
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, we denote the norm and inner product in $L^2(X)$ by $\|\cdot\|$ and $\langle \cdot, \cdot \rangle$, respectively.

65 By the Algorithm 1 procedure, we have

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

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

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

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

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

68 Rearranging terms, we get

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

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

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

70 5.1 Option 1: averaging with respect to everything

71 We then treat each term (summation) separately:

- 72 • The first term is bounded using the assumption that $\text{diam } \mathcal{F} = D < \infty$.
- 73 • The bound on the second term depends on bounding $\mathbb{E} [\|u_m\|_{L^2(X)}^2]$ by a constant indepen-
- 74 dent of m or M .
- 75 • The third term must vanish because of the unbiasedness of u_m , but we don't know that our
- 76 u_m is unbiased, and it may very well not be.

Assumption

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

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

78 **Second term** Define \mathcal{D} to be the set of all observed data, that is, all of the variables in $\mathcal{D}_\Phi, \mathcal{D}_{r_0}, \mathcal{D}_\mathcal{T}$
 79 and $\{z_i\}_{i=1}^M$. Let's evaluate $\mathbb{E} [\|u_m\|^2]$:

$$\mathbb{E} [\|u_m\|^2] = \mathbb{E}_\mathcal{D} \left[\mathbb{E}_X \left[\hat{\Phi}(X, z_m; \mathcal{D}_\Phi)^2 \partial_2 \ell \left(\hat{r}_0(z_m; \mathcal{D}_{r_0}), \mathcal{T}[\widehat{h_{m-1}}](z_m; \mathcal{D}_\mathcal{T}) \right)^2 \right] \right],$$

80 where the second expectation is with respect to a copy of X which is independent of \mathcal{D} . Continuing:

$$\begin{aligned} \mathbb{E}_\mathcal{D} \left[\mathbb{E}_X \left[\hat{\Phi}(X, z_m; \mathcal{D}_\Phi)^2 \partial_2 \ell \left(\hat{r}_0(z_m; \mathcal{D}_{r_0}), \mathcal{T}[\widehat{h_{m-1}}](z_m; \mathcal{D}_\mathcal{T}) \right)^2 \right] \right] \\ = \mathbb{E}_\mathcal{D} \left[\partial_2 \ell \left(\hat{r}_0(z_m; \mathcal{D}_{r_0}), \mathcal{T}[\widehat{h_{m-1}}](z_m; \mathcal{D}_\mathcal{T}) \right)^2 \mathbb{E}_X [\hat{\Phi}(X, z_m; \mathcal{D}_\Phi)^2] \right]. \end{aligned}$$

81 If ℓ is quadratic, we have

$$\begin{aligned} \mathbb{E}_\mathcal{D} \left[\partial_2 \ell \left(\hat{r}_0(z_m; \mathcal{D}_{r_0}), \mathcal{T}[\widehat{h_{m-1}}](z_m; \mathcal{D}_\mathcal{T}) \right)^2 \mathbb{E}_X [\hat{\Phi}(X, z_m; \mathcal{D}_\Phi)^2] \right] \\ = \mathbb{E}_\mathcal{D} \left[\left(\mathcal{T}[\widehat{h_{m-1}}](z_m; \mathcal{D}_\mathcal{T}) - \hat{r}_0(z_m; \mathcal{D}_{r_0}) \right)^2 \mathbb{E}_X [\hat{\Phi}(X, z_m; \mathcal{D}_\Phi)^2] \right]. \end{aligned}$$

82

83 **Third term** We have to work with

$$\mathbb{E} [\langle u_m - \nabla \mathcal{R}(\hat{h}_{m-1}), \hat{h}_{m-1} - h^* \rangle].$$

Find a way to finish this bound. Maybe switch the order of expectations? First in X and then in \mathcal{D} .

84 The strategy employed on the SIP paper was to condition on the σ -algebra generated by the training
 85 samples observed up until iteration iteration $m - 1$. In our case, that would be z_1, \dots, z_{m-1} . The
 86 problem which arises is that we no longer have measurability of \hat{h}_{m-1} with respect to this σ -algebra,
 87 as it depends on the datasets $\mathcal{D}_\Phi, \mathcal{D}_\mathcal{T}, \mathcal{D}_{r_0}$, used to estimate $\hat{\Phi}, \hat{\mathcal{T}}$ and \hat{r}_0 in an offline manner.

88 The other option would be to condition on more things, namely the σ -algebra generated by
 89 $z_1, \dots, z_{m-1}, \mathcal{D}_\Phi, \mathcal{D}_\mathcal{T}, \mathcal{D}_{r_0}$. We gain measurability of \hat{h}_{m-1} , but we are no longer integrating
 90 out $\mathcal{D}_\Phi, \mathcal{D}_\mathcal{T}, \mathcal{D}_{r_0}$, which is needed to use some sort of unbiasedness of the estimators $\hat{\Phi}, \hat{\mathcal{T}}, \hat{r}_0$.

91 Let's try the latter and see what we end up with. Define $\mathcal{D}_{m-1} \triangleq \mathcal{D}_\Phi \cup \mathcal{D}_\mathcal{T} \cup \mathcal{D}_{r_0} \cup \{z_1, \dots, z_{m-1}\}$.
 92 Then,

$$\begin{aligned} \mathbb{E}_\mathcal{D} [\langle u_m - \nabla \mathcal{R}(\hat{h}_{m-1}), \hat{h}_{m-1} - h^* \rangle] \\ = \mathbb{E}_{\mathcal{D}_{m-1}} \left[\mathbb{E} [\langle u_m - \nabla \mathcal{R}(\hat{h}_{m-1}), \hat{h}_{m-1} - h^* \rangle \mid \mathcal{D}_{m-1}] \right] \\ = \mathbb{E}_{\mathcal{D}_{m-1}} \left[\langle \mathbb{E}[u_m \mid \mathcal{D}_{m-1}] - \nabla \mathcal{R}(\hat{h}_{m-1}), \hat{h}_{m-1} - h^* \rangle \right] \quad (\text{Justify this properly}). \end{aligned}$$

93 Now we must evaluate the expression inside the inner product. We restrict ourselves to the quadratic
 94 case. Define $\psi(z) = \mathcal{T}[\widehat{h_{m-1}}](z) - r_0(z)$ and $\hat{\psi}(z; \mathcal{D}_{\text{proj}}) = \mathcal{T}[\widehat{h_{m-1}}](z; \mathcal{D}_\mathcal{T}) - \hat{r}_0(z; \mathcal{D}_{r_0})$, where

95 $\mathcal{D}_{\text{proj}} = \mathcal{D}_{\mathcal{T}} \cup \mathcal{D}_{r_0}$. Then:

$$\begin{aligned}
& \mathbb{E}[u_m(x) \mid \mathcal{D}_{m-1}] - \nabla \mathcal{R}(\hat{h}_{m-1})(x) \\
&= \mathbb{E} \left[\hat{\Phi}(x, Z; \mathcal{D}_{\Phi}) \hat{\psi}(Z; \mathcal{D}_{\text{proj}}) \mid \mathcal{D}_{m-1} \right] - \mathbb{E}_Z [\Phi(x, Z) \psi(Z)] \\
&= \mathbb{E}_Z \left[\hat{\Phi}(x, Z; \mathcal{D}_{\Phi}) \hat{\psi}(Z; \mathcal{D}_{\text{proj}}) \right] - \mathbb{E}_Z [\Phi(x, Z) \psi(Z)] \\
&= \mathbb{E}_Z \left[\left(\hat{\Phi}(x, Z; \mathcal{D}_{\Phi}) - \Phi(x, Z) \right) \hat{\psi}(Z; \mathcal{D}_{\text{proj}}) + \left(\hat{\psi}(Z; \mathcal{D}_{\text{proj}}) - \psi(Z) \right) \Phi(x, Z) \right] \\
&= \left\langle \hat{\Phi}(x, \cdot; \mathcal{D}_{\Phi}) - \Phi(x, \cdot), \hat{\psi}(\cdot; \mathcal{D}_{\text{proj}}) \right\rangle_{L^2(Z)} + \left\langle \hat{\psi}(\cdot; \mathcal{D}_{\text{proj}}) - \psi(\cdot), \Phi(x, \cdot) \right\rangle_{L^2(Z)} \\
&\leq \left\| \hat{\Phi}(x, \cdot; \mathcal{D}_{\Phi}) - \Phi(x, \cdot) \right\|_{L^2(Z)} \left\| \hat{\psi}(\cdot; \mathcal{D}_{\text{proj}}) \right\|_{L^2(Z)} \\
&\quad + \left\| \hat{\psi}(\cdot; \mathcal{D}_{\text{proj}}) - \psi(\cdot) \right\|_{L^2(Z)} \left\| \Phi(x, \cdot) \right\|_{L^2(Z)}.
\end{aligned}$$

96 5.2 Option 2: conditioning on $\mathcal{D}_{\Phi, \mathcal{T}, r_0}$ and averaging with respect to z_1, \dots, z_M

97 With this strategy, our aim isn't to get a convergence guarantee analogous to that of the SIP paper, but
 98 some sort of "given $\mathcal{D}_{\Phi, \mathcal{T}, r_0}$, this inequality is true with high probability" guarantee.

99 We similarly treat each of the three terms separately.

100 **First term** It is bounded in the exact same way as before, since this bound is deterministic and does
 101 not involve expectations.

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

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

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

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

105 Reversing back the expectations, we get

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

106 Assuming quadratic loss, we can write this as

$$\begin{aligned}
& \mathbb{E}_{\mathbf{z}_{1:m}} \left[\mathbb{E}_X \left[\hat{\Phi}(X, \mathbf{z}_m)^2 \right] \left(\hat{\mathcal{T}}[\hat{h}_{m-1}](\mathbf{z}_m) - \hat{r}_0(\mathbf{z}_m) \right)^2 \right] \\
&= \mathbb{E}_{\mathbf{z}_{1:m}} \left[\mathbb{E}_X \left[\hat{\Phi}(X, \mathbf{z}_m)^2 \right] \cdot \left(\left(\hat{\mathcal{T}}[\hat{h}_{m-1}](\mathbf{z}_m) - \mathcal{T}[\hat{h}_{m-1}](\mathbf{z}_m) \right) \right. \right. \\
&\quad \left. \left. + (r_0(\mathbf{z}_m) - \hat{r}_0(\mathbf{z}_m)) \right. \right. \\
&\quad \left. \left. + \left(\mathcal{T}[\hat{h}_{m-1}](\mathbf{z}_m) - r_0(\mathbf{z}_m) \right) \right)^2 \right] \\
&\leq 3 \mathbb{E}_{\mathbf{z}_{1:m}} \left[\mathbb{E}_X \left[\hat{\Phi}(X, \mathbf{z}_m)^2 \right] \left(\hat{\mathcal{T}}[\hat{h}_{m-1}](\mathbf{z}_m) - \mathcal{T}[\hat{h}_{m-1}](\mathbf{z}_m) \right)^2 \right. \\
&\quad \left. + \mathbb{E}_X \left[\hat{\Phi}(X, \mathbf{z}_m)^2 \right] (r_0(\mathbf{z}_m) - \hat{r}_0(\mathbf{z}_m))^2 \right. \\
&\quad \left. + \mathbb{E}_X \left[\hat{\Phi}(X, \mathbf{z}_m)^2 \right] \left(\mathcal{T}[\hat{h}_{m-1}](\mathbf{z}_m) - r_0(\mathbf{z}_m) \right)^2 \right].
\end{aligned}$$

107 Don't know what else to do with this for now. My guess is well have to use some boundedness
108 assumptions on the RKHSs used to estimate Φ, \mathcal{T} and r_0 to uniformly bound this expression. The
109 goal is to bound this uniformly with respect to z_1, z_2, \dots and in a way which does not explode as
110 $|\mathcal{D}_{\Phi, \mathcal{T}, r_0}|$ and M grow.

111 **Third term**