

## A The Generalization of Our Models

### A.1 Multiple Confounders

In this section, we show that because we do not impose any independence assumption on the set of confounder, revealing the values of all confounders offers maximal information on the joint distribution of the confounders. In particular, we will illustrate through the case where we have two binary confounders. The extension to multiple categorical confounders is straight forward.

In the case where we have two binary confounders  $Z_1$  and  $Z_2$ , we can express the ATE as follows:

$$\text{ATE} = \sum_{z_1, z_2} \left( P_{Y|T, Z_1, Z_2}(1|1, z_1, z_2) - P_{Y|T, Z_1, Z_2}(1|0, z_1, z_2) \right) P_{Z_1, Z_2}(z_1, z_2).$$

With an infinite amount of confounded data, we are provided with the joint distribution  $P_{Y, T}(y, t)$ . Thus, it remains to estimate the conditional distributions  $P_{Z_1, Z_2|Y, T}$ . In our paper, we consider only the non-adaptive policies, i.e., the number of samples to deconfound in each group  $(y, t)$  is fixed a priori. In the case where the costs of revealing the values of  $Z_1$  and  $Z_2$  are the same and we do not have any prior knowledge on the distributions of  $Z_1$  and  $Z_2$ , the variables  $Z_1$  and  $Z_2$  becomes exchangeable. In the case where the sample selection policies are completely non-adaptive (which is the case that we consider in this paper), by the symmetry of the variables  $Z_1$  and  $Z_2$ , we have that sampling from the joint distribution of  $Z_1$  and  $Z_2$  yields the maximum expected information on the value of the ATE. (Note that if the confounders take categorical values of different sizes and we allow adaptive policies, then we might be able to reduce the total cost of deconfounding to estimate the ATE to within a desired accuracy level.)

### A.2 Pretreatment Covariates

In the case where we have known pretreatment covariates  $X$ , our model can be applied in estimating the individual treatment effect where we make the common ignorability assumption on the pretreatment covariates  $X$  and the confounder  $Z$ : given pretreatment covariates  $X$  and the confounder  $Z$ , the values of outcome variable,  $Y = 0$  and  $Y = 1$ , are independent of treatment assignment. In this case, the distributions  $P_{Y, T}(y, t)$  and  $P_X(x)$  are known and the Individual Treatment Effect (ITE):

$$\begin{aligned} \text{ITE} &= \sum_{z, x} \left( P_{Y|T, Z, X}(1|1, z, x) - P_{Y|T, Z, X}(1|0, z, x) \right) P_{Z, X}(z, x) \\ &= \sum_{z, x} \left( P_{Y|T, Z, X}(1|1, z, x) - P_{Y|T, Z, X}(1|0, z, x) \right) P_{Z|X}(z|x) P_X(x). \end{aligned} \quad (3)$$

Note that in Equation (3) the only distributions we need to estimate are the conditional distributions  $P_{Z|Y, T, X}$ . The values of  $P_{Y|T, Z, X}$  and  $P_{Z|X}$  can be calculated from  $P_{Z|Y, T, X}$  by first conditioning the confounded distributions  $P_{Y, T}$  on the values of the pretreatment covariates  $X$ , i.e., we first subsample all confounded (outcome, treatment) pairs for a fixed value of  $X$ ,  $X = x$ , and then within each subsample, estimate the conditional distributions  $P_{Z|Y, T, X}$  by applying our methods. To obtain ITE, we weight the estimates we obtain from all subsamples by  $P_X(x)$ .

## B Proofs

### B.1 Review of Classical Results in Concentration Inequalities

Before embarking on our proofs, we state some classic results that we will use frequently. The following concentration inequalities are part of a family of results collectively referred to as *Hoeffding's inequality* (e.g., see [Vershynin \(2018\)](#)).

**Lemma 1** (Hoeffding's Lemma). *Let  $X$  be any real-valued random variable with expected value  $\mathbb{E}[X] = 0$ , such that  $a \leq X \leq b$  almost surely. Then, for all  $\lambda \in \mathbb{R}$ ,  $\mathbb{E}[\exp(\lambda X)] \leq \exp\left(\frac{\lambda^2(b-a)^2}{8}\right)$ .*

**Theorem 7** (Hoeffding's inequality for general bounded r.v.s). *Let  $X_1, \dots, X_N$  be independent random variables such that  $X_i \in [m_i, M_i], \forall i$ . Then, for  $t > 0$ , we have  $P\left(\left|\sum_{i=1}^N (X_i - \mathbb{E}[X_i])\right| \geq t\right) \leq 2 \exp\left(-\frac{2t^2}{\sum_{i=1}^N (M_i - m_i)^2}\right)$ .*

To begin, recall the notation introduced in Section 3: we model the binary-valued treatment, the binary-valued outcome, and the categorical confounder as the random variables  $T \in \{0, 1\}$ ,  $Y \in \{0, 1\}$ , and  $Z \in \{1, \dots, k\}$ , respectively. The underlying joint distribution of these three random variables is represented as  $P_{Y,T,Z}(\cdot, \cdot, \cdot)$ . To save on space for terms that are used frequently, we define the following shorthand notation:

$$\begin{aligned} p_{yt}^z &= P_{Y,T,Z}(y, t, z), \\ a_{yt} &= P_{Y,T}(y, t), \\ q_{yt}^z &= P_{Z|Y,T}(z|y, t). \end{aligned}$$

These terms appear frequently because, to estimate the entire joint distribution on  $Y, T, Z$  (the  $p_{yt}^z$ 's), it suffices to estimate the joint distribution on  $Y, T$  (the  $a_{yt}$ 's), along with the conditional distribution of  $Z$  on  $Y, T$  (the  $q_{yt}^z$ 's):

$$p_{yt}^z = a_{yt}q_{yt}^z.$$

Finally, let  $\hat{p}_{yt}^z, \hat{a}_{yt}$ , and  $\hat{q}_{yt}^z$  be the empirical estimates of  $p_{yt}^z, a_{yt}$ , and  $q_{yt}^z$ , respectively, using the MLE.

## B.2 Proof of Theorem 1

**Theorem 1.** (*Upper Bound*) *Using deconfounded data alone,  $P\left(\left|\widehat{\text{ATE}} - \text{ATE}\right| \geq \epsilon\right) < \delta$  is satisfied if the deconfounded sample size  $m$  is at least*

$$m_{\text{base}} := \max_{t,z} C \left( \sum_y p_{yt}^z \right)^{-2} = \max_{t,z} \frac{1}{P_{T,Z}(t, z)^2} C.$$

*Proof of Theorem 1.* This proof proceeds as follows: first, we prove a sufficient (deterministic) condition, on the errors of our estimates of  $p_{yt}^z$ 's, under which  $|\widehat{\text{ATE}} - \text{ATE}|$  is small. Second, we show that the errors of our estimates of  $p_{yt}^z$ 's are indeed small with high probability.

**Step 1:** First, we can write the ATE in terms of the  $p_{yt}^z$ 's as follows:

$$\text{ATE} = \sum_z (P_{Y|T,Z}(1|1, z) - P_{Y|T,Z}(1|0, z)) P_Z(z) = \sum_z \left( \left( \frac{p_{11}^z}{\sum_y p_{y1}^z} - \frac{p_{10}^z}{\sum_y p_{y0}^z} \right) \left( \sum_{y,t} p_{yt}^z \right) \right).$$

In order for the ATE to be well-defined, we assume  $\sum_y p_{yt}^z \in (0, 1)$  for all  $t, z$  throughout. We can then decompose  $|\widehat{\text{ATE}} - \text{ATE}|$ :

$$\begin{aligned} |\widehat{\text{ATE}} - \text{ATE}| &= \left| \sum_z \left( \left( \frac{\hat{p}_{11}^z}{\sum_y \hat{p}_{y1}^z} - \frac{\hat{p}_{10}^z}{\sum_y \hat{p}_{y0}^z} \right) \left( \sum_{y,t} \hat{p}_{yt}^z \right) - \left( \frac{p_{11}^z}{\sum_y p_{y1}^z} - \frac{p_{10}^z}{\sum_y p_{y0}^z} \right) \left( \sum_{y,t} p_{yt}^z \right) \right) \right| \\ &\leq \sum_z \left| \left( \frac{\hat{p}_{11}^z}{\sum_y \hat{p}_{y1}^z} - \frac{\hat{p}_{10}^z}{\sum_y \hat{p}_{y0}^z} \right) \left( \sum_{y,t} \hat{p}_{yt}^z \right) - \left( \frac{p_{11}^z}{\sum_y p_{y1}^z} - \frac{p_{10}^z}{\sum_y p_{y0}^z} \right) \left( \sum_{y,t} p_{yt}^z \right) \right|. \end{aligned}$$

Thus, in order to upper bound  $|\widehat{\text{ATE}} - \text{ATE}|$  by some  $\epsilon$ , it suffices to show that

$$\left| \left( \frac{\hat{p}_{11}^z}{\sum_y \hat{p}_{y1}^z} - \frac{\hat{p}_{10}^z}{\sum_y \hat{p}_{y0}^z} \right) \left( \sum_{y,t} \hat{p}_{yt}^z \right) - \left( \frac{p_{11}^z}{\sum_y p_{y1}^z} - \frac{p_{10}^z}{\sum_y p_{y0}^z} \right) \left( \sum_{y,t} p_{yt}^z \right) \right| \leq \frac{\epsilon}{k}, \quad \forall z. \quad (4)$$

**Step 2:** To bound the above terms, we first derive Lemma 2 for bounding the error of the product of two estimates in terms of their two individual errors:

**Lemma 2.** For any  $u, \hat{u} \in [-1, 1]$ , and  $v, \hat{v} \in [0, 1]$ , suppose there exists  $\epsilon, \theta \in (0, 1)$  such that all of the following conditions hold:

1.  $|u - \hat{u}| \leq (1 - \theta)\epsilon$
2.  $|v - \hat{v}| \leq \theta\epsilon$
3.  $u + \epsilon \leq 1$
4.  $v + \epsilon \leq 1$
5.  $\epsilon \leq \min(u, v)$

Then,  $|uv - \hat{u}\hat{v}| \leq \epsilon$ .

*Proof of Lemma 2.* Since  $|u - \hat{u}| \leq (1 - \theta)\epsilon$ , we have  $\hat{u} \in [u - (1 - \theta)\epsilon, u + (1 - \theta)\epsilon]$ , and similarly, from  $|v - \hat{v}| \leq \theta\epsilon$ , we have  $\hat{v} \in [v - \theta\epsilon, v + \theta\epsilon]$ . Thus,

$$\begin{aligned}
 |uv - \hat{u}\hat{v}| &\leq \max(|uv - (u + (1 - \theta)\epsilon)(v + \theta\epsilon)|, |uv - (u - (1 - \theta)\epsilon)(v - \theta\epsilon)|) && \text{(because } v, \hat{v} \geq 0) \\
 &= \max(|\theta u\epsilon + (1 - \theta)v\epsilon + (1 - \theta)\theta\epsilon^2|, |\theta u\epsilon + (1 - \theta)v\epsilon - (1 - \theta)\theta\epsilon^2|) \\
 &= |\theta u\epsilon + (1 - \theta)v\epsilon + (1 - \theta)\theta\epsilon^2| && \text{(because } (1 - \theta)\theta\epsilon^2 > 0) \\
 &\leq |\theta(u + \epsilon)\epsilon + (1 - \theta)v\epsilon| && \text{(because } \theta\epsilon^2 > (1 - \theta)\theta\epsilon^2) \\
 &\leq \epsilon && \text{(because } u + \epsilon \in [-1, 1], \text{ and } v \leq 1).
 \end{aligned}$$

□

We can apply Lemma 2 directly to the terms in (4) by setting

$$\begin{aligned}
 u_z &= \frac{p_{11}^z}{\sum_y p_{y1}^z} - \frac{p_{10}^z}{\sum_y p_{y0}^z}, \\
 \hat{u}_z &= \frac{\hat{p}_{11}^z}{\sum_y \hat{p}_{y1}^z} - \frac{\hat{p}_{10}^z}{\sum_y \hat{p}_{y0}^z}, \\
 v_z &= \sum_{y,t} p_{yt}^z, \\
 \hat{v}_z &= \sum_{y,t} \hat{p}_{yt}^z,
 \end{aligned}$$

and noting that  $u_z, \hat{u}_z \in [-1, 1]$ , and  $v_z, \hat{v}_z \in [0, 1]$ . Lemma 2 implies that the upper bound in (4) holds if, for some  $\theta \in (0, 1)$ , we have

$$|v_z - \hat{v}_z| < \frac{\theta}{k}\epsilon \quad \text{and} \quad |u_z - \hat{u}_z| < \frac{1 - \theta}{k}\epsilon.$$

While we can apply standard concentration results to the  $|v_z - \hat{v}_z|$  terms, the  $|u_z - \hat{u}_z|$  terms will need to be further decomposed:

$$\begin{aligned}
 |u_z - \hat{u}_z| &= \left| \frac{p_{11}^z}{\sum_y p_{y1}^z} - \frac{p_{10}^z}{\sum_y p_{y0}^z} - \frac{\hat{p}_{11}^z}{\sum_y \hat{p}_{y1}^z} + \frac{\hat{p}_{10}^z}{\sum_y \hat{p}_{y0}^z} \right| \\
 &\leq \left| \frac{p_{11}^z}{\sum_y p_{y1}^z} - \frac{\hat{p}_{11}^z}{\sum_y \hat{p}_{y1}^z} \right| + \left| \frac{p_{10}^z}{\sum_y p_{y0}^z} - \frac{\hat{p}_{10}^z}{\sum_y \hat{p}_{y0}^z} \right|.
 \end{aligned}$$

It will suffice to show that for each  $t$  and  $z$ ,

$$\left| \frac{p_{1t}^z}{\sum_y p_{yt}^z} - \frac{\hat{p}_{1t}^z}{\sum_y \hat{p}_{yt}^z} \right| < \frac{1-\theta}{2k} \epsilon. \quad (5)$$

**Step 3:** To bound these terms, we derive Lemma 3. Recall that  $p_{1t}^z + p_{0t}^z, \hat{p}_{1t}^z + \hat{p}_{0t}^z \in (0, 1)$ .

**Lemma 3.** For any  $w + s, \hat{w} + \hat{s} \in (0, 1)$ , if  $|w + s - \hat{w} - \hat{s}| \leq (w + s)\epsilon$  and  $|w - \hat{w}| \leq (w + s)\epsilon$ , then

$$\left| \frac{w}{w + s} - \frac{\hat{w}}{\hat{w} + \hat{s}} \right| \leq 2\epsilon.$$

*Proof of Lemma 3.* First, since  $|w + s - \hat{w} - \hat{s}| \leq (w + s)\epsilon$ , we have that

$$\left| \frac{w + s}{\hat{w} + \hat{s}} - 1 \right| \leq \frac{w + s}{\hat{w} + \hat{s}} \epsilon,$$

or equivalently,

$$1 - \frac{w + s}{\hat{w} + \hat{s}} \epsilon \leq \frac{w + s}{\hat{w} + \hat{s}} \leq 1 + \frac{w + s}{\hat{w} + \hat{s}} \epsilon.$$

We can apply this inequality and rearrange terms as follows to conclude the proof:

$$\begin{aligned} \left| \frac{w}{w + s} - \frac{\hat{w}}{\hat{w} + \hat{s}} \right| &= \left| \frac{1}{w + s} \left| w - \hat{w} \frac{w + s}{\hat{w} + \hat{s}} \right| \right| \\ &\leq \left| \frac{1}{w + s} \right| \max \left( \left| w - \hat{w} \left( 1 - \frac{w + s}{\hat{w} + \hat{s}} \epsilon \right) \right|, \left| w - \hat{w} \left( 1 + \frac{w + s}{\hat{w} + \hat{s}} \epsilon \right) \right| \right) \\ &= \left| \frac{1}{w + s} \right| \max \left( \left| w - \hat{w} + \frac{w + s}{\hat{w} + \hat{s}} \hat{w} \epsilon \right|, \left| w - \hat{w} - \frac{w + s}{\hat{w} + \hat{s}} \hat{w} \epsilon \right| \right) \\ &= \max \left( \left| \frac{w - \hat{w}}{w + s} + \frac{\hat{w}}{\hat{w} + \hat{s}} \epsilon \right|, \left| \frac{w - \hat{w}}{w + s} - \frac{\hat{w}}{\hat{w} + \hat{s}} \epsilon \right| \right) \\ &\leq \left| \frac{w - \hat{w}}{w + s} \right| + \left| \frac{\hat{w}}{\hat{w} + \hat{s}} \right| \epsilon \\ &\leq \left| \frac{w + s}{w + s} \right| \epsilon + \left| \frac{\hat{w}}{\hat{w} + \hat{s}} \right| \epsilon \\ &\leq 2\epsilon. \end{aligned}$$

The second to last inequality follows from the assumption that  $|w - \hat{w}| \leq (w + s)\epsilon$ .  $\square$

Lemma 3 implies that (5) is satisfied if

$$|p_{1t}^z - \hat{p}_{1t}^z| < \frac{(\sum_y p_{yt}^z)(1-\theta)}{4k} \epsilon \quad \text{and} \quad |p_{1t}^z + p_{0t}^z - \hat{p}_{1t}^z - \hat{p}_{0t}^z| < \frac{(\sum_y p_{yt}^z)(1-\theta)}{4k} \epsilon.$$

**Step 4:** We've shown above that  $|\widehat{\text{ATE}} - \text{ATE}| \leq \epsilon$  is satisfied when

$$|v_z - \hat{v}_z| < \frac{\theta}{k} \epsilon, \quad |p_{1t}^z - \hat{p}_{1t}^z| < \frac{(\sum_y p_{yt}^z)(1-\theta)}{4k} \epsilon,$$

and

$$|p_{1t}^z + p_{0t}^z - \hat{p}_{1t}^z - \hat{p}_{0t}^z| < \frac{(\sum_y p_{yt}^z)(1-\theta)}{4k} \epsilon, \quad \forall t, z.$$

Note that if  $\forall t, |p_{1t}^z + p_{0t}^z - \hat{p}_{1t}^z - \hat{p}_{0t}^z| = \left| \sum_y p_{yt}^z - \sum_y \hat{p}_{yt}^z \right| < \frac{(\sum_y p_{yt}^z)(1-\theta)}{4k} \epsilon$  then

$$|v_z - \hat{v}_z| = \left| \sum_{y,t} p_{yt}^z - \sum_{y,t} \hat{p}_{yt}^z \right| \leq \sum_t \left| \sum_y p_{yt}^z - \sum_y \hat{p}_{yt}^z \right| < \frac{(\sum_{y,t} p_{yt}^z)(1-\theta)}{4k} \epsilon \leq \frac{(1-\theta)}{4k} \epsilon.$$

Thus, to remove the first constraint  $|v_z - \hat{v}_z| < \frac{\theta}{k}\epsilon$ , we set

$$\frac{\theta}{k}\epsilon = \frac{(1-\theta)}{4k}\epsilon,$$

and obtain  $\theta = \frac{1}{5}$ .

**Step 5:** To summarize so far, Lemmas 2 and 3 allow us to upper bound the error of our estimated ATE in terms of upper bounds on the error of our estimates of its constituent terms:

$$P\left(|\widehat{\text{ATE}} - \text{ATE}| < \epsilon\right) \geq P\left(\bigcap_{t,z} \left\{|p_{1t}^z - \hat{p}_{1t}^z| < \frac{\sum_y p_{yt}^z}{5k}\epsilon\right\} \bigcap_{t,z} \left\{|p_{1t}^z + p_{0t}^z - \hat{p}_{1t}^z - \hat{p}_{0t}^z| < \frac{\sum_y p_{yt}^z}{5k}\epsilon\right\}\right),$$

or equivalently,

$$P\left(|\widehat{\text{ATE}} - \text{ATE}| \geq \epsilon\right) \leq P\left(\bigcup_{t,z} \left\{|p_{1t}^z - \hat{p}_{1t}^z| \geq \frac{\sum_y p_{yt}^z}{5k}\epsilon\right\} \bigcup_{t,z} \left\{|p_{1t}^z + p_{0t}^z - \hat{p}_{1t}^z - \hat{p}_{0t}^z| \geq \frac{\sum_y p_{yt}^z}{5k}\epsilon\right\}\right).$$

Applying a union bound, we have

$$P\left(|\widehat{\text{ATE}} - \text{ATE}| \geq \epsilon\right) \leq \sum_{t,z} P\left(|p_{1t}^z - \hat{p}_{1t}^z| \geq \frac{\sum_y p_{yt}^z}{5k}\epsilon\right) + P\left(|p_{1t}^z + p_{0t}^z - \hat{p}_{1t}^z - \hat{p}_{0t}^z| \geq \frac{\sum_y p_{yt}^z}{5k}\epsilon\right). \quad (6)$$

**Step 6:** Finally, we can apply Hoeffding's inequality (Theorem 7) to obtain the upper bound for the inequality above. Let  $X_{yt}^z$  be the random variable that maps the event  $(Y = y, T = t, Z = z) \mapsto \{0, 1\}$ . Then,  $X_{yt}^z$  is a Bernoulli random variable with parameter  $p_{yt}^z$ . Let  $m$  denote the total number of deconfounded samples that we have. Since  $\hat{p}_{yt}^z$  is estimated through the MLE, we have  $\hat{p}_{yt}^z = \frac{\sum_{i=1}^m X_{yt}^z}{m}$ . Applying Theorem 7, we obtain:

$$P\left(\left|\frac{\sum_{i=1}^m X_{yt}^z}{m} - p_{yt}^z\right| \geq \frac{\sum_y p_{yt}^z}{5k}\epsilon\right) \leq 2 \exp\left(-2m \frac{\left(\sum_y p_{yt}^z\right)^2 \epsilon^2}{25k^2}\right), \quad \text{and} \quad (7)$$

$$P\left(\left|\frac{\sum_{i=1}^m X_{1t}^z + X_{0t}^z}{m} - p_{1t}^z - p_{0t}^z\right| \geq \frac{\sum_y p_{yt}^z}{5k}\epsilon\right) \leq 2 \exp\left(-2m \frac{\left(\sum_y p_{yt}^z\right)^2 \epsilon^2}{25k^2}\right). \quad (8)$$

Combining (6), (7), and (8), we have

$$\begin{aligned} P\left(|\widehat{\text{ATE}} - \text{ATE}| \geq \epsilon\right) &\leq \sum_{t,z} P\left(|p_{1t}^z - \hat{p}_{1t}^z| \geq \frac{\sum_y p_{yt}^z}{5k}\epsilon\right) + P\left(|p_{1t}^z + p_{0t}^z - \hat{p}_{1t}^z - \hat{p}_{0t}^z| \geq \frac{\sum_y p_{yt}^z}{5k}\epsilon\right) \\ &\leq 4k \max_{t,z} \left(2 \exp\left(-2m \frac{\left(\sum_y p_{yt}^z\right)^2 \epsilon^2}{25k^2}\right)\right) \\ &= 8k \max_{t,z} \exp\left(-2m \frac{\left(\sum_y p_{yt}^z\right)^2 \epsilon^2}{25k^2}\right) \\ &\leq \delta, \end{aligned}$$

where the second line follows from the fact that, since  $t$  is binary, there are  $4k$  terms in total. Solving the above equation, we conclude that  $P(|\widehat{\text{ATE}} - \text{ATE}| \geq \epsilon) < \delta$  is satisfied when the sample size  $m$  is at least

$$m \geq \frac{12.5k^2 \ln\left(\frac{8k}{\delta}\right)}{\epsilon^2} \max_{t,z} \frac{1}{\left(\sum_y p_{yt}^z\right)^2}.$$

□

### B.3 Proof of Proposition 1

**Proposition 1.** *For every  $\mathbf{a}$ , there exists some  $\epsilon, \delta$  such that for any fixed number of deconfounded samples  $m$ , we can always construct a pair of  $\mathbf{q}$ 's, say  $\mathbf{q}_1$  and  $\mathbf{q}_2$ , such that no algorithm can distinguish these two conditional distributions with probability more than  $1 - \delta$ , and their corresponding ATE values are  $\epsilon$  away:  $|\text{ATE}_{\mathbf{a}}(\mathbf{q}_1) - \text{ATE}_{\mathbf{a}}(\mathbf{q}_2)| \geq \epsilon$ .*

*Proof of Proposition 1.* It suffices to show for the case where confounder takes binary value. The extension to categorical confounder is straightforward as illustrated in the proof of Theorem 6 in Appendix B.7. Let  $q_{yt} = P(Z = 1|Y = y, T = t)$ . To show that Proposition 1 is true, it is sufficient to show that there exist a positive constant  $c$  (that depends on  $\mathbf{a}$ ) such that for all fixed  $\mathbf{a}$ , there exists a pair of  $\mathbf{q}$  and  $\mathbf{q}'$  such that  $\|\text{ATE}_{\mathbf{a}}(\mathbf{q}) - \text{ATE}_{\mathbf{a}}(\mathbf{q}')\| > c$ , with  $\mathbf{q}$  and  $\mathbf{q}'$  close in distribution. We proceed by construction. For fixed  $\mathbf{a}$ , consider the following  $\mathbf{q}$  pairs:  $\mathbf{q} = (q_{00}, 0, q_{10}, \gamma)$  and  $\mathbf{q}' = (q_{00}, \gamma, q_{10}, 0)$ . Then, we have

$$\begin{aligned} \text{ATE}_{\mathbf{a}}(\mathbf{q}) &= (a_{00}q_{00} + a_{10}q_{10} + a_{11}\gamma) + \frac{a_{11}(1-\gamma)}{a_{11}(1-\gamma) + a_{01}}(1 - a_{00}q_{00} - a_{10}q_{10} - a_{11}\gamma) - \\ &\frac{a_{10}q_{10}}{a_{10}q_{10} + a_{00}q_{00}}(a_{00}q_{00} + a_{10}q_{10} + a_{11}\gamma) - \frac{a_{10}(1-q_{10})}{a_{10}(1-q_{10}) + a_{00}(1-q_{00})}(1 - a_{00}q_{00} - a_{10}q_{10} - a_{11}\gamma), \end{aligned}$$

and similarly, we have

$$\begin{aligned} \text{ATE}_{\mathbf{a}}(\mathbf{q}') &= \frac{a_{11}}{a_{11} + a_{01}(1-\gamma)}(1 - a_{00}q_{00} - a_{01}\gamma - a_{10}q_{10}) - \frac{a_{10}q_{10}}{a_{10}q_{10} + a_{00}q_{00}}(a_{00}q_{00} \\ &+ a_{01}\gamma + a_{10}q_{10}) - \frac{a_{10}(1-q_{10})}{a_{10}(1-q_{10}) + a_{00}(1-q_{00})}(1 - a_{00}q_{00} - a_{01}\gamma - a_{10}q_{10}). \end{aligned}$$

In particular,

$$\lim_{\gamma \rightarrow 0} \text{ATE}_{\mathbf{a}}(\mathbf{q}) - \text{ATE}_{\mathbf{a}}(\mathbf{q}') = a_{00}q_{00} + a_{10}q_{10} \leq a_{00} + a_{10}, \quad (9)$$

where we can choose  $q_{00}$  and  $q_{10}$  to be 1.

On the other hand, we can show that the number of samples needed to distinguish  $\mathbf{q}$  from  $\mathbf{q}'$  is at least  $\Omega(1/\gamma)$ : since  $\mathbf{q}$  and  $\mathbf{q}'$  are the same in two of the entries and symmetric on the rest two, to distinguish  $\mathbf{q}$  and  $\mathbf{q}'$  is to distinguish a Bernoulli random variable with parameter 0 (denoting this variable  $B_0$ ) from a Bernoulli random variable with parameter  $\gamma$  (denoting this random variable  $B_\gamma$ ). Let  $f$  be any estimator of the Bernoulli random variable, and  $x_1, \dots, x_m$  be the sequence of  $m$  observations. Then we have  $|\mathbb{E}_{X \sim B_0^m}[f] - \mathbb{E}_{X \sim B_\gamma^m}[f]| \leq \|B_0^m - B_\gamma^m\|_1 \leq \sqrt{2(\ln 2)\text{KL}(B_0^m \| B_\gamma^m)} \leq 2\sqrt{(\ln 2)\gamma m}$ , where the last inequality is because when given  $m$  samples,  $\text{KL}(B_0^m \| B_\gamma^m) \leq (2\gamma \ln 2 + (1-2\gamma) \ln \frac{1-2\gamma}{1-\gamma})m \leq 2\gamma m$ . On the other hand, any hypothesis test that takes  $n$  samples and distinguishes between  $H_0 : X_1, \dots, X_n \sim P_0$  and  $H_1 : X_1, \dots, X_n \sim P_1$  has probability of error lower bounded by  $\max(P_0(1), P_1(0)) \geq \frac{1}{4}e^{-n\text{KL}(P_0 \| P_1)}$ , where  $P_0(1)$  indicates the probability that we identify class  $H_0$  while the true class is  $H_1$ . Since  $P_0(1) + P_1(0) \leq \delta$ , by contradiction, we can show that  $m \sim \Omega(\ln(\delta^{-1})\gamma^{-1})$ .

Note that this lower bound on  $m$  can be arbitrarily large by choosing  $\gamma$  to be sufficiently small. However their ATE values stay constant away as observed in Equation (9). Thus, for every fixed confounded distribution encoded by  $\mathbf{a}$  and fixed number of deconfounded samples  $m$ , we can always construct a pair of conditional distributions encoded by  $\mathbf{q}$  and  $\mathbf{q}'$  such that their corresponding ATEs are constant away while the probability that we correctly identify the true conditional distribution from  $\mathbf{q}$  and  $\mathbf{q}'$  is less than  $1 - \delta$ . In particular,  $\epsilon = c = a_{00} + a_{10}$  in the above example. (Here, we implicitly assume that  $a_{00} + a_{10}$  is strictly greater than zero, i.e.,  $a_{00} + a_{10} > 0$ .)  $\square$

### B.4 Proof of Theorem 2

**Theorem 2.** (Lower Bound) *For any estimator and sample selection policy, the number of deconfounded samples  $m$  needed to achieve  $P\left(\left|\widehat{\text{ATE}} - \text{ATE}\right| \geq \epsilon\right) < \delta$  is at least  $\Omega(\epsilon^{-2} \log(\delta^{-1}))$ .*

*Proof of Theorem 2.* Again, it suffices to show for the case where the confounder is binary. The extension to categorical confounder is straightforward as illustrated in the proof of Theorem 6 in Appendix B.7. Let

$q_{yt} = P(Z = 1 | Y = y, T = t)$ . We will proceed by construction. Consider  $\mathbf{q} = (q_{00}, q_{01}, \beta, \beta + \gamma)$  and  $\mathbf{q}' = (q_{00}, q_{01}, \beta + \gamma, \beta)$ , for some small  $\gamma$ . Then

$$\begin{aligned} \text{ATE}_{\mathbf{a}}(\mathbf{q}) &= \frac{a_{11}(\beta + \gamma)}{a_{11}(\beta + \gamma) + a_{01}q_{01}}(a_{00}q_{00} + a_{01}q_{01} + a_{10}\beta + a_{11}(\beta + \gamma)) + \frac{a_{11}(1 - \beta - \gamma)}{a_{11}(1 - \beta - \gamma) + a_{01}(1 - q_{01})} \\ &\quad (1 - a_{00}q_{00} - a_{01}q_{01} - a_{10}\beta - a_{11}(\beta + \gamma)) - \frac{a_{10}\beta}{a_{10}\beta + a_{00}q_{00}}(a_{00}q_{00} + a_{01}q_{01} + a_{10}\beta + a_{11}(\beta + \gamma)) - \\ &\quad \frac{a_{10}(1 - \beta)}{a_{10}(1 - \beta) + a_{00}(1 - q_{00})}(1 - a_{00}q_{00} - a_{01}q_{01} - a_{10}\beta - a_{11}(\beta + \gamma)), \end{aligned}$$

and similarly, we have

$$\begin{aligned} \text{ATE}_{\mathbf{a}}(\mathbf{q}') &= \frac{a_{11}\beta}{a_{11}\beta + a_{01}q_{01}}(a_{00}q_{00} + a_{01}q_{01} + a_{10}(\beta + \gamma) + a_{11}\beta) + \frac{a_{11}(1 - \beta)}{a_{11}(1 - \beta) + a_{01}(1 - q_{01})}(1 - a_{00}q_{00} - \\ &\quad a_{01}q_{01} - a_{10}(\beta + \gamma) - a_{11}\beta) - \frac{a_{10}(\beta + \gamma)}{a_{10}(\beta + \gamma) + a_{00}q_{00}}(a_{00}q_{00} + a_{01}q_{01} + a_{10}(\beta + \gamma) + a_{11}\beta) - \\ &\quad \frac{a_{10}(1 - \beta - \gamma)}{a_{10}(1 - \beta - \gamma) + a_{00}(1 - q_{00})}(1 - a_{00}q_{00} - a_{01}q_{01} - a_{10}(\beta + \gamma) - a_{11}\beta). \end{aligned}$$

Ignoring the  $\gamma$  in the denominator, we have that

$$\begin{aligned} \text{ATE}_{\mathbf{a}}(\mathbf{q}) - \text{ATE}_{\mathbf{a}}(\mathbf{q}') &= \left( \frac{a_{11}}{a_{11}\beta + a_{01}q_{01}} + \frac{a_{10}}{a_{10}\beta + a_{00}q_{00}} \right) (a_{00}q_{00} + a_{01}q_{01} + a_{10}\beta + a_{11}\beta)\gamma \\ &\quad - \left( \frac{a_{11}}{a_{11}(1 - \beta) + a_{01}(1 - q_{01})} + \frac{a_{10}}{a_{10}(1 - \beta) + a_{00}(1 - q_{00})} \right) (1 - a_{00}q_{00} - a_{01}q_{01} - a_{10}\beta - a_{11}\beta)\gamma \\ &\quad + \frac{a_{11}^2 - a_{11}a_{10}}{a_{11}\beta + a_{01}q_{01}}\beta\gamma - \frac{a_{11}^2 - a_{11}a_{10}}{a_{11}(1 - \beta) + a_{01}(1 - q_{01})}(1 - \beta)\gamma \\ &\quad + \frac{a_{10}^2 - a_{11}a_{10}}{a_{10}\beta + a_{00}q_{00}}\beta\gamma - \frac{a_{10}^2 - a_{11}a_{10}}{a_{10}(1 - \beta) + a_{00}(1 - q_{00})}(1 - \beta)\gamma \\ &\quad + \frac{a_{11}^2}{a_{11}\beta + a_{01}q_{01}}\gamma^2 + \frac{a_{11}^2}{a_{11}(1 - \beta) + a_{01}(1 - q_{01})}\gamma^2 + \frac{a_{10}^2}{a_{10}\beta + a_{00}q_{00}}\gamma^2 + \frac{a_{10}^2}{a_{10}(1 - \beta) + a_{00}(1 - q_{00})}\gamma^2 \quad (10) \end{aligned}$$

Similar to the proof above, let  $B_1$  denote the Bernoulli random variable with parameter  $\beta$ , and let  $B_2$  denote the Bernoulli random variable with parameter  $\beta + \gamma$ . Then, given  $m$  deconfounded samples, we have  $\text{KL}(B_1^m \| B_2^m) \leq m\beta \ln(\frac{\beta}{\beta + \gamma}) + m(1 - \beta) \ln(\frac{1 - \beta}{1 - \beta - \gamma}) \leq m \ln(1 + \frac{\gamma}{1 - \beta - \gamma}) \leq m(\frac{\gamma}{1 - \beta - \gamma} - \frac{\gamma^2}{2(1 - \beta - \gamma)^2})$ . Thus, we have  $m \sim \Omega(\frac{\ln(\delta^{-1})}{\gamma^2})$ . From Equation (10), we observe that  $\epsilon = \|\text{ATE}_{\mathbf{a}}(\mathbf{q}) - \text{ATE}_{\mathbf{a}}(\mathbf{q}')\| \sim \Omega(\gamma)$ . Combining above, we have  $m \sim \Omega(\frac{\ln(\delta^{-1})}{\epsilon^2})$ .  $\square$

## B.5 Proof of Theorems 3 and 5

**Theorem 3.** (*Upper Bound*) *When incorporating (infinite) confounded data,  $P(|\widehat{\text{ATE}} - \text{ATE}| \geq \epsilon) < \delta$  is satisfied if the number of deconfounded samples  $m$  is at least*

$$m_{\text{nsp}} := \max_{t,z} \frac{C \sum_y a_{yt}}{\left( \sum_y a_{yt} q_{yt}^z \right)^2} = \max_{t,z} \frac{P_T(t)}{P_{T,Z}(t,z)^2} C. \quad (2)$$

**Theorem 5.** (*Upper Bound*) *Under the uniform selection policy, with (infinite) confounded data incorporated,  $P(|\widehat{\text{ATE}} - \text{ATE}| \geq \epsilon) < \delta$  is satisfied if  $\mu_{\text{usp}}$  is at least*

$$m_{\text{usp}} := \max_{t,z} \frac{C \sum_y 4a_{yt}^2}{\left( \sum_y a_{yt} q_{yt}^z \right)^2} = \max_{t,z} \frac{4 \sum_y P_{Y,T}(y,t)^2}{P_{T,Z}(t,z)^2} C.$$

Similarly, for the outcome-weighted selection policy:

$$m_{\text{owsp}} := \max_{t,z} \frac{2C \left( \sum_y a_{yt} \right)^2}{\left( \sum_y a_{yt} q_{yt}^z \right)^2} = \max_{t,z} \frac{2}{P_{Z|T}(z|t)^2} C.$$

*Proof of Theorems 3 and 5.* In these theorems, we derive the concentration of the  $\widehat{\text{ATE}}$  assuming infinite confounded data, and parametrize  $p_{yt}^z$  by  $p_{yt}^z = a_{yt} q_{yt}^z$ . Since under infinite confounded data,  $a_{yt}$ 's are known, and thus we only need to estimate the  $q_{yt}^z$ 's. The key difference between Theorem 5 and Theorem 1 is that now we define the random variables  $X_{yt}^z$  to map the event  $(Z = z|Y = y, T = t)$  to  $\{0, 1\}$ . Thus,  $X_{yt}^z$  is distributed according to  $\text{Bernoulli}(q_{yt}^z)$ . Thus, to decompose  $|a_{1t} q_{1t}^z + a_{0t} q_{0t}^z - a_{1t} \hat{q}_{1t}^z - a_{0t} \hat{q}_{0t}^z|$ , we first show the following lemma:

**Lemma 4.** *Let  $X_1, \dots, X_{x_1 m}$  and  $Y_1, \dots, Y_{x_2 m}$  be independent random variables in  $[0, 1]$ . Then for any  $t > 0$ , we have*

$$P \left( \left| \alpha \frac{\sum_{i=1}^{x_1 m} X_i - \mathbb{E}[X_i]}{x_1 m} + \beta \frac{\sum_{j=1}^{x_2 m} Y_j - \mathbb{E}[Y_j]}{x_2 m} \right| \geq \alpha t + \beta k \right) \leq 2 \exp \left( - \frac{2m(\alpha t + \beta k)^2}{\left( \frac{\alpha^2}{x_1} + \frac{\beta^2}{x_2} \right)} \right).$$

*Proof of Lemma 4.* First observe that

$$\begin{aligned} & P \left( \alpha \frac{\sum_{i=1}^{x_1 m} X_i - \mathbb{E}[X_i]}{x_1 m} + \beta \frac{\sum_{j=1}^{x_2 m} Y_j - \mathbb{E}[Y_j]}{x_2 m} \geq \alpha t + \beta k \right) \\ &= P \left( \frac{\alpha}{x_1} \sum_{i=1}^{x_1 m} (X_i - \mathbb{E}[X_i]) + \frac{\beta}{x_2} \sum_{j=1}^{x_2 m} (Y_j - \mathbb{E}[Y_j]) \geq m\alpha t + m\beta k \right). \end{aligned}$$

Now, let  $Z_i = \frac{\alpha}{x_1} X_i$  if  $i \in [1, x_1 m]$ , and  $Z_i = \frac{\beta}{x_2} Y_i$  if  $i \in [x_1 m + 1, (x_1 + x_2)m]$ . Then applying Theorem 7, we have

$$\begin{aligned} & P \left( \left| \sum_{i=1}^{(x_1+x_2)m} (Z_i - \mathbb{E}[Z_i]) \right| \geq m\alpha t + m\beta k \right) \leq 2 \exp \left( - \frac{2m^2(\alpha t + \beta k)^2}{\sum_{i=1}^{(x_1+x_2)m} (M_i - m_i)^2} \right) \\ &= 2 \exp \left( - \frac{2m(\alpha t + \beta k)^2}{\frac{\alpha^2}{x_1} + \frac{\beta^2}{x_2}} \right). \end{aligned}$$

□

As defined in Section 3, let  $x_{yt}$  denote the percentage data we sample from the group  $yt$ .

Recall that from the proof of Theorem 1, we have

$$\begin{aligned} & P \left( |\widehat{\text{ATE}} - \text{ATE}| \geq \epsilon \right) \leq \sum_{t,z} P \left( |p_{1t}^z - \hat{p}_{1t}^z| \geq \frac{\sum_y p_{yt}^z}{5k} \epsilon \right) + P \left( |p_{1t}^z + p_{0t}^z - \hat{p}_{1t}^z - \hat{p}_{0t}^z| \geq \frac{\sum_y p_{yt}^z}{5k} \epsilon \right) \\ &= \sum_{t,z} P \left( |a_{1t} q_{1t}^z - a_{1t} \hat{q}_{1t}^z| \geq \frac{\sum_y a_{yt} q_{yt}^z}{5k} \epsilon \right) + P \left( |a_{1t} q_{1t}^z + a_{0t} q_{0t}^z - a_{1t} \hat{q}_{1t}^z - a_{0t} \hat{q}_{0t}^z| \geq \frac{\sum_y a_{yt} q_{yt}^z}{5k} \epsilon \right) \\ &= \sum_{t,z} P \left( |q_{1t}^z - \hat{q}_{1t}^z| \geq \frac{\sum_y a_{yt} q_{yt}^z}{5k a_{1t}} \epsilon \right) + P \left( |a_{1t} q_{1t}^z + a_{0t} q_{0t}^z - a_{1t} \hat{q}_{1t}^z - a_{0t} \hat{q}_{0t}^z| \geq \frac{\sum_y a_{yt} q_{yt}^z}{5k} \epsilon \right) \\ &\leq 4k \max_{t,z} \left( 2 \exp \left( -2x_{1t} m \frac{\left( \sum_y a_{yt} q_{yt}^z \right)^2 \epsilon^2}{25k^2 a_{1t}^2} \right), 2 \exp \left( -2m \frac{\left( \sum_y a_{yt} q_{yt}^z \right)^2 \epsilon^2}{25k^2 \sum_y \frac{a_{yt}^2}{x_{yt}}} \right) \right) \\ &\leq \delta, \end{aligned}$$

where the second to last line follows from applying Lemma 4 to the second half of the line above it.



Solving the equation above, we have

$$m \geq \frac{12.5k^2 \ln(\frac{8k}{\delta})}{\epsilon^2} \max_{t,z} \left( \frac{a_{1t}^2/x_{1t}}{\left(\sum_y a_{yt} q_{yt}^z\right)^2}, \frac{\sum_y (a_{yt}^2/x_{yt})}{\left(\sum_y a_{yt} q_{yt}^z\right)^2} \right) = \frac{12.5k^2 \ln(\frac{8k}{\delta})}{\epsilon^2} \max_{t,z} \frac{\sum_y (a_{yt}^2/x_{yt})}{\left(\sum_y a_{yt} q_{yt}^z\right)^2}.$$

The last equality is because  $a_2^2/x_2, a_1^2/x_1 > 0$ . Under NSP,  $x_{yt} = a_{yt}$ . Thus, we have

$$m_{\text{NSP}} := \frac{12.5k^2 \ln(\frac{8k}{\delta})}{\epsilon^2} \max_{t,z} \frac{\sum_y a_{yt}}{\left(\sum_y a_{yt} q_{yt}^z\right)^2}.$$

Similarly, under USP,  $x_{yt} = \frac{1}{4}$ , and we have

$$m_{\text{USP}} := \frac{12.5k^2 \ln(\frac{8k}{\delta})}{\epsilon^2} \max_{t,z} \frac{\sum_y 4a_{yt}^2}{\left(\sum_y a_{yt} q_{yt}^z\right)^2}.$$

Lastly, under OWSP,  $x_{yt} = \frac{a_{yt}}{2\sum_y a_{yt}}$ , and we have

$$m_{\text{OWSP}} := \frac{12.5k^2 \ln(\frac{8k}{\delta})}{\epsilon^2} \max_{t,z} \frac{2(\sum_y a_{yt})^2}{\left(\sum_y a_{yt} q_{yt}^z\right)^2}.$$

□

## B.6 Proof of Theorem 4

**Theorem 4.** *For any fixed  $\epsilon \in [0, 0.5 - 2\beta(1 - \beta)]$  and any fixed  $\delta < 1$ , there exist distributions where  $\mu_{\text{OWSP}}/\mu_{\text{NSP}}$  is arbitrarily close to zero. In addition, for any estimator and every distribution,  $\mu_{\text{OWSP}}/\mu_{\text{NSP}} \leq 2$ .*

*Proof of Theorem 4.* We proceed by construction. For simplicity, we illustrate the correctness of Theorem 4 for binary confounders. The extension to the multi-valued confounder is straightforward and will be demonstrated in the proof of Theorem 6.

Consider the following example:  $a_{01} = a_{10} = a_{11} = \eta$ ,  $a_{00} = 1 - 3\eta$ , and consider the following pair of  $\mathbf{q}$ 's:  $\mathbf{q} = (\beta, \beta, \beta, c\beta)$  and  $\mathbf{q}' = (\beta, \beta, \beta, \beta)$ , where  $c \leq \frac{1-\beta}{\beta}$  is some constant. Here, one of the  $\mathbf{q}$  and  $\mathbf{q}'$  represents the true ATE, and the other represents the estimated ATE using the best estimator. Without loss of generality, we assume that we have already identified three components of the true conditional distribution. (In general, we can always construct an instance by modifying the values of  $a_{01}$  and  $a_{10}$  so that the majority error is induced by estimation error on  $q_{11}$ .) Then, we have  $\text{ATE}_{\mathbf{a}}(\mathbf{q}) = \frac{c\beta}{1+c} + \frac{(1-c\beta)(1-\beta)}{2-c\beta-\beta} - \frac{\eta}{1-2\eta}$ , and  $\text{ATE}_{\mathbf{a}}(\mathbf{q}') = \frac{1}{2} - \frac{\eta}{1-2\eta}$ . Thus,  $\Delta\text{ATE} := |\text{ATE}_{\mathbf{a}}(\mathbf{q}) - \text{ATE}_{\mathbf{a}}(\mathbf{q}')|$ :

$$\Delta\text{ATE} = \left| \frac{1}{2} - \frac{c\beta}{c+1} - \frac{(1-c\beta)(1-\beta)}{2-c\beta-\beta} \right|.$$

Note that when  $c = \frac{1-\beta}{\beta}$ ,  $\Delta\text{ATE} = 0.5 - 2\beta(1 - \beta) \approx 0.5$ . Thus, for any  $\epsilon \in [0, 0.5 - 2\beta(1 - \beta)]$ , there exists some  $c$  such that  $\epsilon = \Delta\text{ATE}$ . Then, for any  $\delta$ , let  $\mu$  denote the minimum expected number of samples that we need to distinguish  $\mathbf{q}$  from  $\mathbf{q}'$  under the best estimator. Then under NSP, the minimum number of samples that we need under the best estimator equals to  $\mu_{\text{NSP}} := \mu/\eta$ , and under OWSP, the minimum number of samples that we need under the best estimator equals to  $\mu_{\text{OWSP}} = 4\mu$ . (Note that  $\mathbf{x}_{yt} = (\frac{1-3\eta}{2(1-2\eta)}, \frac{1}{4}, \frac{\eta}{2(1-2\eta)}, \frac{1}{4})$  under OWSP in this example.) Thus,  $\mu_{\text{OWSP}}/\mu_{\text{NSP}} = 4\eta$ . Since in this example,  $\eta$  is at most  $1/4$ ,  $\mu_{\text{OWSP}}/\mu_{\text{NSP}} \leq 1$  and can be arbitrarily close to 0 as  $\eta \rightarrow 0$ . (Intuitively, the first statement is true because when  $\sum_t a_{0t} \ll \sum_t a_{1t}$  and  $a_{00} \approx a_{01}$ , it is equally important to estimate  $q_{0t}^z$ 's and  $q_{1t}^z$ 's according to the ATE expression. However, under this setup, the number of samples allocated to groups  $(0, t)$ 's decreases as  $a_{0,t}$ 's approach to 0 under NSP, while under OWSP, half of the deconfounded samples are always dedicated to estimate the  $q_{0t}^z$ 's.)

Next, we show the last sentence in Theorem 4 is true. For any fixed  $\epsilon, \delta < 1$ , let  $\mu_{\text{nsp}}$  be the minimum expected number of samples needed to achieve  $P(|\widehat{\text{ATE}} - \text{ATE}| \geq \epsilon) < \delta$  under natural selection policy for the best estimator, then when  $w_{\text{owsp}} := 2\mu_{\text{nsp}} \max_t \sum_y a_{yt}$  also achieves  $P(|\widehat{\text{ATE}} - \text{ATE}| \geq \epsilon) < \delta$  under the outcome-weighted selection policy. The reason is that when using  $w_{\text{owsp}}$  number of deconfounded samples, the number of deconfounded data allocated to each  $yt$  group is at least as much as those under the natural selection policy. Thus, we have  $\mu_{\text{owsp}} \leq w_{\text{owsp}} \leq 2\mu_{\text{nsp}}$ , where the last inequality is because  $\max_t \sum_y a_{yt} < 1$ .  $\square$

## B.7 Proof of Theorem 6

**Theorem 6.** (Lower Bound) For every  $\mathbf{a}$ , there exists a  $\mathbf{q}$  such that  $\mu_{\text{nsp}}$  is at least

$$w_{\text{nsp}} := \frac{C_1}{\beta^2} \max_t \left( \frac{a_{1t}(\sum_y a_{y\bar{t}})^2}{(\sum_y a_{yt})^2}, \frac{a_{0t}(\sum_y a_{y\bar{t}})^2}{(\sum_y a_{yt})^2} \right);$$

similarly for uniform selection policy:

$$w_{\text{usp}} := \frac{C_1}{\beta^2} \max_t \left( 4 \frac{a_{1t}^2(\sum_y a_{y\bar{t}})^2}{(\sum_y a_{yt})^2}, 4 \frac{a_{0t}^2(\sum_y a_{y\bar{t}})^2}{(\sum_y a_{yt})^2} \right);$$

similarly for outcome-weighted sample selection policy:

$$w_{\text{owsp}} := \frac{C_1}{\beta^2} \max_t \left( 2 \frac{a_{1t}(\sum_y a_{y\bar{t}})^2}{\sum_y a_{yt}}, 2 \frac{a_{0t}(\sum_y a_{y\bar{t}})^2}{\sum_y a_{yt}} \right),$$

where  $\bar{t} = 1 - t$  and  $C_1 \propto (k\beta - 1)^2 \ln(\delta^{-1})\epsilon^{-2}$ .

*Proof.* Consider  $\mathbf{q} = (q_{00}^z, q_{01}^z, q_{10}^z, q_{11}^z)$  where  $q_{01}^1 = \beta$ ,  $q_{11}^1 = \beta + \gamma$ , and  $q_{11}^z = q_{01}^z - \gamma/(k-1)$  for  $z = 2, \dots, k$ , with  $\sum_z q_{01}^z = \sum_z q_{11}^z = 1$ . We assume that  $q_{11}^z, q_{01}^z \in [\beta, 1 - \beta]$  for some suitable  $\beta$  and  $\gamma$  for all values of  $Z$ . Similarly, we consider the  $\mathbf{q}'$  where the entries of  $q_{01}^z$  and  $q_{11}^z$  are flipped, i.e.,  $\mathbf{q}' = (q_{00}^z, q_{11}^z, q_{10}^z, q_{01}^z)$ , for some small  $\gamma$ , where the  $q_{yt}^z$ 's are defined above. Then,

$$\begin{aligned} \text{ATE}_{\mathbf{a}}(\mathbf{q}) &= \sum_z \left( \left( \frac{a_{11}q_{11}^z}{\sum_y a_{y1}q_{y1}^z} - \frac{a_{10}q_{10}^z}{\sum_y a_{y0}q_{y0}^z} \right) \sum_{y,t} a_{yt}q_{yt}^z \right) \\ &= \frac{a_{11}(\beta + \gamma)}{a_{11}(\beta + \gamma) + a_{01}\beta} (a_{00}q_{00}^1 + a_{01}\beta + a_{10}q_{10}^1 + a_{11}(\beta + \gamma)) - \frac{a_{10}q_{10}^1}{a_{10}q_{10}^1 + a_{00}q_{00}^1} (a_{00}q_{00}^1 + a_{01}\beta + a_{10}q_{10}^1 + \\ & a_{11}(\beta + \gamma)) + \sum_{z=2}^k \frac{a_{11} \left( q_{01}^z - \frac{\gamma}{k-1} \right)}{a_{11} \left( q_{01}^z - \frac{\gamma}{k-1} \right) + a_{01}q_{01}^z} \left( a_{00}q_{00}^z + a_{01}q_{01}^z + a_{10}q_{10}^z + a_{11} \left( q_{01}^z - \frac{\gamma}{k-1} \right) \right) - \\ & \sum_{z=2}^k \frac{a_{10}q_{10}^z}{a_{10}q_{10}^z + a_{00}q_{00}^z} \left( a_{00}q_{00}^z + a_{01}q_{01}^z + a_{10}q_{10}^z + a_{11} \left( q_{01}^z - \frac{\gamma}{k-1} \right) \right), \end{aligned}$$

and similarly, we have

$$\begin{aligned} \text{ATE}_{\mathbf{a}}(\mathbf{q}') &= \frac{a_{11}\beta}{a_{11}\beta + a_{01}(\beta + \gamma)} (a_{00}q_{00}^1 + a_{01}(\beta + \gamma) + a_{10}q_{10}^1 + a_{11}\beta) - \frac{a_{10}q_{10}^1}{a_{10}q_{10}^1 + a_{00}q_{00}^1} (a_{00}q_{00}^1 + a_{01}(\beta + \gamma) + \\ & a_{10}q_{10}^1 + a_{11}\beta) + \sum_{z=2}^k \frac{a_{11}q_{01}^z}{a_{11}q_{01}^z + a_{01} \left( q_{01}^z - \frac{\gamma}{k-1} \right)} \left( a_{00}q_{00}^z + a_{01} \left( q_{01}^z - \frac{\gamma}{k-1} \right) + a_{10}q_{10}^z + a_{11}q_{01}^z \right) - \\ & \sum_{z=2}^k \frac{a_{10}q_{10}^z}{a_{10}q_{10}^z + a_{00}q_{00}^z} \left( a_{00}q_{00}^z + a_{01} \left( q_{01}^z - \frac{\gamma}{k-1} \right) + a_{10}q_{10}^z + a_{11}q_{01}^z \right) \end{aligned}$$

Ignoring the  $\gamma$  in the denominator, we have that

$$\begin{aligned}
 \text{ATE}_{\mathbf{a}}(\mathbf{q}) - \text{ATE}_{\mathbf{a}}(\mathbf{q}') &\approx \frac{a_{11}}{a_{11}\beta + a_{01}\beta} (a_{00}q_{00}^1 + a_{01}\beta + a_{10}q_{10}^1 + a_{11}\beta)\gamma + \frac{a_{10}q_{10}^1(a_{01} - a_{11})}{a_{10}q_{10}^1 + a_{00}q_{00}^1}\gamma \\
 &- \left( \sum_{z=2}^k \left( \frac{a_{11}/k - 1}{a_{11}q_{01}^z + a_{01}q_{01}^z} (a_{00}q_{00}^z + a_{10}q_{10}^z + (a_{01} + a_{11})q_{10}^z) \right) \right) \gamma - \sum_{z=2}^k \frac{a_{10}q_{10}^z(a_{01} - a_{11})}{a_{10}q_{10}^z + a_{00}q_{00}^z} \frac{1}{k-1}\gamma \\
 &+ \frac{a_{11}^2}{a_{11}\beta + a_{01}\beta} \gamma^2 + \sum_{z=2}^k \frac{a_{11}^2}{a_{11}q_{01}^z + a_{01}q_{01}^z} \frac{\gamma^2}{(k-1)^2} \\
 &= \frac{a_{11}}{a_{11}\beta + a_{01}\beta} (a_{00}q_{00}^1 + a_{10}q_{10}^1)\gamma + \frac{a_{10}q_{10}^1(a_{01} - a_{11})}{a_{10}q_{10}^1 + a_{00}q_{00}^1}\gamma - \frac{a_{11}}{k-1} \sum_{z=2}^k \left( \frac{a_{00}q_{00}^z + a_{10}q_{10}^z}{a_{11}q_{01}^z + a_{01}q_{01}^z} \right) \gamma \\
 &- \frac{1}{k-1} \sum_{z=2}^k \frac{a_{10}q_{10}^z(a_{01} - a_{11})}{a_{10}q_{10}^z + a_{00}q_{00}^z} \gamma + \frac{a_{11}^2}{a_{11}\beta + a_{01}\beta} \gamma^2 + \sum_{z=2}^k \frac{a_{11}^2}{a_{11}q_{01}^z + a_{01}q_{01}^z} \frac{\gamma^2}{(k-1)^2} \tag{11}
 \end{aligned}$$

Since the second order terms in  $\gamma$  is dominated by the first order terms in  $\gamma$ , thus to find the highest lower bound for sample complexity in this instance is to find the largest coefficient in front of  $\gamma$ .

Assuming that  $\beta \ll k$  and  $k\beta < 1$ , then the maximum of Equation (11) is achieved when  $q_{00}^z = q_{10}^z = \beta$ ,  $q_{01}^z = q_{11}^z = 1 - k\beta$ , and  $q_{01}^z = (1 - \beta)/(k - 1)$ , and the coefficient in front of  $\gamma$  is

$$\frac{a_{11}}{a_{11} + a_{01}} (a_{00} + a_{10}) \left( \frac{1}{\beta} - \frac{k - \beta}{1 - \beta} \right) \approx \frac{a_{11}}{a_{11} + a_{01}} (a_{00} + a_{10}) \left( \frac{1}{\beta} - k \right).$$

Similar to the proof of Theorem 2, we have  $m \sim \Omega\left(\frac{\ln(\delta^{-1})}{\gamma^2}\right)$ . From Equation (10), we observe that  $\epsilon = \|\text{ATE}_{\mathbf{a}}(\mathbf{q}) - \text{ATE}_{\mathbf{a}}(\mathbf{q}')\| \sim \Omega(\gamma)$ . Combining above, we have  $m \sim \Omega\left(\frac{\ln(\delta^{-1})}{\epsilon^2}\right)$ . In the case above,  $\epsilon \approx \frac{a_{11}}{a_{11} + a_{01}} (a_{00} + a_{10}) \frac{1}{\beta} \gamma$ , thus, the number of deconfounded samples needed is approximately

$$m \propto \frac{\ln(\delta^{-1}) a_{11}^2 (a_{00} + a_{10})^2}{\epsilon^2 (a_{11} + a_{01})^2} \left( \frac{1}{\beta} - k \right)^2.$$

Let  $C_1 \propto (k\beta - 1)^2 \ln(\delta^{-1}) \epsilon^{-2}$ . Then  $m \sim \Omega\left(\frac{C_1}{\beta^2} \frac{a_{11}^2 (a_{00} + a_{10})^2}{(a_{11} + a_{01})^2}\right)$ .

If we flip the values of  $q_{01}^z$  and  $q_{11}^z$  with the values of  $q_{00}^z$  and  $q_{10}^z$  in both  $\mathbf{q}$  and  $\mathbf{q}'$ , then we have  $m \sim \frac{C_1}{\beta^2} \frac{a_{10}^2 (a_{01} + a_{11})^2}{(a_{10} + a_{00})^2}$ . Note that this is because that the estimation error on ATE and  $1 - \text{ATE}$  is symmetric. In addition, under natural selection policy, we need at least  $\frac{m}{a_{11}}$  samples; uniform selection policy, we need at least  $4m$  deconfounded samples; under outcome-weighted selection policy, we need at least  $2 \frac{a_{11} + a_{01}}{a_{11}} m$  deconfounded samples. Combining all of the above, we obtained Theorem 6.  $\square$

## C Finite Confounded Data

In this case, *deconfounding* reveals the value of  $Z$  for one (initially confounded) sample, and thus we gain no additional information about  $\mathcal{P}_{Y,T}$ . Thus, these  $n$  confounded data provide us with an *estimate* of the confounded distribution,  $\hat{P}_{Y,T}(y, t)$ , which we denote  $\hat{a}_{yt}$ , and thus provide us an estimated OWSP. Similarly, we estimate  $\hat{a}_{yt}$  using the MLE from the confounded data. To check the robustness of OWSP, we extend our analysis to handle finite confounded data. With  $x_{yt}$  defined as in Section 3.2, we can derive a theorem analogous to Theorems 1-5:

**Theorem 8.** (*Upper Bound*) Given  $n$  confounded and  $m$  deconfounded samples, with  $n \geq m$ ,  $P(|\widehat{\text{ATE}} - \text{ATE}| \geq \epsilon) \leq \delta$  is satisfied when

$$\min_{y,t,z} \frac{\left( \sum_y a_{yt} q_{yt}^z \right)^2}{\frac{1}{x_{yt}m} + \frac{(q_{yt}^z)^2}{n}} = \min_{y,t,z} \left( \frac{P_{T,Z}(t, z)^2}{\frac{1}{x_{yt}m} + \frac{(q_{yt}^z)^2}{n}} \right) \geq 4C. \tag{12}$$

The proof of Theorem 8 (Appendix C.1) requires a bound we derive (Appendix, Lemma 5) for the product of two independent random variables. A few results follow from Theorem 8. First, a quick calculation shows that when  $m$  is held constant,  $P(|\text{ATE} - \widehat{\text{ATE}}| \geq \epsilon)$  remains positive as  $n \rightarrow \infty$ . This means that for a certain combinations of  $\epsilon, \delta, n$ , there does not necessarily exist a sufficiently large  $m$  s.t.  $P(|\text{ATE} - \widehat{\text{ATE}}| \geq \epsilon) \leq \delta$  can be satisfied. However, when there exists such an  $m$ , then

$$m \geq \max_{y,t,z} x_{yt}^{-1} \left( \frac{P_{T,Z}(t,z)^2}{4C} - \frac{(q_{yt}^z)^2}{n} \right)^{-1}.$$

Although Theorem 8 does not recover Theorems 3 and 5 exactly when  $n \rightarrow \infty$ ,<sup>1</sup> it provides us with insights into relative performance of our sampling policies. Theorem 8 implies that when  $n \gg (q_{yt}^z)^2 x_{yt} m \forall y, t$ , the majority of the estimation error comes from not deconfounding enough data. This is because when the number of confounded data that we have is more than  $\Omega(m)$ , the error on the ATE in Equation (12) is dominated by fact that we have not deconfounded enough data. To put it another way, for a given  $m$ , having  $n = \Omega(m)$  confounded samples is sufficient.

### C.1 Proof of Theorem 8

**Theorem 8.** (*Upper Bound*) *Given  $n$  confounded and  $m$  deconfounded samples, with  $n \geq m$ ,  $P(|\text{ATE} - \widehat{\text{ATE}}| \geq \epsilon) \leq \delta$  is satisfied when*

$$\min_{y,t,z} \frac{\left( \sum_y a_{yt} q_{yt}^z \right)^2}{\frac{1}{x_{yt}m} + \frac{(q_{yt}^z)^2}{n}} = \min_{y,t,z} \left( \frac{P_{T,Z}(t,z)^2}{\frac{1}{x_{yt}m} + \frac{(q_{yt}^z)^2}{n}} \right) \geq 4C. \quad (12)$$

*Proof of Theorem 8.* In this theorem, we derive the concentration for the  $\widehat{\text{ATE}}$  under finite confounded data. The difference between Theorem 5 and Theorem 8 is that now we need to estimate  $a_{yt}$  in addition to  $q_{yt}^z$ . Thus, to decompose  $|a_{yt} q_{yt}^z - \hat{a}_{yt} \hat{q}_{yt}^z|$ , we first derive Lemma 5.

#### C.1.1 Lemma 5

**Lemma 5** (Sample complexity for two independent r.v.s with two independent sampling processes). *Let  $X_1, \dots, X_n$  and  $Y_1, \dots, Y_m$  be two sequences of Bernoulli random variables independently drawn from distribution  $p_1$  and  $p_2$ , respectively. Let  $S_X = \sum_{i=1}^n X_i, S_Y = \sum_{i=1}^m Y_i$ . Then,*

$$P\left( \left| S_X S_Y - \mathbb{E}[S_X] \mathbb{E}[S_Y] \right| \geq nmt \right) \leq 2 \exp\left( \frac{-2t^2}{\frac{1}{m} + \frac{p_2^2}{n}} \right).$$

<sup>1</sup>We could apply Lemma 2 (Appendix B) to obtain a bound that recovers Theorems 3 and 5 exactly as  $n \rightarrow \infty$ . However, this method does not give us sufficient insights into the comparative performance of our sampling policies.

*Proof of Lemma 5.* The proof follows the proof of Hoeffding's inequality:

$$P\left(S_X S_Y - \mathbb{E}[S_X]\mathbb{E}[S_Y] \geq nmt\right) = P\left(\exp(aS_X S_Y - a\mathbb{E}[S_X]\mathbb{E}[S_Y])\right) \geq \exp(anmt) \quad (13)$$

$$\leq \exp(-anmt)\mathbb{E}\left[\exp(aS_X S_Y - a\mathbb{E}[S_X]\mathbb{E}[S_Y])\right], \quad (\text{because of Markov's inequality}) \quad (14)$$

$$= \exp(-anmt)\mathbb{E}\left[\exp(aS_X(S_Y - \mathbb{E}[S_Y]) + a\mathbb{E}[S_Y](S_X - \mathbb{E}[S_X]))\right] \quad (15)$$

$$\leq \exp(-anmt)\mathbb{E}\left[\exp(a \max(S_X)(S_Y - \mathbb{E}[S_Y]) + a\mathbb{E}[S_Y](S_X - \mathbb{E}[S_X]))\right] \quad (\text{because } S_X \geq 0) \quad (15)$$

$$= \exp(-anmt)\mathbb{E}\left[\exp(an(S_Y - \mathbb{E}[S_Y]) + a\mathbb{E}[S_Y](S_X - \mathbb{E}[S_X]))\right] \quad (16)$$

$$= \exp(-anmt)\mathbb{E}\left[\exp(an(S_Y - \mathbb{E}[S_Y]))\right]\mathbb{E}\left[\exp(a\mathbb{E}[S_Y](S_X - \mathbb{E}[S_X]))\right] \quad (\text{because } X \perp\!\!\!\perp Y) \quad (16)$$

$$= \exp(-anmt)\prod_{i=1}^m \prod_{j=1}^n \mathbb{E}\left[\exp(an(Y_i - \mathbb{E}[Y_i]))\right]\mathbb{E}\left[\exp(a\mathbb{E}[S_Y](X_j - \mathbb{E}[X_j]))\right] \quad (17)$$

$$\leq \exp(-anmt)\prod_{i=1}^m \exp\left(\frac{a^2}{8}n^2\right)\prod_{j=1}^n \exp\left(\frac{a^2}{8}\mathbb{E}[S_Y]^2\right) \quad (17)$$

$$= \exp\left(-anmt + \frac{a^2}{8}mn^2 + \frac{a^2}{8}nm^2p_2^2\right) \quad (\text{because the minimum is achieved at } a = \frac{4t}{n + mp_2^2}) \quad (18)$$

$$\leq \exp\left(-\frac{2mnt^2}{n + mp_2^2}\right) = \exp\left(-\frac{2t^2}{\frac{1}{m} + \frac{p_2^2}{n}}\right).$$

Line (17) is because  $Y_i - \mathbb{E}[Y_i] \in \{-\mathbb{E}[Y_i], 1 - \mathbb{E}[Y_i]\}$ , and thus  $n(Y_i - \mathbb{E}[Y_i]) \in [-n\mathbb{E}[Y_i], n(1 - \mathbb{E}[Y_i])]$ . Furthermore,  $\mathbb{E}[S_Y](X_i - \mathbb{E}[X_i]) \in (-\mathbb{E}[X]\mathbb{E}[S_Y], (1 - \mathbb{E}[X])\mathbb{E}[S_Y])$ . Finally, applying Hoeffding's Lemma (Lemma 1), we obtain line (17).  $\square$

Now we are ready to prove Theorem 8.

### C.1.2 Proof of Theorem 8

In this theorem, we assume that the number of confounded data is finite. Thus, instead of  $a_{yt}$ , we have estimates of them, namely  $\hat{a}_{yt}$ . Let  $n_{yt}$  denote the number of samples in the confounded data such that  $(Y = y, T = t)$ . Let  $m_{yt}^z$  be the number of samples in the deconfounded data such that  $(Y = y, T = t, Z = z)$ . Furthermore, let  $n = \sum_{y,t} n_{yt}$ ,  $m = \sum_{y,t,z} m_{yt}^z$ . Then, under our setup, we estimate  $a_{yt}$  and  $q_{yt}^z$  as follows:

$$\hat{a}_{yt} = \frac{n_{yt}}{n}, \quad \text{and} \quad \hat{q}_{yt}^z = \frac{m_{yt}^z}{\sum_z m_{yt}^z}.$$

Thus, following the proof of Theorem 1, we have

$$\begin{aligned} P\left(|\widehat{\text{ATE}} - \text{ATE}| < \epsilon\right) &\geq P\left(\bigcap_{t,z} \left\{|p_{1t}^z - \hat{p}_{1t}^z| < \frac{\sum_y p_{yt}^z}{5k}\epsilon\right\} \bigcap_{t,z} \left\{|p_{1t}^z + p_{0t}^z - \hat{p}_{1t}^z - \hat{p}_{0t}^z| < \frac{\sum_y p_{yt}^z}{5k}\epsilon\right\}\right) \\ &= P\left(\bigcap_{t,z} \left\{|a_{1t}q_{1t}^z - \hat{a}_{1t}\hat{q}_{1t}^z| < \frac{\sum_y a_{yt}q_{yt}^z}{5k}\epsilon\right\} \bigcap_{t,z} \left\{|a_{1t}q_{1t}^z + a_{0t}q_{0t}^z - \hat{a}_{1t}\hat{q}_{1t}^z - \hat{a}_{0t}\hat{q}_{0t}^z| < \frac{\sum_y a_{yt}q_{yt}^z}{5k}\epsilon\right\}\right). \end{aligned}$$

Notice that  $|a_{1t}q_{1t}^z + a_{0t}q_{0t}^z - \hat{a}_{1t}\hat{q}_{1t}^z - \hat{a}_{0t}\hat{q}_{0t}^z| < \frac{\sum_y a_{yt}q_{yt}^z}{5k}\epsilon$  is satisfied when both

$$|a_{1t}q_{1t}^z - \hat{a}_{1t}\hat{q}_{1t}^z| < \frac{\sum_y a_{yt}q_{yt}^z}{10k}\epsilon, \quad \text{and} \quad |a_{0t}q_{0t}^z - \hat{a}_{0t}\hat{q}_{0t}^z| < \frac{\sum_y a_{yt}q_{yt}^z}{10k}\epsilon.$$

We have:

$$\begin{aligned} P\left(|\widehat{\text{ATE}} - \text{ATE}| < \epsilon\right) &\geq P\left(\bigcap_{t,z} \left\{|a_{1t}q_{1t}^z - \hat{a}_{1t}\hat{q}_{1t}^z| < \frac{\sum_y a_{yt}q_{yt}^z}{10k}\epsilon\right\} \bigcap_{t,z} \left\{|a_{0t}q_{0t}^z - \hat{a}_{0t}\hat{q}_{0t}^z| < \frac{\sum_y a_{yt}q_{yt}^z}{10k}\epsilon\right\}\right) \\ &= P\left(\bigcap_{y,t,z} \left\{|a_{yt}q_{yt}^z - \hat{a}_{yt}\hat{q}_{yt}^z| < \frac{\sum_y a_{yt}q_{yt}^z}{10k}\epsilon\right\}\right). \end{aligned}$$

Lemma 5 suggests that

$$P(|a_{yt}q_{yt}^z - \hat{a}_{yt}\hat{q}_{yt}^z| \geq t) \leq 2 \exp\left(-\frac{2t^2}{\frac{1}{x_{yt}m} + \frac{(q_{yt}^z)^2}{n}}\right).$$

Thus, applying a union bound and Lemma 5, we have

$$\begin{aligned} P\left(|\widehat{\text{ATE}} - \text{ATE}| \geq \epsilon\right) &\leq \sum_{y,t,z} P\left(|a_{yt}q_{yt}^z - \hat{a}_{yt}\hat{q}_{yt}^z| < \frac{\sum_y a_{yt}q_{yt}^z}{10k} \epsilon\right) \\ &\leq 8k \max_{y,t,z} \exp\left(-2 \frac{\left(\sum_y a_{yt}q_{yt}^z\right)^2 \epsilon^2}{\left(\frac{1}{x_{yt}m} + \frac{(q_{yt}^z)^2}{n}\right) 100k^2}\right) \\ &\leq \delta. \end{aligned}$$

Simplifying the equations above, we have

$$\min_{y,t,z} \frac{\left(\sum_y a_{yt}q_{yt}^z\right)^2}{\left(\frac{1}{x_{yt}m} + \frac{(q_{yt}^z)^2}{n}\right)} \geq \frac{50k^2 \ln\left(\frac{8k}{\delta}\right)}{\epsilon^2}.$$

□

## D Corresponding Stories

In this section, we will provide an example for each selection method such that this particular sampling performs the worst when compared with the other two methods. For the purpose of illustration, we consider binary confounder throughout this section. To ease notation, let  $q_{yt}$  denote  $q_{yt}^1$ .

**A Scenario in Which NSP Performs the Worst** A drug repositioning start-up discovered that drug  $T$  can potentially cure a disease  $\gamma$ . which has no known drug cure and goes away without treatments once a while. Since drug  $T$  is commonly used to treat another disease  $\eta$ , the majority patients who has disease  $\gamma$  do not receive any treatment. Among the ones who received drug  $T$ , the start-up discovered that the health outcomes of the majority of patients have improved. The start-up proposes to bring drug  $T$  to an observational study to verify whether drug  $T$  could treat disease  $\gamma$  while not controlling for patient’s treatment adherence levels. As in most cases, patient’s treatment adherence levels could influence doctors’ decision of whether to prescribe drug  $T$  and whether the treatment for disease  $\gamma$  will be successful. Translating this scenario into our notations, we have  $a_{01} = \epsilon_1$ ,  $a_{10} = \epsilon_2$ ,  $a_{11} = \epsilon_3$ , and  $a_{00} = 1 - \sum_{i=1}^3 \epsilon_i$ , say  $\mathbf{a} = (0.9, 0.02, 0.01, 0.07)$ . Now, imagine in the clinical trial, the patients are given a drug case containing drug  $T$  such that the drug case automatically records the frequency that the patient takes the drug. Somehow we know a priori that the patients who do not have health improvement have on average poor treatment adherence, e.g.,  $q_{00} = 0.9$ ,  $q_{01} = 0.7$ ; furthermore, those who have health improvement on average have good treatment adherence, e.g.,  $q_{10} = 0.01$ ,  $q_{11} = 0.3$ . Deconfounding according to NSP, i.e.,  $\mathbf{x} = (a_{00}, a_{01}, a_{10}, a_{11})$ , in this case, will select most samples from the group ( $Y = 0, T = 0$ ). Since the ATE depends on the estimation that relies on both  $T = 0$ , and  $T = 1$ , one would expect that NSP and OWSP will outperform NSP. The left column in Figure 3 confirms this hypothesis.

**A Scenario in Which USP Performs the Worst** A group biostatisticians discovered that mutations on gene  $T$  is likely to cause cancer  $Y$  in patients with a particular type of heart disease. In particular, they discovered that among the those heart disease patients, 79% of patients have neither mutation on  $T$  nor cancer  $Y$ ; 18% patients have both mutation on  $T$  and cancer  $Y$ . In other words,  $a_{00} = 0.79$ ,  $a_{11} = 0.18$ . Furthermore, we have  $a_{01} = 0.01$ ,  $a_{10} = 0.02$ . This group of biostatisticians want to run a small experiment to confirm whether gene  $T$  causes cancer  $Y$ . In particular, they are interested in knowing whether those patients also have mutations on gene  $Z$ , which is also suspected by the same group of biostatisticians to cause cancer  $Y$ . Somehow, we know a priori that  $q_{00} = 0.5$ ,  $q_{01} = 0.01$ ,  $q_{10} = 0.05$ ,  $q_{11} = 0.5$ . From the calculation of the ATE, it is not difficult to observe that the error on the ATE is dominated by the estimation errors on  $q_{00}, q_{11}$ . Thus, we should sample more from the groups ( $Y = 0, T = 0$ ) and ( $Y = 1, T = 1$ ).

**A Scenario in Which OWSP Performs the Worst** A team wants to reposition drug  $T$  to cure diabetes. Drug  $T$  has been used to treat a common comorbid condition of diabetes that appears in 31% of the diabetic patient population. Among those patients who receive drug  $T$ , about 97% has improved health, that is  $a_{01} = 0.01$  and  $a_{11} = 0.3$ . Among the patients who have never received drug  $T$ , about 70% have no health improvement, that is  $a_{00} = 0.5$ , and  $a_{10} = 0.19$ . Let  $q_{00} = 0.05$ ,  $q_{01} = 0.5$ ,  $q_{10} = 0.055$ , and  $q_{11} = 0.4$ . In the ATE, it is easy to observe that  $\frac{a_{11}q_{11}}{a_{11}q_{11}+a_{01}q_{01}}$  and  $\frac{a_{11}(1-q_{11})}{a_{11}(1-q_{11})+a_{01}(1-q_{01})}$  are both dominated by 1 regardless of the estimates of  $q_{11}$  and  $q_{01}$ . In this case, USP outperforms OWSP and NSP when the sample size is larger than 200. On the other hand, the bottom figure in the third column of Figure 3 shows that, when averaged over all possible values of  $\mathbf{q}$ , OWSP performs the best.

## E Approximate Sampling Policies Under Finite Confounded Data

To deconfound according to NSP with finite confounded data is to deconfound the first  $m$  confounded data. For USP, we split the samples to the 4 groups as evenly as possible. That is, we max out the bottleneck group/groups and distribute the excess data as evenly as possible among the remaining groups.

For OWSP, we have  $x_{yt} = \frac{\hat{a}_{yt}}{\sum_y \hat{a}_{yt}}$ , and when implementing OWSP, we will first ensure that the deconfounded samples are split as evenly as possible across treatment groups, and then within the each group, we split the samples close as possible to the outcome ratio.