Supplementary Material for Machine Learning for Variance Reduction in Online Experiments

Yongyi Guo Department of Operations Research and Financial Engineering Princeton University Princeton, NJ 08544 yongyig@princeton.edu

Dominic Coey Facebook 1 Hacker Way, Menlo Park, CA 94025 coey@fb.com Mikael Konutgan Facebook 1 Hacker Way, Menlo Park, CA 94025 kmikael@fb.com

Wenting Li Facebook 1 Hacker Way, Menlo Park, CA 94025 wentingli@fb.com Chris Schoener Facebook 1 Hacker Way, Menlo Park, CA 94025 chrissc@fb.com

Matt Goldman Facebook 1 Hacker Way, Menlo Park, CA 94025 mattgoldman@fb.com

In this supplementary material, we provide the proof of all theoretical results stated in the paper.

1 Proof of Proposition 1

For any (deterministic) $g \in \mathcal{G}$, we have

$$P[Z(g)Z(g)^{\top}] = M_1(g) \otimes M_2,$$

where \otimes denotes the Kronecker product,

$$M_1(g) = \begin{pmatrix} 1 & Eg(X) \\ Eg(X) & Eg(X)^2 \end{pmatrix}, \quad M_2 = \begin{pmatrix} 1 & p \\ p & p \end{pmatrix}.$$

Therefore, any eigenvalue of $P[Z(g)Z(g)^{\top}]$ is the product of one eigenvalue of $M_1(g)$ and one eigenvalue of M_2 . It's easy to verify from Assumption 1 that all eigenvalues of $M_1(g)$ and M_2 are nonnegative and bounded. Thus, we only need to show $\inf_{g \in \mathcal{G}} \lambda_{min}(M_1(g)) > 0$, $\lambda_{min}(M_2) > 0$.

Through some calculations, one can find out that

$$\begin{split} \lambda_{\min}(M_1(g)) &= \frac{1}{2} \Big\{ (Eg(X)^2 + 1) - \sqrt{(Eg(X)^2 + 1)^2 - 4Var(g(X))} \Big\} \\ &= \frac{2Var(g(X))}{(Eg(X)^2 + 1) + \sqrt{(Eg(X)^2 + 1)^2 - 4Var(g(X))}} \geq \frac{Var(g(X))}{Eg(X)^2 + 1} \end{split}$$

35th Conference on Neural Information Processing Systems (NeurIPS 2021), Sydney, Australia.

which leads to

$$\inf_{g \in \mathcal{G}} \lambda_{\min}(M_1(g)) \ge \frac{\inf_{g \in \mathcal{G}} Var(g(X))}{\sup_{g \in \mathcal{G}} Eg(X)^2 + 1} > 0.$$

On the other hand, $\lambda_{min}(M_2) > 0$ can be deduced from $p \in (0, 1)$. By combining the above two inequalities, we conclude the proof.

2 **Proof of Proposition 2**

For compactness we may write the random variables $Z(\hat{g}_k)$ as \hat{Z}_k and $Z(g_0)$ as Z. Similarly for any observation *i* we write $Z_i(\hat{g}_k)$ as $\hat{Z}_{k,i}$ and $Z_i(g_0)$ as Z_i . We are only interested in convergence in probability, so we can assume that the inverse matrices in the definition of $\hat{\beta}(\{\hat{g}_k\}_{k=1}^K)$ and $\hat{\beta}(g_0)$ exist, as this happens with probability approaching 1 according to Lemma 2. We have $\hat{\beta}(\{\hat{g}_k\}_{k=1}^K) - \beta(\{\hat{g}_k\}_{k=1}^K) = A + B$, where

$$A = \underbrace{\left[\left[\frac{1}{N} \sum_{k} \sum_{i \in I_{k}} \widehat{Z}_{k,i} \widehat{Z}_{k,i}^{\top} \right]^{-1} - \left[\frac{1}{K} \sum_{k} P[\widehat{Z}_{k} \widehat{Z}_{k}^{\top}] \right]^{-1} \right]}_{F_{0}} \cdot \left[\frac{1}{N} \sum_{k} \sum_{i \in I_{k}} \widehat{Z}_{k,i} Y_{i} \right],$$

and

$$B = \left[\frac{1}{K}\sum_{k} P[\widehat{Z}_{k}\widehat{Z}_{k}^{\top}]\right]^{-1} \underbrace{\left[\frac{1}{N}\sum_{k}\sum_{i\in I_{k}} [\widehat{Z}_{k,i}Y_{i} - P[\widehat{Z}_{k}Y]]\right]}_{G_{0}}$$

Similarly, $\widehat{\beta}(g_0) - \beta(g_0) = C + D$, where

$$C = \underbrace{\left[\left[\frac{1}{N}\sum_{i}Z_{i}Z_{i}^{\top}\right]^{-1} - \left[P[ZZ^{\top}]\right]^{-1}\right]}_{F_{1}} \left[\frac{1}{N}\sum_{i}Z_{i}Y_{i}\right]$$

and

$$D = \left[P[ZZ^{\top}]\right]^{-1} \underbrace{\left[\frac{1}{N}\sum_{i} [Z_{i}Y_{i} - P[ZY]]\right]}_{G_{1}}.$$

We can write $[\hat{\beta}(\{\hat{g}_k\}_{k=1}^K) - \beta(\{\hat{g}_k\}_{k=1}^K)] - [\hat{\beta}(g_0) - \beta(g_0)] = A - C + B - D$. We show that $\sqrt{N} \|A - C\| \rightarrow_p 0$ and $\sqrt{N} \|B - D\| \rightarrow_p 0$. From the definitions of F_0 and F_1 above, we have $A - C = [F_0 - F_1] \left[\frac{1}{N} \sum_k \sum_{i \in I_k} \hat{Z}_{k,i} Y_i \right] + F_1 \left[\frac{1}{N} \sum_k \sum_{i \in I_k} (\hat{Z}_{k,i} - Z_i) Y_i \right]$. If

1.
$$\left\|\sqrt{N}[F_0 - F_1]\right\| = o_p(1)$$

2. $\left\|\frac{1}{N}\sum_k \sum_{i \in I_k} \widehat{Z}_{k,i} Y_i\right\| = O_p(1)$
3. $\left\|\sqrt{N}F_1\right\| = O_p(1)$
4. $\left\|\frac{1}{N}\sum_k \sum_{i \in I_k} (\widehat{Z}_{k,i} - Z_i) Y_i\right\| = o_p(1),$

then
$$\sqrt{N} \|A - C\| = o_p(1)$$
 as desired. Similarly we write $B - D$ as $B - D = \left[\left[\frac{1}{K} \sum_k P[\widehat{Z}_k \widehat{Z}_k^\top] \right]^{-1} - \left[P[ZZ^\top] \right]^{-1} \right] G_0 + \left[P[ZZ^\top] \right]^{-1} [G_0 - G_1]$. If
5. $\left\| \left[\frac{1}{K} \sum_k P[\widehat{Z}_k \widehat{Z}_k^\top] \right]^{-1} - \left[P[ZZ^\top] \right]^{-1} \right\| = o_p(1)$

6.
$$\left\|\sqrt{N}G_{0}\right\| = O_{p}(1)$$

7. $\left\|P[ZZ^{\top}]^{-1}\right\| = O_{p}(1)$
8. $\left\|\sqrt{N}[G_{0} - G_{1}]\right\| = o_{p}(1)$

then $\sqrt{N} \|B - D\| = o_p(1)$ as desired. We complete the proof in 8 steps by showing statements 1 - 8 above.

Step 1. We apply Lemma 3 by letting $M_{1n} = \frac{1}{N} \sum_{k} \sum_{i \in I_k} \widehat{Z}_{k,i} \widehat{Z}_{k,i}^{\top}, B_n = M_{2n} = P[ZZ^{\top}], A_n = M_{3n} = \frac{1}{K} \sum_{k} P[\widehat{Z}_k \widehat{Z}_k^{\top}], M_{4n} = \frac{1}{N} \sum_{k} \sum_{i \in I_k} Z_i Z_i^{\top}$. Consequently, Step 1 amounts to verifying the conditions of Lemma 3. In fact, these conditions are guaranteed by Lemma 1 as well as the following fact: For each $k = 1, \ldots, K$,

$$\left\| \frac{1}{\sqrt{n}} \sum_{i \in I_k} \left[\widehat{Z}_{k,i} \widehat{Z}_{k,i}^\top - P[\widehat{Z}_k \widehat{Z}_k^\top] - Z_i Z_i^\top + P[ZZ^\top] \right] \right\| \to_p 0.$$
⁽¹⁾

We now prove (1). Define $W_{k,i} = \hat{Z}_{k,i} \hat{Z}_{k,i}^{\top} - P[\hat{Z}_k \hat{Z}_k^{\top}] - Z_i Z_i^{\top} + P[ZZ^{\top}]$, and note that conditional on the data in I_k^c , the function \hat{g}_k is non-random, and the $W_{k,i}$ are mean zero matrices, uncorrelated across observations in I_k . With slight abuse of notation, we use $E[\cdot | I_k^c]$ to denote expectations conditional on the observations with indices belonging to the set I_k^c . For any k = 1, 2, ..., K,

$$E\left[\left\|\frac{1}{\sqrt{n}}\sum_{i\in I_{k}}W_{k,i}\right\|^{2}\left|I_{k}^{c}\right]=\frac{1}{n}E\left[\operatorname{tr}\left(\sum_{i,j\in I_{k}}W_{k,i}^{\top}W_{k,j}\right)\left|I_{k}^{c}\right]\right]$$
(2)

$$= \frac{1}{n} E\left[\sum_{i \in I_k} \operatorname{tr}\left(W_{k,i}^{\top} W_{k,i}\right) \middle| I_k^c\right]$$
(3)

$$\leq \frac{1}{n} E\left[\sum_{i \in I_k} \left\| \left(\widehat{Z}_{k,i} \widehat{Z}_{k,i}^\top - Z_i Z_i^\top\right) \right\|^2 |I_k^c\right]$$
(4)

$$= P\left[\left\|\widehat{Z}_{k}\widehat{Z}_{k}^{\top} - ZZ^{\top}\right\|^{2}\right].$$
(5)

If the RHS of (5) is $o_p(1)$, we can use Lemma 6.1 of [1] to conclude that $\|\frac{1}{\sqrt{n}} \sum_{i \in I_k} W_{k,i}\|$ is $o_p(1)$ as required. Some calculations give

$$\left\|\widehat{Z}_{k}\widehat{Z}_{k}^{\top} - ZZ^{\top}\right\|^{2} \le 12[(\widehat{g}_{k}(X) - g_{0}(X))^{2} + (\widehat{g}_{k}(X)^{2} - g_{0}(X)^{2})^{2}].$$
(6)

Then $P\left[(\widehat{g}_k - g_0)^2\right] \leq \sqrt{P[(\widehat{g}_k - g_0)^4]} \rightarrow_p 0$. Also

$$P\left[(\hat{g}_k^2 - g_0^2)^2\right] = P[(\hat{g}_k - g_0)^2(\hat{g}_k + g_0)^2] \tag{7}$$

$$\leq \sqrt{P[(\hat{g}_k - g_0)^4]} \sqrt{P[(\hat{g}_k + g_0)^4]} \tag{8}$$

$$\leq \sqrt{P[(\hat{g}_k - g_0)^4]} \sqrt{\sup_{g \in \mathcal{G}} P[g^4]} \tag{9}$$

$$\rightarrow_p 0,$$
 (10)

where the second-to-last line follows because $\hat{g}_k + g_0 \in \mathcal{G}$ as \mathcal{G} is a vector space. We conclude from (6) that the RHS of (5) is $o_p(1)$.

Step 2. By the Cauchy-Schwarz inequality,

$$\left\|\frac{1}{N}\sum_{k}\sum_{i\in I_{k}}Z_{i}(\widehat{g}_{k})Y_{i}\right\| \leq \sqrt{\frac{1}{N}\sum_{k}\sum_{i\in I_{k}}\|Z_{i}(\widehat{g}_{k})\|^{2}}\sqrt{\frac{1}{N}\sum_{k}\sum_{i\in I_{k}}Y_{i}^{2}}.$$
(11)

As $E[Y^2] < \infty$, the second term on the RHS is $O_p(1)$ by Markov's inequality. Also for $i \in I_k$, $E\left[\|Z_i(\widehat{g}_k)\|^2\right] = E[1 + T_i + \widehat{g}_k(X_i)^2 + T_i\widehat{g}_k(X_i)^2] \le \sup_{g \in \mathcal{G}} E[2[1 + g(X_i)^2]] < \infty$, and by Markov's inequality the first term on the RHS is also $O_p(1)$. **Step 3.** By the central limit theorem, $\sqrt{N} \left[\sum_{i} \frac{Z_{i}Z_{i}^{\top}}{N} - P[ZZ^{\top}] \right]$ is asymptotically normal. By the delta method and invertibility of $P[ZZ^{\top}]$, $\sqrt{N} \left[\left[\sum_{i} \frac{Z_{i}Z_{i}^{\top}}{N} \right]^{-1} - P[ZZ^{\top}]^{-1} \right]$ is also, and hence its norm is $O_{p}(1)$.

Step 4. We show that for any k, $\frac{1}{n} \sum_{i \in I_k} (\widehat{g}_k(X_i) - g_0(X_i)) Y_i = o_p(1)$, from which the result follows. By Cauchy-Schwarz,

$$\frac{1}{n} \sum_{i \in I_k} (\widehat{g}_k(X_i) - g_0(X_i)) Y_i \le \sqrt{\frac{1}{n} \sum_{i \in I_k} (\widehat{g}_k(X_i) - g_0(X_i))^2} \sqrt{\frac{1}{n} \sum_{i \in I_k} Y_i^2}$$

As Y has finite second moment by assumption, it remains to show the first term on the RHS is $o_p(1)$. We have

$$\frac{1}{n} \sum_{i \in I_k} (\widehat{g}_k(X_i) - g_0(X_i))^2 = \frac{1}{n} \sum_{i \in I_k} \left[(\widehat{g}_k(X_i) - g_0(X_i))^2 - P[(\widehat{g}_k - g_0)^2] \right] + P[(\widehat{g}_k - g_0)^2].$$
(12)

From Lemma 6.1 in [1], the first term on the RHS in (12) is $o_p(1)$ and by the convergence assumption on \hat{g}_k , the second term is too.

Step 5. By the continuous mapping theorem it suffices to show that $\|\frac{1}{K}\sum_{k} \left[P[Z(\hat{g}_k)Z(\hat{g}_k)^{\top}] - P[Z(g_0)Z(g_0)^{\top}]\right]\| = o_p(1)$. From the argument in Step 1, both $P[[\hat{g}_k - g_0]^2]$ and $P[[\hat{g}_k^2 - g_0^2]^2]$ are $o_p(1)$ for all k, and hence $P[\hat{g}_k - g_0]$ and $P[\hat{g}_k^2 - g_0^2]$ are both $o_p(1)$ for all k. The other entries in the matrix are straightforwardly $o_p(1)$.

Step 6. This follows from Step 8 and the fact that by Chebyshev's inequality, $\|\frac{1}{\sqrt{N}}\sum_{i} [Z_iY_i - P[ZY]] \| = O_p(1).$

Step 7. $P[ZZ^{\top}]$ is invertible by assumption.

=

Step 8. The reasoning here is similar to Step 1. For any k and $i \in I_k$, define $W_{k,i} = \hat{Z}_{k,i}Y_i - P[\hat{Z}_kY] - Z_iY_i + P[ZY]$, and note that conditional on the data in I_k^c , the $W_{k,i}$ are mean zero matrices, uncorrelated across observations in I_k . Then

$$E\left[\left\|\frac{1}{\sqrt{n}}\sum_{i\in I_k}W_{k,i}\right\|^2 \left|I_k^c\right| \le \frac{1}{n}E\left[\sum_{i\in I_k}\left\|\left(\widehat{Z}_{k,i}Y_i - Z_iY_i\right)\right\|^2 \left|I_k^c\right| \le P\left[\left\|\widehat{Z}_kY - ZY\right\|^2\right].\right]\right]$$

Because $P[(\hat{g}_k(X) - g_0(X))^2 Y^2] \leq \sqrt{P[(\hat{g}_k - g_0)^4]} \sqrt{P[Y^4]} \rightarrow_p 0$, the RHS of (2) is $o_p(1)$. We use Lemma 6.1 of [1] to conclude that $\left\| \frac{1}{\sqrt{n}} \sum_{i \in I_k} W_{k,i} \right\|$ is also $o_p(1)$, from which the result follows.

3 Proof of Theorem 1

We have

$$\widehat{\alpha}_1(\{\widehat{g}_k\}_{k=1}^K) - \widehat{\alpha}_1(g_0) = \left[\widehat{\alpha}_1(\{\widehat{g}_k\}_{k=1}^K) - \beta_1(\{\widehat{g}_k\}_{k=1}^K) - \beta_3(\{\widehat{g}_k\}_{k=1}^K) \frac{1}{K} \sum_{k=1}^K P\widehat{g}_k\right]$$
(13)

$$-\left[\widehat{\alpha}_{1}(g_{0}) - \beta_{1}(g_{0}) - \beta_{3}(g_{0})Pg_{0}\right]$$
(14)

$$A+B,$$
(15)

where

$$A = [\widehat{\beta_1}(\{\widehat{g}_k\}_{k=1}^K) - \beta_1(\{\widehat{g}_k\}_{k=1}^K)] - [\widehat{\beta_1}(g_0) - \beta_1(g_0)],$$
(16)

and

$$B = \underbrace{\left[\widehat{\beta_{3}}(\{\widehat{g}_{k}\}_{k=1}^{K})\frac{1}{N}\sum_{i}\widehat{g}_{k(i)}(X_{i}) - \beta_{3}(\{\widehat{g}_{k}\}_{k=1}^{K})\frac{1}{K}\sum_{k=1}^{K}P\widehat{g}_{k}\right]}_{C} - \underbrace{\left[\widehat{\beta_{3}}(g_{0})\frac{1}{N}\sum_{i}g_{0}(X_{i}) - \beta_{3}(g_{0})Pg_{0}\right]}_{D}.$$
(17)

Proposition 1 has established that $A = o_p(1/\sqrt{N})$. Moreover

$$C = \underbrace{\left(\widehat{\beta_{3}}(\{\widehat{g}_{k}\}_{k=1}^{K}) - \beta_{3}(\{\widehat{g}_{k}\}_{k=1}^{K})\right) \frac{1}{N} \sum_{i} \widehat{g}_{k(i)}(X_{i})}_{C_{1}} + \underbrace{\beta_{3}(\{\widehat{g}_{k}\}_{k=1}^{K}) \left(\frac{1}{N} \sum_{i} \left[\widehat{g}_{k(i)}(X_{i}) - P \mathfrak{G}_{k}(i)\right]\right)}_{C_{2}}}_{C_{2}}$$

and

$$D = \underbrace{\left(\widehat{\beta}_{3}(g_{0}) - \beta_{3}(g_{0})\right) \frac{1}{N} \sum_{i} g_{0}(X_{i})}_{D_{1}} + \underbrace{\left(\beta_{3}(g_{0}) \frac{1}{N} \sum_{i} [g_{0}(X_{i}) - Pg_{0}]\right)}_{D_{2}}.$$
 (19)

We show $C_1 - D_1$ and $C_2 - D_2$ are $o_p(1/\sqrt{N})$ to conclude. In fact

$$C_{1} - D_{1} = \left(\widehat{\beta}_{3}(\{\widehat{g}_{k}\}_{k=1}^{K}) - \beta_{3}(\{\widehat{g}_{k}\}_{k=1}^{K}) - \widehat{\beta}_{3}(g_{0}) + \beta_{3}(g_{0})\right) \frac{1}{N} \sum_{i} \widehat{g}_{k(i)}(X_{i}) + \left(\widehat{\beta}_{3}(g_{0}) - \beta_{3}(g_{0})\right) \frac{1}{N} \sum_{i} \left[\widehat{g}_{k(i)}(X_{i}) - g_{0}(X_{i})\right] = o_{p}(1/\sqrt{N}).$$
(20)

This is because

- $\widehat{\beta_3}(\{\widehat{g}_k\}_{k=1}^K) \beta_3(\{\widehat{g}_k\}_{k=1}^K) \widehat{\beta_3}(g_0) + \beta_3(g_0) = o_p(1/\sqrt{N})$ from Proposition 1;
- $\frac{1}{N}\sum_i \widehat{g}_{k(i)}(X_i) = \frac{1}{N}\sum_i g_0(X_i) + \frac{1}{N}\sum_i (\widehat{g}_{k(i)}(X_i)) g_0(X_i)) = O_p(1)$ from the LLN and the same logic bounding (12) above;
- $\widehat{\beta}_3(g_0) \beta_3(g_0) = O_p(1/\sqrt{N})$ from the CLT and the fact that $P(Z(g_0)Z(g_0)\top)$ has all eigenvalues bounded away from 0;

•
$$\frac{1}{N}\sum_{i}(\widehat{g}_{k(i)}(X_i) - g_0(X_i)) = o_p(1)$$
 again from bounding argument applied to (12)

Similarly,

$$C_{2} - D_{2} = \beta_{3}(\{\widehat{g}_{k}\}_{k=1}^{K}) \left(\frac{1}{N} \sum_{i} \left[\left[\widehat{g}_{k(i)}(X_{i}) - P\widehat{g}_{k(i)}\right] - \left[g_{0}(X_{i}) - Pg_{0}\right]\right]\right) + \left(\left(\beta_{3}(\{\widehat{g}_{k}\}_{k=1}^{K}) - \beta_{3}(g_{0})\right) \frac{1}{N} \sum_{i} \left[g_{0}(X_{i}) - Pg_{0}\right]\right) = o_{p}(1/\sqrt{N}), \quad (21)$$

which results from the following facts:

- $\beta_3(\{\widehat{g}_k\}_{k=1}^K) = \beta_3(g_0) + (\beta_3(\{\widehat{g}_k\}_{k=1}^K) \beta_3(g_0)) = O_p(1);$
- $\frac{1}{N}\sum_{i} \left[\left[\widehat{g}_{k(i)}(X_i) P\widehat{g}_{k(i)} \right] \left[g_0(X_i) Pg_0 \right] \right] = o_p(1/\sqrt{N})$ from the same reasoning applied to bound (1);
- $\beta_3(\{\widehat{g}_k\}_{k=1}^K) \beta_3(g_0) = o_p(1)$ due to convergence of \widehat{g}_k to g_0 , continuity of $\beta_3(\cdot)$, and the continuous mapping theorem;
- $\frac{1}{N} \sum_{i} [g_0(X_i) Pg_0] = O_p(1/\sqrt{N})$ from the CLT.

Combining the above arguments, we conclude that $B = o_p(1/\sqrt{N})$.

4 **Proof of Proposition 4**

We first show that $\widehat{Var}(\widehat{g}_{k(i)}(X_i)) \rightarrow_p \sigma_q^2$. We have

$$\widehat{Var}(\widehat{g}_{k(i)}(X_i)) = \frac{1}{K} \sum_k \frac{1}{n} \sum_{i \in I_k} \widehat{g}_k(X_i)^2 - \left[\frac{1}{K} \sum_k \frac{1}{n} \sum_{i \in I_k} \widehat{g}_k(X_i)\right]^2.$$
 (22)

By the same logic as in Step 1 of the proof of Proposition 1, for each k = 1, 2, ..., K,

$$E\left[\left\|\frac{1}{n}\sum_{i\in I_k} [\widehat{g}_k(X_i)^2 - P\widehat{g}_k^2]\right\|^2 \middle| I_k^c\right] \to_p 0,$$

and so $\frac{1}{n} \sum_{i \in I_k} \widehat{g}_k(X_i)^2 - P \widehat{g}_k^2 \to_p 0$. Since $P \widehat{g}_k^2 \to_p P g_0^2$, it follows that $\frac{1}{n} \sum_{i \in I_k} \widehat{g}_k(X_i)^2 \to_p P g_0^2$. Similarly $\frac{1}{n} \sum_{i \in I_k} \widehat{g}_k(X_i) \to_p P g_0$. Hence $\widehat{Var}(\widehat{g}_{k(i)}(X_i)) \to_p \sigma_g^2$. Also, by Proposition 1,

$$\left\|\widehat{\beta}(\{\widehat{g}_k\}_{k=1}^K) - \beta(\{\widehat{g}_k\}_{k=1}^K)\right\| \to_p 0$$
(23)

and by continuity of $\beta(\cdot)$ and the continuous mapping theorem,

$$\left\|\beta(\{\widehat{g}_k\}_{k=1}^K) - \beta(g_0)\right\| \to_p 0.$$
 (24)

Consequently $\left\|\widehat{\beta}(\{\widehat{g}_k\}_{k=1}^K) - \beta(g_0)\right\| \to_p 0$. By the continuous mapping theorem, we conclude that $\widehat{\sigma}^2 \to_p \sigma^2$.

5 Proof of auxiliary lemmas

Lemma 1. Given Assumption 1,

$$\left\|\frac{1}{N}\sum_{k}\sum_{j\in I_{k}}\widehat{Z}_{k,j}\widehat{Z}_{k,j}^{\top}-\frac{1}{K}\sum_{k}P(\widehat{Z}_{k}\widehat{Z}_{k}^{\top})\right\|=O_{p}(1/\sqrt{n}).$$

Proof. Since the number of splits K is bounded, we only need to verify for any $k \in \{1, 2, ..., K\}$,

$$\left\|\frac{1}{n}\sum_{j\in I_k}\widehat{Z}_{k,j}\widehat{Z}_{k,j}^{\top} - P(\widehat{Z}_k\widehat{Z}_k^{\top})\right\| = O_p(1/\sqrt{n}).$$

Below we'll prove

$$\frac{1}{n} \sum_{j \in I_k} T_j^2 \widehat{g}_k^2(X_j) - E[T_j^2 \widehat{g}_k^2(X_j) | I_k^c] = O_p(1/\sqrt{n}).$$
(25)

The other terms can be derived in the similar manner.

First, since $P(\hat{g}_k - g_0)^4 \to_p 0$ as $n \to \infty$, we know that for any subsequence $\{n_l\}$ of \mathbb{N} , it further has a subsequence $\{n_l\}$, such that $P(\hat{g}_k - g_0)^4 \to 0$ a.s. as $l \to \infty$. Our next step is to prove

$$\frac{1}{\sqrt{n_l'}} \sum_{j \in I_k} T_j^2 \hat{g}_k^2(X_j) - E[T_j^2 \hat{g}_k^2(X_j) | I_k^c] = O_p(1)$$
(26)

as $l \to \infty$.

For notational simplicity, define $V_{k,j} := T_j^2 \hat{g}_k^2(X_j) - E[T_j^2 \hat{g}_k^2(X_j)|I_k^c]$. Since $\{V_{k,j}\}_{j \in I_k}$ are independent conditioned on I_k^c , for any $t \in \mathbb{R}$ we have

$$E \exp\left(it/\sqrt{n'_l} \cdot \sum_{j \in I_k} V_{k,j}\right) = EE\left[\exp\left(it/\sqrt{n'_l} \cdot \sum_{j \in I_k} V_{k,j}\right) \middle| I^c_k\right]$$
$$= E\left\{E\left[\exp\left(it/\sqrt{n'_l} \cdot V_{k,j}\right) \middle| I^c_k\right]\right\}^{n'_l}.$$

Furthermore,

$$\lim_{l \to \infty} E \exp\left(it/\sqrt{n_l'} \cdot \sum_{j \in I_k} V_{k,j}\right) = \lim_{l \to \infty} E\left\{E\left[\exp\left(it/\sqrt{n_l'} \cdot V_{k,j}\right) \middle| I_k^c\right]\right\}^{n_l'}$$
$$= E \lim_{l \to \infty} \left\{E\left[\exp\left(it/\sqrt{n_l'} \cdot V_{k,j}\right) \middle| I_k^c\right]\right\}^{n_l'}.$$
(27)

Our goal is now to derive the limit in the last term so that we can infer the limiting distribution of $1/\sqrt{n'_l} \cdot \sum_{j \in I_k} V_{k,j}$.

First, we conduct the Taylor expansion

$$\exp\left(it/\sqrt{n'_{l}} \cdot V_{k,j}\right) = 1 + it.\sqrt{n'_{l}} \cdot V_{k,j} - \frac{t^{2}}{2n'_{l}}V_{k,j}^{2} + R_{k,j}.$$

Here

$$R_{k,j} = \exp\left(it/\sqrt{n'_{l}} \cdot V_{k,j}\right) - \left[1 + it/\sqrt{n'_{l}} \cdot V_{k,j} - \frac{t^{2}}{2n'_{l}}V_{k,j}^{2}\right].$$

Thus

$$E\left[\exp\left(it/\sqrt{n_{l}'} \cdot V_{k,j}\right) \middle| I_{k}^{c}\right] = 1 + it/\sqrt{n_{l}'} \cdot E[V_{k,j}|I_{k}^{c}] - \frac{t^{2}}{2n_{l}'} E[V_{k,j}^{2}|I_{k}^{c}] + E[R_{k,j}|I_{k}^{c}] = 1 - \frac{t^{2}}{2n_{l}'} E[V_{k,j}^{2}|I_{k}^{c}] + E[R_{k,j}|I_{k}^{c}]$$
(28)

First, with probability 1,

$$\lim_{l \to \infty} E[V_{k,j}^2 | I_k^c] = \lim_{l \to \infty} \left\{ E[T_j^4 \widehat{g}_k^4(X_j) | I_k^c] - E[T_j^2 \widehat{g}_k^2(X_j) | I_k^c]^2 \right\}$$
$$= p \cdot Pg_0^4 - p^2 \cdot (Pg_0^2)^2.$$
(29)

Next, we bound $|E[R_{k,j}|I_k^c]|$. In fact,

$$R_{k,j} \leq \begin{cases} \frac{2t^3}{n_l'^{3/2}} V_{k,j}^3 & \text{when } |V_{k,j}| \leq \frac{\sqrt{n_l'}}{2t}, \\ 2 + \frac{t}{\sqrt{n_l'}} |V_{k,j}| + \frac{t^2}{2n_l'} |V_{k,j}|^2 & \text{otherwise.} \end{cases}$$

This means

$$|E[R_{k,j}|I_k^c]| \le E[R_{k,j}^{(1)}|I_k^c] + E[R_{k,j}^{(2)}|I_k^c],$$

where
$$R_{k,j}^{(1)} = \frac{2t^3}{n_l^{13/2}} |V_{k,j}|^3 \mathbb{1}_{\{|V_{k,j}| \le \sqrt{n_l'}/(2t)\}},$$

 $R_{k,j}^{(2)} = (2 + \frac{t}{\sqrt{n_l'}} |V_{k,j}| + \frac{t^2}{2n_l'} |V_{k,j}|^2) \mathbb{1}_{\{|V_{k,j}| > \sqrt{n_l'}/(2t)\}}.$

On the one hand,

$$\begin{split} & E[R_{k,j}^{(1)}|I_k^c] \le \frac{2t^3}{{n_l'}^{3/2}} E\bigg[|V_{k,j}|^{2+\delta/2} \cdot \left(\sqrt{n_l'}/2t\right)^{1-\delta/2} \bigg| I_k^c\bigg] \\ &= \frac{2^{\delta/2}t^{2+\delta/2}}{{n_l'}^{1+\delta/4}} E\bigg[|T_j^2 \hat{g}_k^2(X_j) - ET_j^2 \hat{g}_k^2(X_j)|^{2+\delta/2} \bigg| I_k^c\bigg] \le \frac{2^{2+\delta}t^{2+\delta/2}}{{n_l'}^{1+\delta/4}} P|\hat{g}_k|^{4+\delta}. \end{split}$$

On the other hand, by Markov's inequality,

$$\begin{split} E[R_{k,j}^{(2)}|I_k^c] &\leq 2E\Big[\Big(2t/\sqrt{n_l'}\Big)^{2+\delta/2}|V_{k,j}|^{2+\delta/2}\Big|I_k^c\Big] + t/\sqrt{n_l'} \cdot \\ E\Big[|V_{k,j}|\cdot\Big(2t/\sqrt{n_l'}\Big)^{1+\delta/2}|V_{k,j}|^{1+\delta/2}\Big|I_k^c\Big] + \frac{t^2}{2n_l'} \cdot \\ E\Big[|V_{k,j}|^2\cdot\Big(2t/\sqrt{n_l'}\Big)^{\delta/2}|V_{k,j}|^{\delta/2}\Big|I_k^c\Big] &\leq \frac{2^{6+\delta}t^{2+\delta/2}}{n_l'^{1+\delta/4}}P|\widehat{g}_k|^{4+\delta}. \end{split}$$

Combining the above two bounds, we deduce that

$$|E[R_{k,j}|I_k^c]| \le \frac{2^{7+\delta}t^{2+\delta/2}}{{n'_l}^{1+\delta/4}} P|\widehat{g}_k|^{4+\delta}.$$

Thus with probability 1, $E[R_{k,j}|I_k^c] = o(1/n'_l)$.

Combining the above bound, (28) and (29), we obtain that with probability 1,

$$\begin{split} &\lim_{l \to \infty} n'_l \log E \left[\left. \exp \left(it / \sqrt{n'_l} \cdot V_{k,j} \right) \right| I^c_k \right] \\ &= \lim_{l \to \infty} n'_l \log \left(1 - \frac{t^2}{2n'_l} E[V^2_{k,j} | I^c_k] + E[R_{k,j} | I^c_k] \right) \\ &= -\frac{t^2}{2n'_l} [p \cdot Pg^4_0 - p^2 \cdot (Pg^2_0)^2]. \end{split}$$

Finally we plug the above into (27) and conclude that

$$\lim_{l \to \infty} E \exp\left(it/\sqrt{n'_{l}} \cdot \sum_{j \in I_{k}} V_{k,j}\right) = \exp\left\{-\frac{t^{2}}{2n'_{l}}[p \cdot Pg_{0}^{4} - p^{2} \cdot (Pg_{0}^{2})^{2}]\right\}.$$

This implies that $\frac{1}{\sqrt{n'_l}} \sum_{j \in I_k} V_{k,j}$ converges in distribution to a centered normal random variable with variance $p \cdot Pg_0^4 - p^2 \cdot (Pg_0^2)^2$, and (26) follows.

Finally, since for any subsequence $\{n_l\}$ of \mathbb{N} , it further has a subsequence $\{n'_l\}$ such that (26) holds, it can only be the case that (25) is true.

Lemma 2. The following hold with probability tending to 1:

$$\lambda_{\min}\left(\frac{1}{n}\sum_{i\in I_k}\widehat{Z}_{k,i}\widehat{Z}_{k,i}^{\top}\right) \ge \frac{1}{2}\inf_{g\in\mathcal{G}}\lambda_{\min}(P[Z(g)Z(g)^{\top}]) \quad \forall k\in\{1,2,\ldots,K\};$$
(30)

$$\lambda_{\min}\left(\frac{1}{N}\sum_{i=1}^{N}\widehat{Z}_{i}\widehat{Z}_{i}^{\top}\right) \geq \frac{1}{2}\inf_{g\in\mathcal{G}}\lambda_{\min}(P[Z(g)Z(g)^{\top}]).$$
(31)

Proof. According to Weyl's inequality,

$$\begin{split} \lambda_{\min} & \left(\frac{1}{n} \sum_{i \in I_k} \widehat{Z}_{k,i} \widehat{Z}_{k,i}^\top \right) \ge \lambda_{\min}(P(\widehat{Z}_k \widehat{Z}_k^\top)) - \left\| \frac{1}{n} \sum_{j \in I_k} \widehat{Z}_{k,j} \widehat{Z}_{k,j}^\top - P(\widehat{Z}_k \widehat{Z}_k^\top) \right\| \\ \ge & \inf_{g \in \mathcal{G}} \lambda_{\min}(P[Z(g)Z(g)^\top]) - \left\| \frac{1}{n} \sum_{j \in I_k} \widehat{Z}_{k,j} \widehat{Z}_{k,j}^\top - P(\widehat{Z}_k \widehat{Z}_k^\top) \right\|. \end{split}$$

On the other hand, from the proof of Lemma 1 we know

$$\left\|\frac{1}{n}\sum_{j\in I_k}\widehat{Z}_{k,j}\widehat{Z}_{k,j}^{\top} - P(\widehat{Z}_k\widehat{Z}_k^{\top})\right\| = O_p(1/\sqrt{n}).$$

This implies that

$$\lim_{n \to \infty} P\left(\left\| \frac{1}{n} \sum_{j \in I_k} \widehat{Z}_{k,j} \widehat{Z}_{k,j}^\top - P(\widehat{Z}_k \widehat{Z}_k^\top) \right\| \ge \frac{1}{2} \inf_{g \in \mathcal{G}} \lambda_{min}(P[Z(g)Z(g)^\top]) \right) = 0.$$

Combining the above, we obtain (30). (31) can be proved in a similar way.

Lemma 3. Let $\{M_{1n}\}, \{M_{2n}\}, \{M_{3n}\}, \{M_{4n}\}, \{A_n\}, \{B_n\}$ be sequences of random real symmetric matrices of fixed dimension. Assume that with probability 1, $\lambda_0 := \inf_n \lambda_{\min}(B_n) > 0$, and $||A_n - B_n|| = o_p(1)$. Moreover, assume that

$$||M_{1n} - A_n|| = O_p(1/\sqrt{n}), ||M_{3n} - A_n|| = O_p(1/\sqrt{n}), ||M_{2n} - B_n|| = O_p(1/\sqrt{n}), ||M_{4n} - B_n|| = O_p(1/\sqrt{n}).$$

If in addition,

$$\sqrt{n} \| M_{1n} + M_{2n} - M_{3n} - M_{4n} \| \to_p 0,$$

then

$$\sqrt{n} \|M_{1n}^{-1} + M_{2n}^{-1} - M_{3n}^{-1} - M_{4n}^{-1}\| \to_p 0.$$

Proof. Define the event

$$E_n := \{ \|A_n - B_n\| \ge \lambda_0/2 \} \cup \{ \max\{\|M_{1n} - A_n\|, \|M_{3n} - A_n\|\} \ge \lambda_0/2 \} \\ \cup \{ \max\{\|M_{2n} - B_n\|, \|M_{4n} - B_n\|\} \ge \lambda_0/2 \}.$$

Then $\lim_{n\to\infty} P(E_n) = 0$. Now on E_n^c , according to a Neumann series expansion,

$$M_{1n}^{-1} = [A_n + (M_{1n} - A_n)]^{-1}$$

= $A_n^{-1/2} [I - A_n^{-1/2} (M_{1n} - A_n) A_n^{-1/2} + D_{1n}] A_n^{-1/2}$

Here $D_{1n} = \sum_{j \ge 2} [-A_n^{-1/2} (M_{1n} - A_n) A_n^{-1/2}]^j$, and we have on E_n^c

$$\|D_{1n}\| \leq \sum_{j\geq 2} \|A_n^{-1/2} (M_{1n} - A_n) A_n^{-1/2} \|^j$$

$$\leq \frac{\|A_n^{-1}\|^2 \|M_{1n} - A_n\|^2}{1 - \|A_n^{-1}\| \|M_{1n} - A_n\|} \leq \frac{8}{\lambda_0^2} \|M_{1n} - A_n\|^2.$$
(32)

Here we use the fact that on E_n^c

$$||A_n^{-1/2}(M_{1n} - A_n)A_n^{-1/2}|| \le ||A_n^{-1/2}||^2 ||M_{1n} - A_n|| < \frac{2}{\lambda_0} \cdot \frac{\lambda_0}{2} = 1$$

Similar expansions hold for M_{2n} , M_{3n} and M_{4n} , and we define D_{2n} , D_{3n} and D_{4n} accordingly. Using some simple algebra, we deduce that on E_n^c ,

$$M_{1n}^{-1} + M_{2n}^{-1} - M_{3n}^{-1} - M_{4n}^{-1} = J_{1n} + J_{2n} + J_{3n} + J_{4n},$$

where

$$J_{1n} = -A_n^{-1} [M_{1n} + M_{2n} - M_{3n} - M_{4n}] A_n^{-1},$$

$$J_{2n} = -A_n^{-1} (M_{4n} - M_{2n}) A_n^{-1} + B_n^{-1} (M_{4n} - M_{2n}) B_n^{-1},$$

$$J_{3n} = A_n^{-1/2} (D_{1n} - D_{3n}) A_n^{-1/2},$$

$$J_{4n} = B_n^{-1/2} (D_{2n} - D_{4n}) B_n^{-1/2}.$$

For any $\epsilon > 0$,

$$P(\sqrt{n}\|M_{1n}^{-1} + M_{2n}^{-1} - M_{3n}^{-1} - M_{4n}^{-1}\| > \epsilon) < P(E_n) + \sum_{\ell=1}^{4} P(E_n^c \cap \{\sqrt{n}\|J_{\ell n}\| > \epsilon/4\}).$$
(33)

Combining the fact that $\lim_{n\to\infty} P(E_n) = 0$, we only need to prove that each of the rest of the terms on the the RHS of (33) has limit 0.

First, $\lim_{n\to\infty} P(E_n^c \cap \{\sqrt{n} ||J_{1n}|| > \epsilon/4\}) = 0$ follows from our assumption. For J_{2n} , observe that $J_{2n} = J_{2n}^{(1)} + J_{2n}^{(2)}$, where

$$J_{2n}^{(1)} = (B_n^{-1} - A_n^{-1})(M_{4n} - M_{2n})A_n^{-1}, J_{2n}^{(2)} = B_n^{-1}(M_{4n} - M_{2n})(B_n^{-1} - A_n^{-1}).$$

We bound the limit of $||J_{2n}^{(1)}||$ as follows: For any $\delta > 0$, there exists M > 0 such that $\forall n$, $P(\sqrt{n}||M_{4n} - M_{2n}|| > M) < \frac{\delta}{2}$. According to our assumption, there further exists $N \in \mathbb{N}$ such that for all n > N, $P(||A_n - B_n|| > \frac{\lambda_0^3 \epsilon}{32M}) < \frac{\delta}{2}$. Therefore for all n > N,

$$P(E_n^c \cap \{\sqrt{n} \| J_{2n}^{(1)} \| > \epsilon/8\})$$

$$\leq P(E_n^c \cap \{\sqrt{n} \| A_n^{-1} (A_n - B_n) B_n^{-1} (M_{4n} - M_{2n}) A_n^{-1} \| > \epsilon/8\})$$

$$\leq P(E_n^c \cap \{ \| A_n - B_n \| \cdot \sqrt{n} \| M_{4n} - M_{2n} \| > \lambda_0^3 \epsilon/32\})$$

$$\leq P(\sqrt{n} \| M_{4n} - M_{2n} \| > M) + P(\| A_n - B_n \| > \lambda_0^3 \epsilon/(32M)) < \delta.$$

The above argument implies that $\lim_{n\to+\infty} P(E_n^c \cap \{\sqrt{n} || J_{2n}^{(1)} || > \epsilon/8\}) = 0$. Similarly we have $\lim_{n\to+\infty} P(E_n^c \cap \{\sqrt{n} || J_{2n}^{(2)} || > \epsilon/8\}) = 0$. Thus

$$\lim_{n \to +\infty} P(E_n^c \cap \{\sqrt{n} \| J_{2n} \| > \epsilon/4\})$$

$$\leq \lim_{n \to +\infty} P(E_n^c \cap \{\sqrt{n} \| J_{2n}^{(1)} \| > \epsilon/8\}) + \lim_{n \to +\infty} P(E_n^c \cap \{\sqrt{n} \| J_{2n}^{(2)} \| > \epsilon/8\}) = 0.$$

Now we proceed to bound the limit of $||J_{3n}||$. In fact we have

$$P(E_n^c \cap \{\sqrt{n} \| J_{3n} \| > \epsilon/4\}) \le P(E_n^c \cap \{\sqrt{n} \| D_{1n} - D_{3n} \| > \epsilon\lambda_0/8\})$$

$$\le P(E_n^c \cap \{\sqrt{n} \| D_{1n} \| > \epsilon\lambda_0/16\}) + P(E_n^c \cap \{\sqrt{n} \| D_{3n} \| > \epsilon\lambda_0/16\})$$

$$\le P(\sqrt{n} \| M_{1n} - A_n \|^2 > \epsilon\lambda_0^3/128) + P(\sqrt{n} \| M_{3n} - A_n \|^2 > \epsilon\lambda_0^3/128).$$

In the last inequality we utilize (32). Combining our assumptions, we have

$$\lim_{n \to \infty} P(E_n^c \cap \{\sqrt{n} \| J_{3n} \| > \epsilon/4\}) = 0.$$

Similarly

$$\lim_{n \to \infty} P(E_n^c \cap \{\sqrt{n} \| J_{4n} \| > \epsilon/4\}) = 0$$

We conclude our proof.

References

[1] CHERNOZHUKOV, Victor; CHETVERIKOV, Denis; DEMIRER, Mert; DUFLO, Esther; HANSEN, Christian; NEWEY, Whitney; ROBINS, James: Double/debiased machine learning for treatment and structural parameters. In: *The Econometrics Journal* 21 (2018), Nr. 1