-1}}\Bigg[\mathbb{E}_X\Bigg[\|\Psi_m\|^2_{L^2(Z)}\left\|\Phi(X,\cdot) - \widehat{\Phi}(X,\cdot)\right\|^2_{L^2(Z)} \\
&\qquad\qquad + \left\|\widehat{\Phi}(X,\cdot)\right\|^2_{L^2(Z)}\left\|\Psi_m - \widehat{\Psi}_m\right\|^2_{L^2(Z)}\Bigg]\Bigg]^{\frac{1}{2}} \\
&\quad= \sqrt{2}D\Bigg(\mathbb{E}_{\boldsymbol{z}_{1:m-1}}\left[\|\Psi_m\|^2_{L^2(Z)}\mathbb{E}_X\left[\left\|\Phi(X,\cdot) - \widehat{\Phi}(X,\cdot)\right\|^2_{L^2(Z)}\right]\right] \\
&\qquad\qquad + \mathbb{E}_{\boldsymbol{z}_{1:m-1}}\left[\left\|\Psi_m - \widehat{\Psi}_m\right\|^2_{L^2(Z)}\mathbb{E}_X\left[\left\|\widehat{\Phi}(X,\cdot)\right\|^2_{L^2(Z)}\right]\right]\Bigg)^{\frac{1}{2}} \\
&\quad= \sqrt{2}D\Bigg(\mathbb{E}_X\left[\left\|\Phi(X,\cdot) - \widehat{\Phi}(X,\cdot)\right\|^2_{L^2(Z)}\right]\mathbb{E}_{\boldsymbol{z}_{1:m-1}}\left[\|\Psi_m\|^2_{L^2(Z)}\right] \\
&\qquad\qquad + \mathbb{E}_X\left[\left\|\widehat{\Phi}(X,\cdot)\right\|^2_{L^2(Z)}\right]\mathbb{E}_{\boldsymbol{z}_{1:m-1}}\left[\left\|\Psi_m - \widehat{\Psi}_m\right\|^2_{L^2(Z)}\right]\Bigg)^{\frac{1}{2}}
\end{aligned}
$$

$$=: \sqrt{2}D(A+B)^{\frac{1}{2}}.$$

We proceed to analyze each term separately:

- To bound A, first notice that

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

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

Create section describing how we are estimating each term.

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

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

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

In total, what we have is

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

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

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

We still need to bound this norm somehow.

Furthermore, we also have

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

Therefore,

$$
\begin{aligned}
B &= \mathbb{E}_X\left[\left\|\widehat{\Phi}(X,\cdot)\right\|^2_{L^2(Z)}\right]\mathbb{E}_{\boldsymbol{z}_{1:m-1}}\left[\left\|\Psi_m-\widehat{\Psi}_m\right\|^2_{L^2(Z)}\right] \\
&\leq \left\|\widehat{\Phi}\right\|^2_{\mathcal{R}_{\mathbb{W}}}\mathbb{E}_{\boldsymbol{z}_{1:m-1}}\left[2\left(M^2\left\|\mathcal{P}-\widehat{\mathcal{P}}\right\|^2_{\mathrm{op}}+\|r_0-\widehat{r_0}\|^2_{L^2(Z)}\right)\right] \\
&= 2\left\|\widehat{\Phi}\right\|^2_{\mathcal{R}_{\mathbb{W}}}\left(M^2\left\|\mathcal{P}-\widehat{\mathcal{P}}\right\|^2_{\mathrm{op}}+\|r_0-\widehat{r_0}\|^2_{L^2(Z)}\right).
\end{aligned}
$$

What's left to do:

- Bound $\left\|\widehat{\Phi}\right\|_{\mathcal{R}_{\mathbb{W}}}$. (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.)
- Use some estimate on $\left\|\mathcal{P}-\widehat{\mathcal{P}}\right\|_{\mathrm{op}}$ (Adapt notation and setup in the KIV paper).

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

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

  with $k_X : \mathbb{X}\times\mathbb{X} \to \mathbf{R}$ being the kernel associated with $\mathcal{H}_X$. Then $\mathcal{P} = \mathcal{P}\circ\iota_X\iota_X^*$ and we can directly apply the result on KIV's paper, since $\mathcal{P}\circ i_X$ can be seen as the restriction of $\mathcal{P}$ to $\mathcal{H}_X$. We then also need the further hypothesis that $\mathrm{Im}(\mathcal{P}\circ\iota_X)\subseteq\mathcal{H}_Z$, or something like this (because, rigorously speaking, $\mathcal{P}f$ is an equivalence class of functions, so in what way can we say that this equivalence class is "in $\mathcal{H}_Z$"?). This hypothesis is implicitly made in the KIV paper, when they say that $E : \mathcal{H}_{\mathcal{X}} \to \mathcal{H}_Z$ without providing any assumptions on $\mathcal{H}_X$ and $\mathcal{H}_Z$, other than saying that they are RKHS. Who can guarantee that $(z \mapsto \mathbb{E}[f(X) \mid Z = z]) \in \mathcal{H}_Z$ for every $f \in \mathcal{H}_X$?
- Find way to estimate r_0 which gives estimate on $\|r_0-\widehat{r_0}\|_{L^2(Z)}$. Maybe use the same estimation technique we have for $\mathcal{P}$ as an operator from $L^2(Y)\to L^2(Z)$ applied to the identity and employ the same bound?

For the rest of the paper:

- Create section which describes, in detail, how we are estimating Φ, $\mathcal{P}$ 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 $\mathcal{P}$.
- 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.

References

[1] Masashi Sugiyama, Taiji Suzuki, and Takafumi Kanamori. *Density Ratio Estimation in Machine Learning*. Cambridge University Press, 2012. DOI: 10.1017/CBO9781139035613.