# Optimal Stratification of Survey Experiments\*

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March 1, 2024

#### Abstract

This paper studies a two-stage model of experimentation, where the researcher first samples representative units from an eligible pool, then assigns each sampled unit to treatment or control. To implement balanced sampling and assignment, we introduce a new family of finely stratified designs that generalize matched pairs randomization to propensities  $p(x) \neq 1/2$ . We show that two-stage stratification nonparametrically dampens the variance of treatment effect estimation. We formulate and solve the optimal stratification problem with heterogeneous costs and fixed budget, providing simple heuristics for the optimal design. In settings with pilot data, we show that implementing a consistent estimate of this design is also efficient, minimizing asymptotic variance subject to the budget constraint. We also provide new asymptotically exact inference methods, allowing experimenters to fully exploit the efficiency gains from both stratified sampling and assignment. An application to nine papers recently published in top economics journals demonstrates the value of our methods.

Keywords: Matched Pairs, Blocking, Survey Sampling, Robust Standard Error, Treatment Effects.

*JEL Codes*: C10, C14, C90

<sup>\*</sup>I wish to thank Alberto Abadie, Anna Mikusheva, and Victor Chernozhukov for their support and guidance during this project. This paper also benefited from conversations with Isaiah Andrews, Mert Demirer, and numerous seminar participants. The current work replaces an earlier version of my job market paper titled "Designing Representative and Balanced Experiments by Local Randomization."

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#### 1 Introduction

Randomized controlled trials (RCTs) are now common in economics research, with thousands of active experiments in the AEA RCT registry spanning a wide range of fields. A key objective of experimental design is to reduce the variance of treatment effect estimation, helping applied researchers make the most efficient use of their limited resources. One way to do this is by covariate-adaptive treatment assignment, which balances observed covariates between the treatment and control group at design-time. This paper contributes to theory of covariate-adaptive treatment assignment, but also models a new dimension of experimental design: the selection of the experimental participants.

The selection of participants, also known as the sampling frame, is an important step in designing an experiment. For example, Abaluck et al. (2021) run an experiment to estimate the effect of mask distribution on covid infection rates in Bangladesh. From a pool of 1000 eligible villages, they first randomly sample 600 to be included in the experiment, then assign the sampled villages to various interventions that promote mask usage. Similarly, Breza et al. (2021) estimate the effect of Facebook ads discouraging holiday travel on covid infection rates. Since their budget for running ads is finite, they first sample a small set of counties in which to run ads and collect outcome data, then randomly assign these sampled counties to low or high intensity of treatment. We show how to increase the efficiency of treatment effect estimation by sampling experimental units that are representative of the broader target population, and provide new inference methods that take full advantage of these precision gains.

To do so, this paper introduces a new family of finely stratified randomization procedures that can be used for both representative sampling of the experimental units and finely balanced treatment assignment. When used for assignment, our method generalizes the principle of matched pairs randomization to propensities  $p(x) \neq 1/2$ , allowing discrete or continuous stratification variables in general dimension. The basic building block is a new algorithm that matches the experimental units into homogeneous groups of k by minimizing an objective function directly linked to estimation efficiency. This matching algorithm also enables finely stratified sampling of the experimental participants. For example, suppose 1000 people respond to an advertisement to participate in an experiment, but the experimental budget only allows for 200 participants. Using observed covariate information, we match the units into homogeneous 5-tuples, sampling q = 1/5 of the units in each tuple to participate, uniformly at random. By finely representing the distribution of treatment effect heterogeneity in the population into

our smaller experiment, this sampling procedure reduces the variance due to treatment effect heterogeneity. More generally, we provide finely stratified designs implementing heterogeneous sampling propensities q(x).

We study a two-stage procedure that (1) samples participants then (2) assigns treatments to the sampled units, using finely stratified designs at both stages. Under finely stratified treatment assignment alone, the difference-of-means estimator  $Y \sim 1 + D$  achieves the Hahn (1998) variance bound for the average treatment effect (ATE), effectively doing nonparametric regression adjustment "by design." Our analysis shows that finely stratified sampling provides an additional nonparametric variance reduction, dampening the variance due to treatment effect heterogeneity. In particular, representative sampling makes this variance component scale with the the number of units we sample from, rather than the smaller true experiment size, boosting the effective sample size for this component of the variance. Extending recent results in Bai (2022), we characterize the optimal stratification variables for sampling and assignment, showing that for sampling one wants to stratify on covariates that are most predictive of treatment effect heterogeneity. In an extension, we also study estimation of the sample average treatment effect (SATE) over the eligible population using design-based asymptotics.

Building on these asymptotic results, we formalize and solve an optimal design problem with fixed experimental budget and heterogeneous costs. In development economics, the cost of including a village in an experiment can vary widely based on observable characteristics such as its distance from the urban center, village size and so on. This forces applied researchers to choose a tradeoff between sample size and sample representativeness when they select where to experiment. We propose a new formalization of this tradeoff, deriving the jointly optimal sampling intensity  $q^*(x)$  and assignment propensity  $p^*(x)$  under finely stratified randomization. Our results provide simple heuristics for optimal sampling of the experimental units, analogous to classical results on sample allocation for coarsely stratified survey design (Cochran (1977)). Under homoskedasticity, for instance, the optimal sampling propensity  $q^*(x) \propto C(x)^{-1/2}$ , where C(x) is the cost of including a unit of type X = x in the experiment. We show that an oracle design that implements discretizations of  $q^*(x)$  and  $p^*(x)$  using fine stratification minimizes the asymptotic variance of our estimator over all stratified designs, subject to the experimental budget constraint.

We also briefly investigate exact optimality in finite samples. For fixed propensity p = 1/2, we prove that the globally optimal covariate-adaptive randomization takes the

form of a novel "alternating design", assigning a certain optimal allocation vector  $(d_i^*)_{i=1}^n$  and its mirror image  $(1-d_i^*)_{i=1}^n$  each with probability 1/2. The optimal allocation  $(d_i^*)_{i=1}^n$  solves the well-known Max-Cut graph partitioning problem (Rendl et al. (2008)), with edge weights related to the smoothness of the outome functions.

We apply our optimal stratification results to the problem of two-wave design using data from a pilot experiment, providing the first fully efficient solution to this problem. The basic idea is to estimate the optimal sampling and assignment propensities  $q^*(x)$  and  $p^*(x)$  using the pilot, then implement these estimates in the main experiment using fine stratification. Under large pilot asymptotics, this strategy is as efficient as the oracle design, achieving the budget-constrained minimal asymptotic variance. We also provide results under fixed pilot asymptotics, and briefly discuss potential robustifications. In the case without sampling, the problem of design using a pilot has received considerable attention in the recent literature, see for instance Hahn et al. (2011), Tabord-Meehan (2022), and Bai (2022), and we give a detailed comparison with these results.

Finally, we provide novel asymptotically exact inference for the average treatment effect under joint finely stratified sampling and assignment, using a collapsed-strata<sup>1</sup> type estimator (Hansen et al. (1953)). These inference methods allow experimenters to fully exploit the efficiency gains from both finely stratified sampling and assignment. The use of non-constant sampling proportions q(x) produces discontinuities in the propensity-weighted outcome functions, introducing new technical challenges relative to previous work. Simulations and an empirical application to N = 9 papers recently published in top journals in economics demonstrate the value of our proposed methods.

#### 1.1 Related Literature

Our sampling model is related to the classical literature on survey sampling, e.g. as surveyed in Cochran (1977) and Lohr (2021). Yang et al. (2021) propose a two-stage design using rerandomization for both sampling and assignment.<sup>2</sup> Under rerandomization, difference-of-means estimation is asymptotically slightly less efficient than ex-post linear covariate adjustment. By contrast, we show that two-stage fine stratification is asymptotically equivalent to nonparametric covariate adjustment for the imbalances in both the sampling and assignment variables. Theorem 3.12 provides a formal equivalence

<sup>&</sup>lt;sup>1</sup>See also Abadie and Imbens (2008) and Bai et al. (2021) for related results in the context of matched pairs assignment.

<sup>&</sup>lt;sup>2</sup>This work is contemporaneous with the original version of our paper in Cytrynbaum (2021).

statement.

For an overview of experimental design theory, see Rosenberger and Lachin (2016) or Athey and Imbens (2017). A representative sample of recent work on stratified treatment assignment includes Imai et al. (2009), Bugni et al. (2018), Fogarty (2018), Wang et al. (2021), Bai et al. (2021), de Chaisemartin and Ramirez-Cuellar (2021), Bai (2022), and Tabord-Meehan (2022). For treatment assignment, our work is most related to Bai (2022), who introduces finely stratified designs for constant propensity p = a/k and univariate stratification variables, with inference for the case p = 1/2. Aside from stratification, other recent proposals for balanced treatment assignment include Kasy (2016), Kallus (2017), Li et al. (2018), Krieger et al. (2019), and Harshaw et al. (2021). We explicitly compare with some of these methods in Remark 3.4.

Our results on design using a pilot study is related to previous results in Hahn et al. (2011), Bai (2022), Tabord-Meehan (2022), and Kasy and Sautmann (2021). We provide detailed comparisons in Section 6 below. Our inference results are related to the method of collapsed-strata in Hansen et al. (1953) and its modern variants studied in Abadie and Imbens (2008) and Bai et al. (2021).

The rest of the paper is organized as follows. Section 2 introduces notation and discusses our matching algorithm. Section 3 states our main asymptotic results, including the equivalence with nonparametric adjustment. Section 4 formalizes and solves the optimal stratification and finite sample optimal design problems. Section 6 discusses design using a pilot study. Section 7 provides our inference methods. Our empirical results are presented in Section 8, and recommendations for practice in Section 9.

## 2 Motivation and Description of Method

Consider running an experiment to estimate the average treatment effect (ATE). There are n eligible units, with observed baseline covariates  $(X_i)_{i=1}^n$ . We wish to sample proportion  $q \in (0,1]$  of these units to participate in the experiment. Denote  $T_i = 1$  if a unit is sampled and  $T_i = 0$  otherwise. Sampled units are then assigned to treatment or control  $D_i \in \{0,1\}$ . Let  $Y_i(d)$  denote the potential outcome of unit i for  $d \in \{0,1\}$ .

Since outcomes are only observed for participating units<sup>3</sup> we may write

$$Y_i = T_i[D_iY_i(1) + (1 - D_i)Y_i(0)].$$

We focus on estimation and inference for the population ATE = E[Y(1) - Y(0)], modeling the n eligible units  $(X_i, Y_i(0), Y_i(1))_{i=1}^n \sim F$  as an iid sample from a superpopulation of interest. For example, the eligible units could be n = 1000 respondents to an online advertisement to participate in an experiment with a budget constraint of 100 participants. In this context, the variable  $T_i \in \{0,1\}$  models which of the n = 1000 units we choose to include in the experiment. In some applications, the eligible units may comprise the entire population of interest. For example, the units  $i = 1, \ldots, n$  may be the entire population of villages in a country, which we sample to obtain the participating villages. To accommodate such applications, Section 10.1 in the appendix presents design-based versions of our main results, targeting the sample average treatment effect SATE  $= n^{-1} \sum_{i=1}^{n} Y_i(1) - Y_i(0)$  in the eligible population. Here, we define the SATE over the entire eligible population  $i = 1, \ldots, n$  that we are allowed to sample from, not just the smaller set of units that are chosen to participate in the experiment  $\{i: T_i = 1\}$ .

Our goal is to sample a representative subset of the eligible units and assign them to treatment and control in a way that finely balances the baseline covariates  $(X_i)_{i=1}^n$ . To do so, we introduce a new family of finely stratified designs that generalize the principle of matched pairs randomization to arbitary propensity scores p(x) = P(D = 1|X = x), with continuous or discrete covariates in general dimension. We also use these new designs for finely stratified sampling, allowing us to implement arbitrary heterogeneous sampling propensities q(x) = P(T = 1|X = x), while finely balancing covariates between the sampled and non-sampled units. The basic building block of our method is a matched k-tuples design, which uses the baseline covariates to match units into homogeneous groups of k, randomly assigning a out of k units in each group to T = 1 during sampling or D = 1 during assignment. We formally define the method in the context of finely stratified sampling in the next definition.

**Definition 2.1** (Local Randomization). Let q = a/k with gcd(a, k) = 1. Partition the eligible units into groups with |g| = k, so that  $\{1, \ldots, n\} = \bigcup_g g$  disjointly. In general, there may be one remainder group with |g| < k. Let  $\psi(X) \in \mathbb{R}^d$  be a vector of

<sup>&</sup>lt;sup>3</sup>If control outcomes are costlessly observed for all units, the sampling problem becomes trivial. We still contribute novel assignment designs in this case.

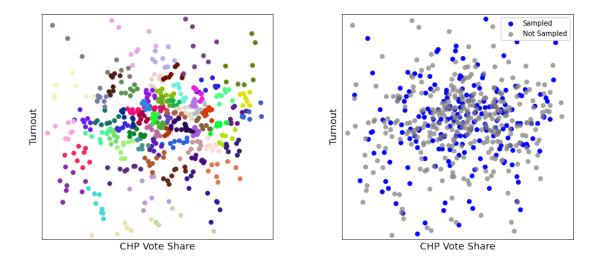


Figure 1: Sampling groups and variables for  $T_{1:n} \sim \text{Loc}(\psi, q)$  with q = 3/8.

stratification variables, and suppose that the groups are homogeneous in the sense that

$$n^{-1} \sum_{q} \sum_{i,j \in q} |\psi(X_i) - \psi(X_j)|_2^2 = o_p(1)$$
(2.1)

Require that the groups only depend on the stratification variable values  $\psi_{1:n} = (\psi(X_i))_{i=1}^n$ , and data-independent randomness  $\pi_n$ , so that  $g = g(\psi_{1:n}, \pi_n)$ . Independently over all groups with |g| = k, draw sampling variables  $(T_i)_{i \in g}$  by setting  $T_i = 1$  for exactly a out of k units, completely at random. For units in the remainder group with |g| < k, draw  $T_i$  iid with  $P(T_i = 1) = a/k$ . We say that such a design implements q locally with respect to  $\psi(x)$ , denoting  $T_{1:n} \sim \text{Loc}(\psi, q)$ .

Remark 2.2. Equation 2.1 was introduced in Bai et al. (2021) for matched pairs treatment assignment, k=2 (without stratified sampling). Bai (2022) justifies Equation 2.1 for p=a/k and  $\dim(\psi)=1$  by stratifying on sorted covariate values. We extend such results to multivariate stratification at both the sampling and assignment stages  $(\dim(\psi) \neq 1)$ , deriving novel rates even for the classical case of matched pairs. In Section 3.2, we further extend this definition to allow  $T_{1:n} \sim \operatorname{Loc}(\psi, q(\psi))$ , with non-constant propensity  $q(\psi)$ , characterizing the efficient  $q(\psi)$  in a model with heterogeneous sampling costs in Section 4. Our theory uses novel asymptotics where group size  $k_n$  and number of propensity levels  $|L_n| = |\operatorname{Image}(q(\cdot))|$  may grow with n.

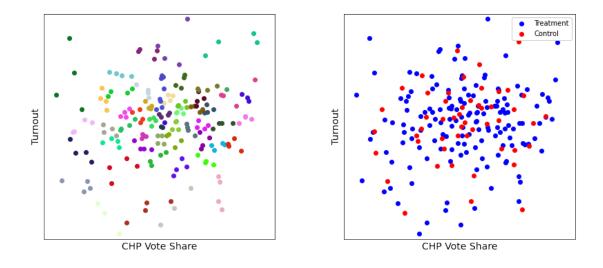


Figure 2: Assignment groups and variables for  $D_{1:n} \sim \text{Loc}(\psi, p)$  with p = 3/4.

We discuss matching algorithms and their associated homogeneity rates in Section 2.1 below. Consider sampling and assignment propensities q = a/k and p = a'/k'. In the rest of the paper, we study treatment effect estimation under a two-stage procedure:

- (1) Sample eligible units  $T_{1:n} \sim \text{Loc}(\psi, q)$ .
- (2) Assign treatments  $D_{1:n} \sim \text{Loc}(\psi, p)$  to the sampled units  $\{i : T_i = 1\}$ .

This two-stage procedure is illustrated in Figures 1 and 2, using data from an election experiment in Turkey reported in Baysan (2022). Each color represents a different group of units formed during sampling and assignment. For example, in Figure 1 we form groups of size |g| = 8, randomly sampling 3 out of 8 units from each group to "represent" that group in the experiment. The sampled units are shown in blue in the figure on the right. In figure 2, we match the sampled units into groups of k' = 4, assigning 3 out of 4 to D = 1 in each group.

Section 3.2 presents the most general version of our method, allowing different stratification variables  $\psi_1$  and  $\psi_2$  to be used for sampling and assignment, as well as varying sampling and assignment propensities q(x), p(x). Optimal choice of stratification variables for sampling and assignment is discussed in Section 3. Our framework enables unified asymptotics and inference for a wide variety of different designs, as shown in the examples below.

**Example 2.3** (Matched Tuples). Suppose n=1000 individuals from a target population sign up to participate in an experiment, providing basic demographic information  $(X_i)_{i=1}^n$ . There are only resources for 300 units to be enrolled, so q=3/10. Among these 300 units, p=1/4 will be assigned to the more costly treatment and 3/4 to control. We sample using the design  $T_{1:n} \sim \text{Loc}(\psi, 3/10)$ , which matches the 1000 eligible units into homogeneous groups of 10 and randomly sets  $T_i=1$  for 3 out of 10 units in each group. We assign treatments  $D_{1:n} \sim \text{Loc}(\psi, 1/4)$  to the  $\sum_i T_i = 300$  sampled units, matching them into homogeneous tuples of four and assigning 1 out of 4 in each tuple to  $D_i=1$ .

Example 2.4 (Complete Randomization). We say that variables  $T_{1:n}$  are completely randomized with probability q if  $T_{1:n}$  is drawn uniformly from all vectors  $t_{1:n}$  with  $t_i = 1$  for exactly proportion q of the units. Formally, we have  $P(T_{1:n} = t_{1:n}) = 1/\binom{n}{qn}$  for all such vectors. We denote  $T_{1:n} \sim \operatorname{CR}(q)$  and  $D_{1:n} \sim \operatorname{CR}(p)$  for sampling and assignment, respectively. Complete randomization may be obtained in our framework by setting  $\psi = 1$  and forming groups |g| = k at random, which automatically satisfies Equation 2.1. For example, assigning 2 out of 3 units in each group to treatment gives a "random matched triples" representation of complete randomization with p = 2/3. Proposition 9.15 in the original version of this paper (Cytrynbaum (2021)) provides a formal equivalence result, and our theory explicitly accounts for this extra randomness.

**Example 2.5** (Coarse Stratification). The procedure in Definition 2.1 produces n/k groups of k units that are tightly matched in  $\psi(X)$  space, suggesting fine stratification. However, coarsely stratified designs with a fixed strata  $S(X) \in \{1, ..., m\}$  can also be obtained in this framework by setting  $\psi(X) = S(X)$  and matching units with the same S(X) value into groups at random. Coarse stratification was previously studied using different methods in Bugni et al. (2018). We extend their results in Example 3.5 below, allowing coarse stratification at both the sampling and assignment stages.

Remark 2.6 (Sampling Centroids). It's also possible to reverse the order of our two-stage procedure. For example, if q = a/k and p = a'/k' we can first match the eligible units  $i = 1, \ldots, n$  into groups of size k', forming the group centroids  $\bar{\psi}_g = (k')^{-1} \sum_{i \in g} \psi_i$ . Next, we match these group centroids themselves into homogeneous groups of size k. For each group of k centroids, we randomly sample a of the centroids, and their corresponding groups of k' units, into the experiment. Finally, we assign a' out of k' units in each sampled group to treatment. Intuitively, this procedure allocates more of the finite "match quality" in the data set towards balanced assignment, making the assignment groups as tight as possible. We conjecture that this procedure is asymptotically

equivalent to the one studied in this paper, but leave formal study to future work.

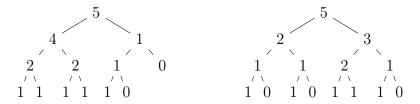
#### 2.1 Matching Algorithms

One possibility is to treat the left hand side of Equation 2.1 as an objective function and minimize it over all partitions of the units into groups of k. Denoting  $d(\psi) = \dim(\psi)$ , Theorem A.1 in the appendix shows that if  $E[|\psi(X)|_2^{\alpha}] < \infty$  for some  $\alpha > d(\psi) + 1$  then the optimal groups satisfy

$$\min_{(g)} n^{-1} \sum_{g} \sum_{i,j \in g} |\psi_i - \psi_j|_2^2 = O_p(n^{2/\alpha - 2/(d(\psi) + 1)}) = o_p(1)$$
(2.2)

If  $\psi(X)$  is bounded this becomes  $O_p(n^{-2/(d(\psi)+1)})$ , sharpening the rate achieved under a boundedness assumption in previous work on matched pairs (Bai et al. (2021)). For k=2, the optimal groups are computable in  $O(n^3)$  time using an algorithm due to Derigs (1988).<sup>4</sup> Efficient algorithms for computing the optimal groups for general k are not available, and we expect the problem to be NP-hard.<sup>5</sup>

Iterative Matching - Instead of calculating the optimal partition, for k > 2 we iteratively apply Derigs' algorithm to match units into larger groups. For fixed k, this procedure can be shown to satisfy the same rate in Equation 2.2 above. There are many ways to implement iterative pairing for each k. For example, k = 5 can be obtained by pairwise matching of 4-tuples to 1-tuples, or 3-tuples to 2-tuples and so on. This is shown in the figure below, where each level of the tree represents a call to the optimal pairing algorithm.



Before the jth algorithm call, we add a certain number of "empty centroids", represented by the 0's in the figure. We also prohibit certain types of matches in order to guarantee the desired sequence of group sizes. For example, at the second level of the tree on the left, we set the distance to  $+\infty$  between groups of size |g| = 2 and |g'| = 1,

<sup>&</sup>lt;sup>4</sup>We use the min-weight-matching implementation from the NetworkX 3.1 module in Python.

<sup>&</sup>lt;sup>5</sup>See Karmakar (2022) for hardness results in a related problem.

size |g| = 1 and |g'| = 1, and size |g| = 0 and |g'| = 0. There are many choices of such cardinality trees for each k, not all of which can be feasibly implemented using these type of constraints. We provide a canonical way of generating such sequences, as well as the required constraints at each algorithm call, that is guaranteed to implement the desired group cardinality k. Technical details are provided in Section 10.2 in the appendix.

Large Experiments. This algorithm is highly tractable for small and medium experiment sizes. For example, matching n = 500 units into 5-tuples takes 23 seconds on a laptop computer, while n = 2000 takes about 24 minutes. However, larger experiments quickly become intractable. For example, Domurat et al. (2021) has n = 87394, which would take about 3.8 years to match using the algorithm described above. To enable fine stratification in larger experiments, one possibility is to exploit the global shape of the baseline covariate data to rule out matches between distant units. To do so, let  $v_1$  be the first principal component of the stratification variables  $(\psi_i)_{i=1}^n$  and consider the following procedure:

- (1) Partition  $(\psi_i)_{i=1}^n$  into K folds by (1/K)th quantile of the sorted projections  $v_1'\psi_i$ .
- (2) Separately in each fold, run the iterative Derigs (1988) procedure above.

Intuitively, we use the first principal component to sort units by their projection along a natural "direction" through the dataset. This exploits the idea that good matches are unlikely between non-adjacent folds: Figure 4 in the appendix gives a visual representation. By parallelizing over K=80 folds, a dataset of size n=87394 can be matched about 5 minutes. The original version of our procedure and this "PCA folds" version are asymptotically equivalent for fixed K. We focus on the original version in the theory that follows.

## 3 Asymptotic Theory

This section contains our main asymptotic results, showing nonparametric efficiency gains from both finely stratified sampling and assignment. First, we state our main assumption.

**Assumption 3.1.** The moments  $E[Y(d)^2] < \infty$  for d = 0, 1 and  $E[|\psi(X)|_2^{\alpha}] < \infty$  hold for some  $\alpha > \dim(\psi) + 1$ .

Previous work on fine stratification has required Lipschitz continuity of the outcome function  $E[Y(d)|\psi(X)=\psi]$  and variance  $Var(Y(d)|\psi(X)=\psi)$ , as well as boundedness of the stratification variables  $\psi(X)$ .<sup>6</sup> We provide a novel technical analysis that allows all of these assumptions to be removed.

Estimation. Let  $\widehat{\theta}$  be the regression coefficient on  $D_i$  in  $Y_i \sim 1 + D_i$ , estimated in the sampled units  $\{i: T_i = 1\}$ . This is just the usual difference-of-means estimator. Before continuing to our asymptotic results, we state a variance decomposition for  $\widehat{\theta}$  that will be used extensively in what follows. Let  $c(\psi) = E[Y(1) - Y(0)|\psi(X) = \psi]$  denote the conditional average treatment effect (CATE) and  $\sigma_d^2(\psi) = \text{Var}(Y(d)|\psi(X) = \psi)$  the heteroskedasticity function. Define the balance function

$$b(\psi; p) = E[Y(1)|\psi(X)] \left(\frac{1-p}{p}\right)^{1/2} + E[Y(0)|\psi(X)] \left(\frac{p}{1-p}\right)^{1/2}.$$
 (3.1)

Suppose that sampling and assignment are both completely randomized,  $T_{1:n} \sim \operatorname{CR}(q)$  and  $D_{1:n} \sim \operatorname{CR}(p)$ , as in Example 2.4. Let  $n_T = \sum_i T_i$  denote the experiment size. Our work shows that  $\sqrt{n_T}(\widehat{\theta} - \operatorname{ATE}) \Rightarrow \mathcal{N}(0, V)$  with variance

$$V = \operatorname{Var}(c(\psi)) + \operatorname{Var}(b(\psi; p)) + E\left[\frac{\sigma_1^2(\psi)}{p} + \frac{\sigma_0^2(\psi)}{1-p}\right]. \tag{3.2}$$

We think of the first term as the variance due to treatment effect heterogeneity, in particular, the heterogeneity predictable by the stratification variables. The second term is the variance due to random assignment, which arises from the chance covariate imbalances between treatment and control units created by complete randomization  $D_{1:n} \sim CR(p)$ . The results in the next section show how stratified sampling and assignment nonparametrically dampen the each component of this variance expansion.

### 3.1 Constant Sampling and Assignment Propensities

In this section we state a central limit theorem for ATE estimation for the simplest case where the sampling and assignment propensities q = a/k and p = a'/k' are constant. This result quantifies the efficiency gains from stratification in each stage of the design. Remarks 3.7 and 3.9 draw connections between our findings and classical results on semi-parametric efficiency in the analysis of observational data. Section 3.2 below provides

<sup>&</sup>lt;sup>6</sup>For example, see Bai et al. (2021), Bai et al. (2023).

the most general version of the results in this section.

**Theorem 3.2.** Require Assumption 3.1. If sampling and assignment designs are locally randomized  $T_{1:n} \sim \text{Loc}(\psi, q)$  and  $D_{1:n} \sim \text{Loc}(\psi, p)$ , then  $\sqrt{n_T}(\widehat{\theta} - \text{ATE}) \Rightarrow \mathcal{N}(0, V)$ 

$$V = q \operatorname{Var}(c(\psi)) + E\left[\frac{\sigma_1^2(\psi)}{p} + \frac{\sigma_0^2(\psi)}{1-p}\right].$$

Comparing to Equation 3.2 above, the variance component  $\operatorname{Var}(b(\psi;p))$  due to covariate imbalance between the treatment arms is now asymptotically negligible. The variance due to treatment effect heterogeneity  $\operatorname{Var}(c(\psi))$  is now dampened by the sampling proportion  $q \in (0,1]$ . To see why, observe that the normalization  $\sqrt{n_T}(\widehat{\theta} - \operatorname{ATE})$  effectively holds the experiment size  $n_T$  constant as we vary q. Holding  $n_T$  constant, the number of eligible units  $n \approx n_T/q$  grows as  $q \to 0$ . For small q, there are many eligible units to sample from, allowing us to choose a highly representative sample of experimental participants. Our theory shows that this reduces the variance due to treatment effect heterogeneity that is predictable by the stratification variables. Another way to understand this is that under finely stratified sampling, the first variance component scales with the larger size n of eligible units, rather than the true experiment size  $n_T$ . This effectively "boosts" the experiment size for this component of the variance.

**Example 3.3** (Matched Tuples). In Example 2.3 above, we sampled  $n_T = 300$  of n = 1000 eligible units using the stratified design  $T_{1:n} \sim \text{Loc}(\psi, q)$  with q = 3/10. Next, we assigned 1/4 of the sampled units to treatment by  $D_{1:n} \sim \text{Loc}(\psi, 1/4)$ . Theorem 3.2 shows that under this design  $\sqrt{n_T}(\widehat{\theta} - \text{ATE}) \Rightarrow \mathcal{N}(0, V)$  with asymptotic variance

$$V = (3/10) \operatorname{Var}(c(\psi)) + E \left[ \frac{\sigma_1^2(\psi)}{1/4} + \frac{\sigma_0^2(\psi)}{3/4} \right].$$

Nonparametric Regression by Design. If q = 1 or sampling is completely randomized  $T_{1:n} \sim CR(q)^7$  then the asymptotic variance in Theorem 3.2 is

$$V = \operatorname{Var}(c(\psi)) + E\left[\frac{\sigma_1^2(\psi)}{p} + \frac{\sigma_0^2(\psi)}{1-p}\right].$$

This is exactly the Hahn (1998) semiparametric variance bound for ATE with iid observations  $(Y, D, \psi(X))$ . We achieve the semiparametric variance bound with a simple

<sup>&</sup>lt;sup>7</sup>The latter statement follows from the more general results in Section 3.2.

<sup>&</sup>lt;sup>8</sup>Recent work in Armstrong (2022) shows that this efficiency bound also holds in settings with

difference-of-means estimator, without the need for nonparametric re-estimation of the known propensity (Hirano et al. (2003)) or covariate adjustment with well-specified outcome models (Robins and Rotnitzky (1995)). We can interpret this result as saying that finely stratified treatment assignment  $D_{1:n} \sim \text{Loc}(\psi, p)$  does nonparametric covariate adjustment "by design." See Theorem 3.12 below for a more formal equivalence result.

Representative Sampling. If sampling is locally randomized  $T_{1:n} \sim \operatorname{Loc}(\psi, q)$ , then the variance due to treatment effect heterogeneity decreases from  $\operatorname{Var}(c(\psi))$  to  $q\operatorname{Var}(c(\psi))$ . In this case, V can be strictly smaller than the classical semiparametric variance bound. Intuitively, by using the additional covariates  $(\psi(X_i))_{i=1}^n$  to select a representative sample, we finely represent the distribution of treatment effect levels  $(c(\psi_i))_{i=1}^n$  in the larger eligible population into our experiment. More formally, consider an oracle setting where we observe the treatment effect level  $c(\psi_i)$  for each sampled unit  $T_i = 1$ , estimating the ATE by the sampled average  $\hat{\theta} = (1/n_T) \sum_i T_i c(\psi_i)$ . Our analysis shows that if  $T_{1:n} \sim \operatorname{Loc}(\psi, q)$  then

$$(1/n_T)\sum_{i=1}^n T_i c(\psi_i) = E_n[c(\psi_i)] + o_p(n^{-1/2}).$$

Because of this, the sampled average  $(1/n_T) \sum_i T_i c(\psi_i)$  behaves like the infeasible average  $E_n[c(\psi_i)]$  over all eligible units, including those not sampled into the experiment. This nonparametrically dampens the variance due to treatment effect heterogeneity from  $\operatorname{Var}(c(\psi))$  to  $q \operatorname{Var}(c(\psi))$  for  $q \in (0,1]$ .

Remark 3.4 (Comparison with Other Designs). For the case without sampling, we can compare our results on fine stratification to other covariate-adaptive assignment designs. Li et al. (2018) shows that under rerandomized treatment assignment,  $\hat{\theta}$  is asymptotically (almost) as efficient as interacted linear regression adjustment, effectively doing linear regression "by design." Bugni et al. (2019) show that coarsely stratified assignment  $\psi(X) \in \{1, ..., m\}$  is asymptotically equivalent to an interacted linear regression adjustment that includes all strata indicators as covariates. Harshaw et al. (2021) suggest a novel Gram-Schmidt walk design with MSE bounded by a quantity related to linear ridge regression. By contrast, we show that the fine stratification  $D_{1:n} \sim \text{Loc}(\psi, p)$  does nonparametric regression adjustment by design.

Extending Bugni et al. (2019), the next example proves an equivalence between covariate-adaptive randomization, including the designs considered here.

coarse stratification and linear regression adjustment in the case where sampling and asignment are both coarsely stratified.

**Example 3.5** (Coarse Stratification). If  $T_{1:n} \sim \text{Loc}(S,q)$  and  $D_{1:n} \sim \text{Loc}(S,p)$  for a fixed stratification  $S(X) \in \{1,\ldots,m\}$ , Theorem 3.2 shows that  $\sqrt{n_T}(\widehat{\theta} - \text{ATE}) \Rightarrow \mathcal{N}(0,V_S)$  with variance

$$V_S = q \operatorname{Var}(c(S)) + E \left[ \frac{\sigma_1^2(S)}{p} + \frac{\sigma_0^2(S)}{1-p} \right].$$
 (3.3)

Alternatively, suppose sampling  $T_{1:n} \sim \operatorname{CR}(q)$  and assignment  $D_{1:n} \sim \operatorname{CR}(p)$  are completely randomized (Example 2.4), and we instead estimate the ATE using ex-post linear adjustment for the covariate imbalances due to both sampling and assignment. To define the adjustment, let  $z_i = (\mathbb{1}(S_i = k))_{k=1}^{m-1}$  denote leave-one-out strata indicators and their de-meaned versions  $\tilde{z}_i = z_i - E_n[z_i|T_i = 1]$ . Consider the linear regression  $Y \sim 1 + D + \tilde{z} + D\tilde{z}$  and let  $\hat{\tau}$  denote the coefficient on D and  $\hat{\beta}$  the coefficient on  $D\tilde{z}$ . Define the sampled covariate mean  $\bar{z}_{T=1} = E_n[z_i|T_i = 1]$  and eligible covariate mean  $\bar{z} = E_n[z_i]$  and consider the doubly-adjusted estimator

$$\widehat{\theta}_{adj} = \widehat{\tau} - \widehat{\beta}'(\bar{z}_{T=1} - \bar{z}). \tag{3.4}$$

We study this estimator in the next theorem.

**Theorem 3.6** (Regression Equivalence). Assume  $E[Y(d)^2] < \infty$  and P(S = k) > 0 for all  $k \in [m]$ . If  $T_{1:n} \sim \operatorname{CR}(q)$  and  $D_{1:n} \sim \operatorname{CR}(p)$  then  $\sqrt{n_T}(\widehat{\theta}_{adj} - \operatorname{ATE}) \Rightarrow \mathcal{N}(0, V_S)$  with  $V_S$  the coarsely stratified variance in Equation 3.5.

This result shows that under coarsely stratified sampling and assignment, the simple difference-of-means estimator  $\hat{\theta}$  behaves like the doubly-adjusted estimator  $\hat{\theta}_{adj}$  under complete randomization. Theorem 3.12 in the next section generalizes this example to the case of fine stratification and nonparametric double adjustment for both sampling and assignment imbalances. The remainder of this subsection provides more intuition for Theorem 3.2, connecting our results on fine stratification to the previous literature on semiparametric efficiency.

Remark 3.7 (Efficient Influence Function). Consider expanding the difference-of-means estimator  $\hat{\theta}$  about the efficient influence function for the ATE. Denote the nonparametric regression residuals  $\epsilon_i^d = Y_i(d) - E[Y_i(d)|\psi_i]$ . Under locally randomized sampling and

assignment

$$\widehat{\theta} = E_n[c(\psi_i)] + E_n \left[ \frac{D_i \epsilon_i^1}{p} + \frac{(1 - D_i) \epsilon_i^0}{1 - p} \middle| T_i = 1 \right] + \underbrace{\text{Cov}_n(T_i, c(\psi_i))}_{\text{Sampling}} / q + \underbrace{\text{Cov}_n(D_i, b(\psi_i) \middle| T_i = 1)}_{\text{Assignment}} / c_p + O_p(n^{-1}).$$

If  $T_i = 1$  for i = 1, ..., n then the first two terms are exactly the efficient influence function for the ATE. The third term is the estimator error due to correlation between the sampling variables  $T_i$  and treatment effect heterogeneity  $c(\psi_i)$  among the eligible units. The fourth term is the estimator error due to correlation between treatment assignments  $D_i$  and outcome heterogeneity among the sampled units. Without stratification, the chance covariate imbalances produce by randomization contribute non-negligible asymptotic variance, and the errors  $\sqrt{n} \operatorname{Cov}_n(T_i, c(\psi_i)) \Rightarrow \mathcal{N}(0, v)$  with v > 0. By contrast, we show that if  $T_{1:n} \sim \operatorname{Loc}(\psi, q)$  then the sampling errors  $\sqrt{n} \operatorname{Cov}_n(T_i, F(\psi_i)) = o_p(1)$  for any function  $E[F(\psi)^2] < \infty$ , and similarly for the assignment term. Because of this, the unadjusted estimator  $\hat{\theta}$  is first-order equivalent to the efficient influence function for the ATE under local randomization if q = 1. If q < 1, the situation is even better, and the first term behaves like the infeasible average  $E_n[c(\psi_i)]$  over all eligible units.

Remark 3.8 (Table One). Applied researchers often report tests of covariate balance in "table one." Consider testing for balance of a covariate  $F(\psi_i)$ . One common approach is to report a p-value for the test that  $\beta = 0$  in the regression  $F(\psi_i) = \hat{a} + \hat{\beta}D_i + e_i$ , using the normal limit  $\sqrt{n}\hat{\beta} \Rightarrow \mathcal{N}(0,v)$ . By contrast, if  $D_{1:n} \sim \text{Loc}(\psi,p)$  then  $\sqrt{n}\hat{\beta} = o_p(1)$  for any covariate  $E[F(\psi)^2] < \infty$ , showing that the level of such a test converges to zero. Intuitively, this shows that fine stratification with respect to  $\psi(X)$  balances any square-integrable transformation  $F(\psi)$  to order  $o_p(n^{-1/2})$ .

Remark 3.9 (Realized Propensity Score). For any set A with  $P(\psi \in A) > 0$  define the realized sampling proportions in A by  $\widehat{q}_A = E_n[T_i|\psi_i \in A]$ . If sampling is completely randomized, the discrepancy between expected and realized propensities  $q - \widehat{q}_A = O_p(n^{-1/2})$ , so that q is implemented with errors of order  $1/\sqrt{n}$ . This is illustrated in Figure 3, where the realized sampling and assignment propensities widely diverge from their nominal levels in certain regions of the space. Such fluctuations of  $\widehat{q}_A$  about q increase estimator variance. One way to fix this problem is to nonparametrically re-estimate the realized sampling and assignment proportions  $\widehat{q}(\psi)$  and  $\widehat{p}(\psi)$  everywhere in the space, as in

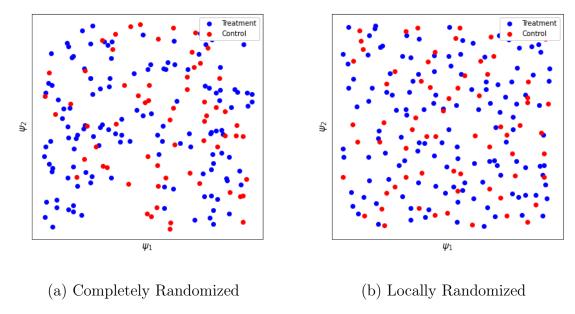


Figure 3: Covariates  $\psi_i \sim \text{Unif}([0,1]^2)$ , n = 1000 and sampling and assignment propensities q = 1/5 and p = 2/3. For complete randomization, the realized propensities (Remark 3.9) widely diverge from q and p in certain parts of the space.

Hirano et al. (2003), using the propensity weighting

$$\widehat{\theta}_{ipw} = E_n \left[ \frac{T_i(D_i - \widehat{p}(\psi_i))Y_i}{\widehat{q}(\psi_i)(\widehat{p} - \widehat{p}^2)(\psi_i)} \right]$$

For experiments, we provide a simpler solution, showing that fine stratification gets the realized propensities right at design-time. In particular, our analysis shows that if  $T_{1:n} \sim \text{Loc}(\psi, q)$  then the gap between the realized and target propensities  $q - \widehat{q}_{A_n} = o_p(n^{-1/2})$ , even for a shrinking sequence of sets with  $P(\psi \in A_n) \to 0$  slowly enough. Because of this, we think of the design  $T_{1:n} \sim \text{Loc}(\psi, q)$  as a "local" implementation of the propensity q with respect to  $\psi(X)$ .

### 3.2 Varying Sampling and Assignment Propensities

This section describes the most general version of our method, providing finely stratified designs with heterogeneous sampling and assignment proportions q(x), p(x). The asymptotics developed in this section allows us to formulate and solve the problem of optimal stratification with heterogeneous costs in Section 4 below. First, we formally define the procedure. Suppose that  $q(x) \in \{a_l/k_l : l \in L\}$  for some finite index set L. Similarly, suppose  $p(x) \in \{a_l'/k_l' : l \in L'\}$  with  $|L'| < \infty$ . Extending our definition, let  $T_{1:n} \sim \text{Loc}(\psi, q(x))$  denote the following double stratification procedure:

- (1) Partition  $\{1, \ldots, n\}$  into propensity strata  $S_l \equiv \{i : q(X_i) = a_l/k_l\}$ .
- (2) In each propensity stratum  $S_l$ , draw samples  $(T_i)_{i \in S_l} \sim \text{Loc}(\psi, a_l/k_l)$ .

Equivalently, we partition each propensity stratum  $S_l$  into groups  $g \subseteq S_l$  of size  $k_l$  such that  $S_l = \bigsqcup_{g \in \mathcal{G}_l} g$  and the homogeneity condition

$$n^{-1} \sum_{g} \sum_{i,j \in g} |\psi_i - \psi_j|_2^2 = n^{-1} \sum_{l} \sum_{g \in \mathcal{G}_l} \sum_{i,j \in g} |\psi_i - \psi_j|_2^2 = o_p(1)$$

In practice, we simply run our matching algorithm separately in each propensity stratum  $S_l$ , and draw  $(T_i)_{i \in g} \sim \operatorname{CR}(a_l/k_l)$  independently for each  $g \in \mathcal{G}_l$ . Treatment assignment  $D_{1:n} \sim \operatorname{Loc}(\psi, p(x))$  is defined identically, partitioning only the units  $\{i : T_i = 1\}$  sampled into the experiment.

Example 3.10 (Budget and Welfare Constraints). Consider a village level experiment, where collecting outcome data is either high cost H or low cost L, depending on village proximity and labor costs. Due to budget constraints, we decide to sample q(L) = 1/2 of the low cost villages but only q(H) = 1/10 of the high cost villages. To do so, we match the high cost villages into 10-tuples and the low cost villages into pairs using publicly available covariates  $\psi_1$ . We randomly sample one village from each 10-tuple and one from each pair. Before assigning treatments, we collect additional survey covariates  $\psi_2$  in each sampled village  $T_i = 1$ . We label the sampled villages as those likely to benefit most M and least L from the intervention according to our prior. Local policymakers insist on the targeted assignment propensity p(M) = 2/3 and p(L) = 1/3. We implement this assignment propensity using matched triples on  $\psi_2$ , assigning D = 1 to 2/3 of the villages in each M-type triple and 1/3 in each L-type triple.

Before stating our main result, we extend the definition of our estimator to accommodate varying propensities. Define the double IPW estimator

$$\widehat{\theta}_2 = E_n \left[ \frac{T_i D_i Y_i}{q(\psi_i) p(\psi_i)} \right] - E_n \left[ \frac{T_i (1 - D_i) Y_i}{q(\psi_i) (1 - p(\psi_i))} \right]$$
(3.5)

If p(x) = p and q(x) = q are constant, then  $\widehat{\theta}_2 = \widehat{\theta} + O_p(n^{-1})$ , where  $\widehat{\theta}$  is the difference-of-means estimator studied in the previous section. Then abusing notation we denote both estimators by  $\widehat{\theta}$ . The following theorem gives our asymptotic results for fine stratification with varying propensities, extending the fixed propensity results in Theorem 3.2 above. We begin with the special case  $\psi_1 = \psi_2 = \psi$  and  $q = q(\psi)$ ,  $p = p(\psi)$ , all non-random.

**Theorem 3.11** (CLT). Suppose Assumption 3.1 holds. Assume sampling and assignment  $T_{1:n} \sim \text{Loc}(\psi, q(\psi))$  and  $D_{1:n} \sim \text{Loc}(\psi, p(\psi))$ . Then  $\sqrt{n_T}(\widehat{\theta} - \text{ATE}) \Rightarrow \mathcal{N}(0, V)$ 

$$V = E[q(\psi)] \left( \text{Var}(c(\psi)) + E\left[ \frac{1}{q(\psi)} \left( \frac{\sigma_1^2(\psi)}{p(\psi)} + \frac{\sigma_0^2(\psi)}{1 - p(\psi)} \right) \right] \right)$$

If q=1 then this is exactly the Hahn (1998) semiparametric variance bound for ATE with iid observations  $(Y, D, \psi(X))$  and propensity  $p(\psi)$ . This shows that under fine stratification the population IPW estimator is already semiparametrically efficient, with no need to nonparametrically re-estimate the known propensities  $q(\psi)$  and  $p(\psi)$  as in Hirano et al. (2003). Next consider the efficiency gain from stratified sampling. The overall sampling proportion  $n_T/n$  has  $n_T/n = E[q(\psi)] + o_p(1)$ . Then defining  $\bar{q} = E[q(\psi)]$ , local randomization reduces the variance due to treatment effect heterogeneity from  $Var(c(\psi))$  to  $\bar{q} Var(c(\psi))$  for  $\bar{q} \in (0, 1]$ , just as in the constant propensity case.

Regression Equivalence. Theorem 3.11 shows that if q=1 then difference-of-means is semiparametrically efficient. To the best of our knowledge, no such efficiency bound is available for joint finely stratified sampling and assignment  $T_{1:n} \sim \text{Loc}(\psi, q(\psi))$  and  $D_{1:n} \sim \text{Loc}(\psi, p(\psi))$  with  $q \neq 1$ . Instead, we show a direct equivalence between unadjusted estimation under fine stratification and nonparametric regression adjustment under an iid design. In particular, the asymptotic variance V above is the same as that achieved by a doubly-robust estimator that adjusts for covariate imbalances during both sampling and assignment. To state the result, consider regression estimators  $\widehat{m}_d(\psi)$  for  $m_d(\psi) = E[Y(d)|\psi]$ . Define the doubly-augmented IPW (2-AIPW) estimator

$$\widehat{\theta}_{adj} = E_n[\widehat{m}_1(\psi_i) - \widehat{m}_0(\psi_i)] + E_n\left[\frac{T_i D_i(Y_i - \widehat{m}_1(\psi_i))}{q(\psi_i)p(\psi_i)} - \frac{T_i(1 - D_i)(Y_i - \widehat{m}_0(\psi_i))}{q(\psi_i)(1 - p(\psi_i))}\right]$$

 $\widehat{\theta}_{adj}$  adjusts for covariate imbalances due to both sampling and assignment. We im-

<sup>&</sup>lt;sup>9</sup>This is because  $E_n[D_i] = p + O(n^{-1})$  for stratified designs. It would be false for  $D_i \stackrel{\text{iid}}{\sim} \text{Bernoulli}(p)$ .

plement the estimator using cross-fitting, similar to Chernozhukov et al. (2017). See the proof for details. If q=1 this reduces to the familiar AIPW estimator for the ATE. The next result provides an equivalence between doubly-robust nonparametric adjustment under an iid design and unadjusted estimation under a finely stratified design.

**Theorem 3.12** (Regression Equivalence). Require Assumption 3.1. Suppose the estimators  $|\widehat{m}_d - m_d|_{2,\psi} = o_p(1)$  are well-specified and consistent. If the design is iid  $T_i \stackrel{\text{iid}}{\sim} \text{Bernoulli}(q(\psi_i))$  and  $D_i \stackrel{\text{iid}}{\sim} \text{Bernoulli}(p(\psi_i))$  then  $\sqrt{n_T}(\widehat{\theta}_{adj} - \text{ATE}) \Rightarrow \mathcal{N}(0, V)$  with the variance V the same as under fine stratification in Theorem 3.11.

Intuitively, Theorem 3.12 shows that finely stratified sampling and assignment makes the unadjusted estimator  $\widehat{\theta}$  as efficient as a more complicated estimator that adjusts nonparametrically for covariate imbalances during both sampling and assignment.

Estimated Design Variables. We wish to formally accommodate the case where design variables  $\psi, q(\psi), p(\psi)$  are estimated using previously collected data. To do so, define the random element  $\xi \perp \!\!\!\perp (X_i, Y_i(1), Y_i(0))_{i=1}^n$  and let  $\psi = \psi(X, \xi), p = p(\psi, \xi)$ , and  $q = q(\psi, \xi)$ . For example, we could let  $\xi = (\widehat{m}_d)_{d=0,1}$  be regression estimates of  $m_d(x) = E[Y(d)|X = x]$  from a pilot experiment and set  $\psi(X, \xi) = (\widehat{m}_0(X), \widehat{m}_1(X))$ . Define  $c(\psi, \xi) = E[Y(1) - Y(0)|\psi, \xi]$  and  $\sigma_d^2(\psi, \xi) = \text{Var}(Y(d)|\psi, \xi)$ . The proof of Theorem 3.11 shows that if  $T_{1:n} \sim \text{Loc}(\psi, q(\psi, \xi))$  and  $D_{1:n} \sim \text{Loc}(\psi, p(\psi, \xi))$  then  $\sqrt{n_T}(\widehat{\theta} - \text{ATE})|\xi \Rightarrow \mathcal{N}(0, V(\xi))$  with conditional asymptotic variance

$$V(\xi) = E[q(\psi, \xi)] \left( \operatorname{Var}(c(\psi, \xi)) + E\left[ \frac{1}{q(\psi, \xi)} \left( \frac{\sigma_1^2(\psi, \xi)}{p(\psi, \xi)} + \frac{\sigma_0^2(\psi, \xi)}{1 - p(\psi, \xi)} \right) \right] \right)$$
(3.6)

All expectations and variances are conditional on  $\xi$ . The inference methods provided in Section 7 are asymptotically exact conditional on  $\xi$ . Note that marginally over both our experiment and the previous data  $\xi$ , the estimator is asymptotically mixed normal  $\sqrt{n_T}(\hat{\theta} - \text{ATE}) \Rightarrow Z$ , where Z has characteristic function  $E[\exp(-\frac{1}{2}t^2V(\xi))]^{10}$ .

Collecting Data After Sampling. In practice, experimenters may want to use different stratification variables  $\psi_1$  for sampling and  $\psi_2$  for assignment with  $\psi_1 \neq \psi_2$ . For example,  $\psi_1$  may include publicly available administrative data, while  $\psi_2$  includes additional survey covariates collected after sampling units into the experiment. To accommodate this, next we state our most general version of Theorem 3.11. Suppose

<sup>&</sup>lt;sup>10</sup>This mixed normal limit was also observed by Cai and Rafi (2023) in a setting with iid treatments.

Assumption 3.1 holds and let sampling and assignment  $T_{1:n} \sim \text{Loc}(\psi_1, q(x))$  and  $D_{1:n} \sim \text{Loc}(\psi_2, p(x))$ . If  $q(x) = q(\psi_1)$ , require  $\psi_1 \subseteq \psi_2$ . Otherwise, require  $(\psi_1, q) \subseteq \psi_2$ . Then  $\sqrt{n_T}(\widehat{\theta} - \text{ATE}) \Rightarrow \mathcal{N}(0, \bar{q}V)$  with  $\bar{q} = E[q(X)]$  and asymptotic variance  $V = V_1 + V_2$ 

$$V_{1} = \operatorname{Var}(c(X)) + E\left[\frac{1}{q(X)} \left(\frac{\sigma_{1}^{2}(X)}{p(X)} + \frac{\sigma_{0}^{2}(X)}{1 - p(X)}\right)\right]$$

$$V_{2} = E\left[\frac{1 - q(X)}{q(X)} \operatorname{Var}(c(X)|\psi_{1}, q)\right] + E\left[\frac{1}{q(X)} \operatorname{Var}(b(X)|\psi_{2}, p)\right]$$
(3.7)

The variance V does not have a simple form like in the special cases considered above if  $\psi_1 \neq \psi_2$ . Instead, we expand V relative to the efficient variance  $V_1$ , which we conjecture is the semiparametric efficiency bound in this setting. If  $\psi_1 = \psi_2 = \psi$ , and  $q = q(\psi)$ ,  $p = p(\psi)$  then V can be rearranged into the form in Theorem 3.11. The requirement that the stratification is increasing<sup>11</sup>  $\psi_1 \subseteq \psi_2$  is subtle. We defer this technical discussion to Remark 10.1 in the appendix.

Optimal Stratification Variables. Inspecting the variance  $V_2$  in Equation 3.7 shows that the minimal dimension efficient stratification variables are  $\psi_1^* = c(X)$  and  $\psi_2^* = (c(X), q(X), b(X))$ . In this case,  $V_2$  is identically zero, and  $V = V_1$ , the conjectured semiparametric efficiency bound. We include q(X) in  $\psi_2^*$  to satisfy the subvector condition  $(\psi_1, q) \subseteq \psi_2$ . If  $q(x) = q(\psi_1)$ , we can just take  $\psi_2^* = (c(X), b(X))$  under the weaker condition  $\psi_1 = h(\psi_2)$  for some measurable h. In practice, these optimal  $\psi_1^*$  and  $\psi_2^*$  are not known. This suggests letting  $\psi_1(X)$  be a small subvector of the baseline covariates expected to be most predictive of treatment effect heterogeneity, and  $\psi_2(X)$  a subvector expected to be predictive of outcomes. If  $c(X) = F(\psi_1(X))$  for some function F, then the choice  $\psi_1(X)$  is asymptotically optimal. If none of the baseline covariates predict treatment effect heterogeneity, so that c(X) is constant, then completely randomized sampling with  $\psi_1^* = 1$  is efficient. We discuss pilot estimation of  $\psi_1^*$  and  $\psi_2^*$  in Section 6.2.

Remark 3.13 (Curse of Dimensionality). Setting  $\psi_1(X) = \psi_2(X) = X$  in Equation 3.7 also minimizes the asymptotic variance V. However, there is a curse of dimensionality when matching on many baseline covariates. In particular, our analysis shows that if E[Y(d)|X=x] is Lipschitz continuous, then the finite sample variance converges to the asymptotic limit at rate  $n \operatorname{Var}(\widehat{\theta}) = V + O_p(n^{-2/(\dim(\psi)+1)})$ , which may be slow

<sup>&</sup>lt;sup>11</sup>In fact, we just require that  $\psi_1 = h(\psi_2)$  for a measurable function h.

<sup>&</sup>lt;sup>12</sup>Since  $b(X; p) \propto E[Y(1)|X]/p + E[Y(0)|X]/(1-p)$ , we should prioritize predicting outcomes in the arm assigned with lowest probability.

even in moderate dimensions. Because of this, for fixed n the variance  $Var(\widehat{\theta})$  may be U-shaped in the dimension of the stratification variables, since matching on many irrelevant variables reduces match quality on the relevant variables. This motivates the search for stratification variables  $\psi_1(x)$  and  $\psi_2(x)$  of small dimension that minimize V.

Remark 3.14 (Sampling Subordinate Assignment). Suppose the sampling propensity q is constant, p=1/2 and consider a matched pair  $g=\{i,j\}$  formed during treatment assignment. For a well-matched pair with  $|\psi_i - \psi_j|_2$  small, the balance function difference  $|b(\psi_i) - b(\psi_j)|$  will also be small as long as  $b(\psi)$  is continuous. This can be shown to reduce the variance due to random assignment. However, if sampling propensity  $q(\psi)$  is not constant, then estimator variance is determined instead by the weighted balance function  $b(\psi)/q(\psi)$ . If  $q(\psi_i) \neq q(\psi_j)$ , e.g. because i and j lie just across the boundary between different sampling propensity strata, then the weighted difference  $|b(\psi_i)/q(\psi_i) - b(\psi_j)/b(\psi_j)|$  may be large even if  $|\psi_i - \psi_j|_2$  is small. Such boundary effects are asymptotically negligible, as shown by our theory, but can significantly inflate finite sample variance in small experiments with many sampling strata and highly predictive covariates. One way to prevent this issue is to match units separately within each sampling stratum  $\{i: q(\psi_i) = a/k\}$  at the assignment stage. We implement this modification in our empirical application in Section 8 below.

## 4 Optimal Stratified Designs

In this section we formulate and solve the problem of optimal stratification in survey experiments, characterizing the optimal sampling and assignment propensities for budget-constrained experimentation with heterogeneous costs. We show how to implement these optimal propensities using fine stratification and prove that such a design is efficient. For simplicity, in what follows we restrict to the case with stratification variables  $\psi_1 = \psi_2 = \psi$  and sampling and assignment propensities  $q = q(\psi)$  and  $p = p(\psi)$ .

### 4.1 Budget-Constrained Sampling Problem

In Section 3, we presented asymptotic results of the form  $\sqrt{n_T}(\widehat{\theta} - \text{ATE}) \Rightarrow \mathcal{N}(0, V)$  normalized by the experiment size  $n_T = \sum_i T_i$ , which is the typical normalization in the previous literature. However, observe that the experiment size  $n_T$  varies with the sampling propensity  $q(\psi)$  in our setting, making this normalization unsuitable for our

current task of optimizing over  $q(\psi)$  to find the efficient sampling propensity. Because of this, in what follows we instead normalize by the number of eligible units n. Since  $n_T/n \xrightarrow{p} E[q(\psi)]$ , this just removes the multiplicative factor  $E[q(\psi)]$  from our previous results, so that  $\sqrt{n}(\widehat{\theta} - ATE) \Rightarrow \mathcal{N}(0, V(q, p))$ 

$$V(q,p) = \operatorname{Var}(c(\psi)) + E\left[\frac{1}{q(\psi)} \left(\frac{\sigma_1^2(\psi)}{p(\psi)} + \frac{\sigma_0^2(\psi)}{1 - p(\psi)}\right)\right]$$
(4.1)

With this fixed normalization in hand, consider minimizing Equation 4.1 over all sampling propensities  $q(\psi)$ . Clearly the unconstrained solution is  $q^*(\psi) = 1$ , making the experiment as large as possible. More generally, we can formalize the problem of experimentation with heterogeneous costs subject to a budget constraint.

**Costs.** Define  $C(\psi; p)$  to be the known, potentially heterogeneous cost of including a unit of type  $\psi(X) = \psi$  in the experiment. One natural cost specification is

$$C(\psi; p) = C_s(\psi) + p(\psi)C_1(\psi) + (1 - p(\psi))C_0(\psi). \tag{4.2}$$

For example, in a development economics context  $C_s(\psi)$  could be the "sampling cost" of paying volunteers to collect outcome data in a village  $\psi_i = \psi$ , while  $C_1(\psi)$  and  $C_0(\psi)$  are the marginal costs of assigning treatment and control, respectively.

To finish setting up the problem, define the ex-ante heteroskedasticity function

$$\bar{\sigma}^2(\psi; p) = \frac{\sigma_1^2(\psi)}{p(\psi)} + \frac{\sigma_0^2(\psi)}{1 - p(\psi)}$$
(4.3)

We interpret  $\bar{\sigma}^2(\psi; p)$  as the expected residual variance from sampling a unit with  $\psi_i = \psi$  into the experiment, prior to realization of its random treatment assignment  $D_i \in \{0,1\}$ , and similarly for the expected costs in Equation 4.2 above. For fixed assignment propensity  $p(\psi)$ , the asymptotic variance objective can be written  $V(q) = \text{Var}(c(\psi)) + E[\bar{\sigma}^2(\psi; p)/q(\psi)]$ . Then the budget-constrained variance minimization problem with budget  $\bar{B}$  can be written

$$\min_{0 < q \le 1} E\left[\frac{\bar{\sigma}^2(\psi; p)}{q(\psi)}\right] \quad \text{s.t.} \quad E[C(\psi; p)q(\psi)] = \bar{B}. \tag{4.4}$$

The next theorem characterizes the interior solutions to this problem. We assume that  $\inf_{\psi} \sigma_d^2(\psi) \geq c > 0$  and costs  $C(\psi; p) \in [C_l, C_u] \subseteq (0, \infty)$ .

**Theorem 4.1.** Define the candidate solution

$$q^*(\psi; p) = \bar{B} \cdot \frac{\bar{\sigma}(\psi; p) C(\psi; p)^{-1/2}}{E[\bar{\sigma}(\psi; p) C(\psi; p)^{1/2}]}.$$
(4.5)

If  $\sup_{\psi} q^*(\psi) \leq 1$ , then  $q^*$  is optimal in Equation 4.4.

If the feasibility constraint  $\sup_{\psi} q^*(\psi) \leq 1$  is violated, the optimal sampling propensity may not have a simple analytical form. Remark 6.5 below provides a rounding procedure that can be used to restore feasibility in this case. To build intuition for the form of the solution, consider the following special cases, suppressing dependence on p.

- (a) Homoskedasticity. Suppose  $\sigma_d^2(\psi) = \sigma_d^2$  constant for  $d \in \{0, 1\}$  and  $p(\psi) = p$ . Then the optimal propensity  $q^*(\psi) = \bar{B} \cdot C(\psi)^{-1/2} / E[C(\psi)^{1/2}]$  has  $q^*(\psi) \propto 1 / \sqrt{C(\psi)}$ . This provides a simple heuristic for sample allocation with heterogeneous costs.
- (b) Homogeneous costs. If  $C(\psi) = 1$ , then  $E[q(\psi)] \leq \bar{B}$  constrains the total proportion of sampled units. In this case write the budget constraint  $\bar{B} = \bar{q}$ . The optimal solution has form  $q^*(\psi) = \bar{q}\bar{\sigma}(\psi)/E[\bar{\sigma}(\psi)]$ , with sampling propensity proportional to the ex-ante standard deviation. In particular, we would like to oversample  $(q^*(\psi) > \bar{q})$  units of type  $\psi(X) = \psi$  that have larger residual standard deviation than the average  $E[\bar{\sigma}(\psi)]$ , and undersample in the opposite case.

Optimal Spending. Under optimal sampling, the total amount spent on units of type  $\psi$  is  $C(\psi)q^*(\psi)dP(\psi) \propto \sqrt{\bar{\sigma}^2(\psi)C(\psi)}dP(\psi)$ . This shows that we should spend more on units with larger ex-ante variance and larger per unit cost. However, since the optimal propensity undersamples high cost units, spending grows as  $\sqrt{C(\psi)}$ , instead of linearly as it would if  $q(\psi) = q$  were constant.

## 4.2 Globally Optimal Stratification

The main result of this section studies implementation of the globally optimal stratified design, subject to the budget constraint. In particular, we show efficiency of a finely stratified implementation of the jointly optimal sampling and assignment propensities  $q^*$  and  $p^*$ . In this section, we restrict to the case with costs  $C(\psi; p) = C(\psi)$  not depending on p. See Remark 4.4 for discussion of the general case.

First, we characterize the optimal assignment propensity. For any fixed sampling propensity  $q(\psi)$ , the global minimizer of Equation 4.1 is the conditional Neyman allo-

cation  $p^*(\psi) = \sigma_1(\psi)/(\sigma_1(\psi) + \sigma_0(\psi))$ . In some cases, we may only be interested in implementing a constant assignment propensity  $p^* \in (0,1)$ . If q is also constant, then

$$p^* = \sqrt{E[\sigma_1^2(\psi)]} \left( \sqrt{E[\sigma_1^2(\psi)]} + \sqrt{E[\sigma_0^2(\psi)]} \right)^{-1}$$
 (4.6)

Compare this to the classical Neyman allocation  $\sigma_1/(\sigma_1+\sigma_0)$  with  $\sigma_d = \mathrm{SD}(Y(d))$ . In our setting, only the residual variances  $\sigma_d^2(\psi) = \mathrm{Var}(Y(d)|\psi)$  enter  $p^*$ , since the fluctuations of Y(d) predictable by  $\psi(X)$  do not contribute to first-order asymptotic variance under fine stratification.

The jointly optimal sampling and assignment propensities are obtained by plugging the conditional Neyman allocation  $p^*(\psi) = \sigma_1(\psi)/(\sigma_1(\psi) + \sigma_0(\psi))$  into the formula for  $q^*(\psi; p)$  above. This gives ex-ante variance  $\bar{\sigma}^2(\psi) = (\sigma_1(\psi) + \sigma_0(\psi))^2$  and jointly optimal sampling and assignment propensities

$$p^*(\psi) = \frac{\sigma_1(\psi)}{\sigma_1(\psi) + \sigma_0(\psi)} \qquad q^*(\psi; p^*) = \bar{B} \frac{(\sigma_1(\psi) + \sigma_0(\psi))C(\psi)^{-1/2}}{E[(\sigma_1(\psi) + \sigma_0(\psi))C(\psi)^{1/2}]}.$$
 (4.7)

The propensities  $p^*(\psi)$  and  $q^*(\psi)$  will generally need to be discretized in order to implement them using fine stratification. To do so, we provide novel asymptotics with both the number of distinct propensity levels  $L_n$  as well as the number of units in each group  $|g| = k_n$  growing with the sample size n.

**Definition 4.2** (Discretization). Let  $q_n^*(\psi)$  and  $p_n^*(\psi)$  take values in the finite approximating propensity set  $\{a_l/k_l: l \in L_n\}$  with levels  $L_n$ . Suppose that  $|q_n^* - q^*|_{\infty} = o(1)$  and  $|p_n^* - p^*|_{\infty} = o(1)$ . Define maximum group size  $\overline{k}_n = \max_{l \in L_n} k_l$  and require that  $\overline{k}_n |L_n| = o(n^{1-\frac{\dim(\psi)+1}{\alpha}})$  for  $E[|\psi(X)|^{\alpha}] < \infty$ .

If  $\psi(X)$  is bounded, the final condition simplifies to  $k_n|L_n|=o(n)$ . For example, one way to satisfy Definition 4.2 is to round the optimal propensities to the nearest  $a/k_n$  for some sequence  $k_n \to \infty$ , setting  $q_n^*(\psi) = \operatorname{argmin}\{|q^*(\psi) - a/k_n| : 1 \le a \le k_n - 1, k_n = \lfloor n^{1/2-\epsilon} \rfloor\}$  and similarly for  $p_n^*(\psi)$ . The main theorem of this section shows that such discretizations are asymptotically efficient.

**Theorem 4.3** (Optimal Stratification). Suppose Assumption 3.1. If  $T_{1:n} \sim \text{Loc}(\psi, q_n^*(\psi))$  and  $D_{1:n} \sim \text{Loc}(\psi, p_n^*(\psi))$ . Then  $\sqrt{n}(\widehat{\theta} - \text{ATE}) \Rightarrow \mathcal{N}(0, V^*)$ 

$$V^* = \text{Var}(c(\psi)) + \min_{\substack{0 < q, p \le 1 \\ E[C(\psi)q(\psi)] = \bar{B}}} E\left[\frac{1}{q(\psi)} \left(\frac{\sigma_1^2(\psi)}{p(\psi)} + \frac{\sigma_0^2(\psi)}{1 - p(\psi)}\right)\right]$$

The design in Theorem 4.3 minimizes the asymptotic variance over all sampling and assignment propensities, subject to the budget constraint. If we set q = 1, then  $V^* = \min_{0 \le p \le 1} V_H(p)$ , minimizing the Hahn (1998) semiparametric efficiency bound for the ATE over all propensities scores. As noted above, Armstrong (2022) shows that this bound also applies to the designs in this paper for the case q = 1.

Remark 4.4 (General Costs). For the specification in Equation 4.2, the restriction to costs  $C(\psi; p) = C(\psi)$  is without loss of efficiency if the marginal costs of assigning treatment and control are similar  $C_1 \approx C_0$ , or if sampling costs are much larger than the cost difference between treatment arms  $C_s \gg |C_1 - C_0|$ . We leave joint optimization of  $q(\psi), p(\psi)$  with general costs  $C(\psi; p)$  to future work. However, for optimization of the sampling propensity  $q(\psi)$  alone with fixed propensity  $p(\psi)$ , e.g. p = 1/2, we can accommodate general costs  $C(\psi; p)$ . We simply use the design  $T_{1:n} \sim \text{Loc}(\psi, q_n^*(\psi; p))$ , discretizing the optimal sampling propensity from Equation 4.5.

## 5 Optimal Covariate-Adaptive Randomization

In this section, we derive the globally optimal covariate-adaptive randomization for treatment assignment with p=1/2, showing that it takes the form of a novel alternating design. In the case q=1 and p(X)=a/k fixed, Bai (2022) showed that if the b(x) were known, then matching units into strata of size k according to their sorted  $b(X_i)$  values minimizes  $\mathrm{MSE}(\widehat{\theta}|X_{1:n})$  over all stratified designs. By contrast, here we show that if b(x) were known, the class of stratified designs itself would generally be suboptimal. To see this, consider the case p=1/2. Define the complete graph  $K_n$  with vertices  $\{1,\ldots,n\}$  and edge weights  $w_{ij}=b(X_i)b(X_j)$ . The Max-Cut optimization problem asks for a partition of the vertices into disjoint sets  $E_1 \cup E_0 = \{1,\ldots,n\}$  such that the weight of cut edges between  $E_1$  and  $E_0$  is maximized

$$\max_{E_0, E_1} \sum_{i,j} b(X_i) b(X_j) \mathbb{1}(i \in E_1, j \in E_0) \quad \text{s.t.} \quad E_0 \sqcup E_1 = \{1, \dots, n\}$$
 (5.1)

For example, see Rendl et al. (2008) for an overview. Let  $E_0^*, E_1^*$  solve the Max-Cut problem in Equation 5.1. Define the optimal treatment allocation  $d_{1:n}^* = d_{1:n}^*(X_{1:n})$  by  $d_i^* = \mathbb{1}(i \in E_1^*)$  for  $1 \leq i \leq n$ . Define the alternating design  $P^*(D_{1:n}|X_{1:n})$  that

alternates between  $d_{1:n}^*$  and its mirror image  $1 - d_{1:n}^*$  by

$$P^*(D_{1:n} = d_{1:n}^*|X_{1:n}) = P^*(D_{1:n} = 1 - d_{1:n}^*|X_{1:n}) = 1/2$$

with  $D_{1:n} \perp \!\!\!\perp W_{1:n}|X_{1:n}$  for the full data  $W_{1:n} = (X_i, Y_i(1), Y_i(0))_{i=1}^n$ . Our next theorem shows that the the alternating design  $P^*$  is globally optimal over the set of all covariate-adaptive designs with fixed treatment probability  $P(D_i = 1) = 1/2$ . We denote this set of designs by  $\mathcal{P}_{1/2} = \{P : P(D_i = 1) = 1/2, \ D_{1:n} \perp \!\!\!\perp W_{1:n}|X_{1:n}\}$ . For simplicity, suppose n = 2m for an integer m.

**Theorem 5.1** (Optimal Design). The design  $P^*$  has  $MSE_{P^*}(\widehat{\theta}|X_{1:n}) \leq MSE_P(\widehat{\theta}|X_{1:n})$  for all  $P \in \mathcal{P}_{1/2}$ .

The inequality is strict if Problem 5.1 has a unique solution up to permutation of set labels. In particular, note that  $P^*$  is not a matched pairs design. Nevertheless, b(x) is not known, so neither the globally optimal design, nor the optimal stratified design from Bai (2022) are feasible. We also caution against plug-in approaches that use a pilot estimate of  $b(X_i)$ . Section 6.2 below shows that such approaches are equivalent to regression adjustment with regressions estimated in the pilot instead of the main sample, which may perform poorly if the pilot is small. For these reasons, we do not further pursue finite sample optimal designs in this paper.

## 6 Design with a Pilot Experiment

In this section, we study a procedure that uses pilot data to estimate and implement the solution to the optimal stratification problem derived in the previous section. We show that this feasible version of the optimal design is asymptotically efficient, achieving the budget-constrained optimal variance of Theorem 4.3. In particular, for the case q=1 our procedure minimizes the semiparametric variance bound over all propensity scores, providing the first asymptotically efficient solution to the question of design using a pilot study (Hahn et al. (2011)). The methods in this section are also relevant when observational data from the target population or a closely related previous experiment are available. Small pilot considerations and potential robustifications are discussed in Remark 6.3 below. Pilot estimation of the optimal stratification variables  $\psi^*$  is discussed in Section 6.2 below.

#### 6.1 Feasible Optimal Stratification

Fix stratification variables  $\psi_1 = \psi_2 = \psi$  and consider estimating the optimal design for the budget-constrained problem in Equation 4.4. This amounts to using pilot or proxy data to estimate the efficient sampling proportions  $q^*(\psi)$  and treatment propensity  $p^*(\psi)$ . As a proof of concept, we first state our result under large pilot asymptotics, allowing consistent estimation of the heteroskedasticity functions  $\sigma_d(\psi)$ . We show that the feasible estimated optimal design is asymptotically efficient in the sense of Theorem 4.3. Fixed pilot asymptotics and small sample considerations are discussed in Remark 6.3 below.

In Section 4 we derived the optimal propensities

$$q^*(\psi) = \bar{B} \frac{(\sigma_1(\psi) + \sigma_0(\psi))C(\psi)^{-1/2}}{E[(\sigma_1(\psi) + \sigma_0(\psi))C(\psi)^{1/2}]} \qquad p^*(\psi) = \frac{\sigma_1(\psi)}{\sigma_1(\psi) + \sigma_0(\psi)}.$$

The sampling propensity  $q^*(\psi)$  is optimal provided the feasibility condition  $\sup_{\psi} q^*(\psi) \le 1$  is satisfied. Consider pilot heteroskedasticity estimates<sup>13</sup>  $\widehat{\sigma}_d^2(\psi)$  for d = 0, 1. Define the propensity estimates<sup>14</sup>

$$\widehat{q}(\psi) = \overline{B} \frac{(\widehat{\sigma}_1(\psi) + \widehat{\sigma}_0(\psi))C(\psi)^{-1/2}}{E_n[(\widehat{\sigma}_1(\psi_i) + \widehat{\sigma}_0(\psi_i))C(\psi_i)^{1/2}]} \qquad \widehat{p}(\psi) = \frac{\widehat{\sigma}_1(\psi)}{\widehat{\sigma}_1(\psi) + \widehat{\sigma}_0(\psi)}.$$

In practice, we may find  $\widehat{q}(\psi_j) > 1$  for some j. This could be because the condition  $\sup_{\psi} q^*(\psi) \leq 1$  is violated and the optimal sampling problem does not have an interior solution, or just due to statistical error. However, we can transform  $\widehat{q}(\psi)$  into an admissible sampling propensity by an iterative rounding procedure, described in Remark 6.5 below. Suppose we have done so and let  $\widehat{q}_n(\psi)$  and  $\widehat{p}_n(\psi)$  be a sequence of discretizations of  $\widehat{q}(\psi)$  and  $\widehat{p}(\psi)$ , satisfying the conditions in Definition 4.2. We require the following technical conditions, including consistency of the pilot heteroskedasticity estimates.

Assumption 6.1. Require pilot estimation rate  $|\sigma_d^2 - \widehat{\sigma}_d^2|_{2,\psi} = O_p(n^{-r})$  for some r > 0. Require the variance regularity condition  $\inf_{\psi} \sigma_d(\psi) > 0$  and  $(\sigma_1/\sigma_0)(\psi) \in [c_l, c_u]$  with  $0 < c_l < c_u < \infty$ . Assume the interior solution condition  $\sup_{\psi} q^*(\psi) \leq 1$ . Require discretization rate  $\overline{k}_n |L_n| = o(n^{1-(\dim(\psi)+1)/\alpha_1})$  and  $\overline{k}_n = \omega(n^{1/\alpha_2})$ . Assume the moments  $E[Y(d)^4] < \infty$ ,  $E[\psi(X)]_2^{\alpha_1} < \infty$  for  $\alpha_1 > \dim(\psi) + 1$ , and  $E[|m_d(\psi)|^{\alpha_2}] < \infty$  for

 $<sup>^{13}</sup>$ In practice, we use a modification of Fan and Yao (1998) to estimate variance functions. See appendix section A.2 for details.

<sup>&</sup>lt;sup>14</sup>Note in  $\widehat{q}(\psi)$  the average is taken over the main experiment covariates, allowing for covariate shift between pilot and main experiment.

 $\alpha_2 \geq 1/r$ . Assume costs  $0 < C(\psi) < \infty$  for all  $\psi$ .

Our main result shows that finely stratified implementation of the optimal propensity estimates is asymptotically fully efficient.

**Theorem 6.2** (Pilot Design). Impose Assumption 6.1. Suppose  $T_{1:n} \sim \text{Loc}(\psi, \widehat{q}_n(\psi))$  and  $D_{1:n} \sim \text{Loc}(\psi, \widehat{p}_n(\psi))$ . Then  $\sqrt{n}(\widehat{\theta} - \text{ATE}) \Rightarrow \mathcal{N}(0, V^*)$ 

$$V^* = \text{Var}(c(\psi)) + \min_{\substack{0 < q, p \le 1 \\ E[C(\psi)q(\psi)] = \bar{B}}} E\left[ \frac{1}{q(\psi)} \left( \frac{\sigma_1^2(\psi)}{p(\psi)} + \frac{\sigma_0^2(\psi)}{1 - p(\psi)} \right) \right]$$

For intuition, it is also helpful to consider certain special cases of Theorem 6.2. If we fix q = 1, the design  $D_{1:n} \sim \text{Loc}(\psi, \widehat{p}_n(\psi))$  asymptotically minimizes the Hahn (1998) variance bound over all propensity scores

$$V^* = \min_{0 \le p \le 1} V_H(p) = \text{Var}(c(\psi)) + \min_{0 \le p \le 1} E\left[\frac{\sigma_1^2(\psi)}{p(\psi)} + \frac{\sigma_0^2(\psi)}{1 - p(\psi)}\right]. \tag{6.1}$$

If  $\widehat{p}^*$  is a consistent pilot estimate of the optimal constant propensity  $p^*$  in Equation 4.6, then the design  $D_{1:n} \sim \operatorname{Loc}(\psi, \widehat{p}_n)$  has  $\sqrt{n}(\widehat{\theta} - \operatorname{ATE}) \Rightarrow \mathcal{N}(0, V)$  with

$$V^* = \text{Var}(c(\psi)) + \min_{p \in (0,1)} E\left[\frac{\sigma_1^2(\psi)}{p} + \frac{\sigma_0^2(\psi)}{1-p}\right]$$

Remark 6.3 (Small Pilots). For small pilots, the asymptotic results in Theorem 6.2 requiring consistent estimation of the variance function  $\sigma_d^2(\psi)$  may not reflect finite sample performance. In practice, we may instead consider an inconsistent variance approximation using the squared residuals from a linear regression. Let  $\hat{\epsilon_i}^d$  be residuals from regressions  $Y(d) \sim 1 + \psi$  in  $\{D_i = d\}$ . For pilot data  $W_{1:m}$  compute residual standard deviation estimate  $\hat{s}_d = E_m[(\hat{\epsilon_i}^d)^2]^{1/2}$  and form the estimated optimal propensity  $\hat{p}^* = \hat{s}_1/(\hat{s}_1 + \hat{s}_0)$ , rounding it to a close rational number  $\hat{p} = a/k$ . By Equation 3.6, if  $D_{1:n} \sim \text{Loc}(\psi, \hat{p})$  then conditioning on the pilot data  $\sqrt{n}(\hat{\theta} - \text{ATE})|W_{1:m} \Rightarrow \mathcal{N}(0, V)$ 

$$V = \operatorname{Var}(c(\psi)) + E \left[ \frac{\sigma_1^2(\psi)}{\widehat{p}} + \frac{\sigma_0^2(\psi)}{1 - \widehat{p}} \middle| W_{1:m} \right]$$

The rounding of  $\hat{p}^*$  to  $\hat{p} = a/k$  adds robustness. For example, if  $p^* = 1/2$  and our pilot estimate  $\hat{p}^* = .57$ , we would round to  $\hat{p} = 1/2$  except in very large experiments. See the discussion of discretization in Remark 6.4 below. In practice, this procedure could

be further robustified by constructing a confidence interval for  $p^*$  and checking that it excludes a baseline choice such as p = 1/2, though we leave this to further work.

**Remark 6.4** (Discretization). Consider a pilot estimate  $\hat{p}(\psi) = .637$ . This could be rounded to any of  $\hat{p} = 2/3$ , 3/5, 13/20, 63/100 and so on. If  $\psi$  is bounded, Assumption 6.1 requires that  $k_n = o(\sqrt{n})$  for the rounding scheme  $a/k_n$ . This condition gives some quantitative guidance about discretization fineness. For example, if n = 400 we might rule out  $\hat{p} = 13/20$ . In our simulations and empirical application, it's often possible to choose a reasonable number of discretization levels just by inspecting the histogram of the estimated  $\hat{p}(\psi)$  and  $\hat{q}(\psi)$  to see how much heterogeneity is needed.

**Remark 6.5** (Feasible Sampling). In practice, we may find that  $\widehat{q}(\psi_j) > 1$  for some j, violating the sampling constraint. To restore feasibility, we can iteratively set  $\widehat{q}(\psi_j) = 1$  for such j and recompute the optimal propensity for the remaining units. To that end, define an index set  $J = \emptyset$  and implement the following iterative rounding procedure. (1) Find the largest  $\widehat{q}(\psi_j) > 1$ . Set  $\widehat{q}(\psi_j) = 1$  and add j to J. (2) Recompute the sampling propensity according to

$$\widehat{q}(\psi_i) = \frac{\overline{B} - (1/n) \sum_{i \in J} C(\psi_i)}{1 - |J|/n} \frac{(\widehat{\sigma}_1(\psi_i) + \widehat{\sigma}_0(\psi_i)) C(\psi_i)^{-1/2}}{E_n[(\widehat{\sigma}_1(\psi_l) + \widehat{\sigma}_0(\psi_l)) C(\psi_l)^{1/2} | l \notin J]} \qquad \forall i \notin J.$$

If  $\max_{i=1}^n \widehat{q}(\psi_i) \leq 1$ , stop. Otherwise, return to (1). This procedure satisfies the insample budget constraint  $E_n[\widehat{q}(\psi_i)C(\psi_i)] = \overline{B}$  after each iteration and terminates with  $\max_{i=1}^n \widehat{q}(\psi_i) \leq 1$ .

Remark 6.6 (Optimal Stratification Trees). Tabord-Meehan (2022) suggests using pilot data to estimate a stratification  $\widehat{S}$  and assignment propensity  $\widehat{p}(\widehat{S})$  over a set of tree partitions  $\widehat{S} \in \mathcal{T}$  of the covariate space. If  $\widehat{S} = \widehat{S}(\psi)$  then in our notation their Theorem 3.1 implies that  $\sqrt{n}(\widehat{\theta} - \text{ATE}) \Rightarrow \mathcal{N}(0, V)$ 

$$V = \operatorname{Var}(c(\psi)) + \min_{S \in \mathcal{T}} \left( E[\operatorname{Var}(b(\psi; p^*(S))|S)] + E\left[ \frac{\sigma_1^2(\psi)}{p^*(S)} + \frac{\sigma_0^2(\psi)}{1 - p^*(S)} \right] \right).$$

The optimal propensity  $p^*(S) = \sigma_1(S)/(\sigma_1(S) + \sigma_0(S))$  with  $\sigma_d^2(S) = \text{Var}(Y(d)|S)$ . The display shows that the optimal stratification tree chooses a compromise between two different forces. In the first term, it tries to minimize the variance due to covariate imbalance by choosing strata S that predict propensity-weighted outcomes well, minimizing  $E[\text{Var}(b(\psi; p^*(S))|S)]$ . In the second term, it tries to minimize the residual variance by choosing strata S such that  $p^*(S)$  is close to the optimal propensity

 $p^*(\psi) = \sigma_1(\psi)/(\sigma_1(\psi) + \sigma_0(\psi))$ . By contrast, we implement a discretized consistent estimate  $\widehat{p}_n(\psi)$  of the optimal propensity  $p^*(\psi)$  using fine stratification. This makes the middle term above asymptotically lower order and globally minimizes the residual term, without any first-order tradeoff (Equation 6.1). Of course, if S = S(X) uses different covariates than our stratification variables  $\psi$ , then the efficiencies cannot be ranked.

#### 6.2 Estimating Stratification Variables

Section 3 showed that the stratification variables  $\psi_1^* = c(X)$  and  $\psi_2^* = (c, b)(X)$  were asymptotically efficient for both sampling and assignment. This suggests setting  $\psi_1(X) = \widehat{c}(X)$  and  $\psi_2(X) = (\widehat{c}(X), \widehat{b}(X))$ , using pilot estimates of the various regression functions. In our notation, the design  $D_{1:n} \sim \operatorname{Loc}(\widehat{b}, p)$  was proposed in Bai (2022) for the case with iid sampling.

Regression vs. Matching on Estimated Functions. Our first result is negative, suggesting that for small pilots such an approach would be dominated by not using the pilot data at all at the design stage, drawing treatments iid and doing regression adjustment in the main sample. For simplicity, set q = 1 and let  $D_{1:n} \sim \text{Loc}(\hat{b}, p)$  be the design with pilot-estimated stratification variables. Let  $\hat{\theta}$  be the difference of means estimator formed using the data  $W_{1:n} = (D_i, X_i, Y_i(D_i))_{i=1}^n$ . Separately, define iid treatments  $\check{D}_i \sim \text{Bernoulli}(p)$  and let  $\widehat{\theta}_{adj}$  be the cross-fit AIPW estimator in Theorem 3.12, estimated using the alternate data  $\check{W}_{1:n} = (\check{D}_i, X_i, Y_i(\check{D}_i))_{i=1}^n$  with regression estimators  $\check{m}_d(\psi)$ . Define  $\check{b}(X)$  by plugging in  $\check{m}_d(\psi)$  to the formula in Equation 3.1. Then with  $c_p = (p - p^2)^{1/2}$  the estimators  $\widehat{\theta}$  and  $\widehat{\theta}_{adj}$  have identical expansions

$$\widehat{\theta} = E_n[c(X_i)] + E_n[(D_i - p)(b - \widehat{b})(X_i)]/c_p + R_n + O_p(n^{-1})$$

$$\widehat{\theta}_{adj} = E_n[c(X_i)] + E_n[(\check{D}_i - p)(b - \check{b})(X_i)]/c_p + \check{R}_n.$$

The residual terms  $\sqrt{n}R_n$ ,  $\sqrt{n}\check{R}_n \Rightarrow \mathcal{N}(0,v)$  for v>0 and are mean-independent of the first term. Denote the imbalance terms  $B_n=E_n[(D_i-p)(b-\hat{b})(X_i)]$  and  $\check{B}_n=E_n[(\check{D}_i-p)(b-\check{b})(X_i)]$ . These terms control estimator error due to covariate imbalances between the treatment arms. With pilot regression error  $r_n^{pilot}=\max_d\|\widehat{m}_d-m_d\|_{2,\psi}$  and main sample regression error  $r_n^{main}=\max_d\|\check{m}_d-m_d\|_{2,\psi}$ , it's easy to show that

$$\sqrt{n}B_n = O_p(r_n^{pilot})$$
 and  $\sqrt{n}\check{B}_n = O_p(r_n^{main}).$ 

We expect pilot estimation error to be larger  $r_n^{pilot} \gg r_n^{main}$  if the pilot is much smaller than the main sample.

Robustified Approach. The discussion above showed that, for small pilots, the design  $D_{1:n} \sim \operatorname{Loc}(\hat{b}, p)$  behaves like a noisy version of the AIPW estimator  $\hat{\theta}_A$ , with regression adjustments estimated using the pilot instead of the main experiment. However, the Bai (2022) approach could still dominate if e.g.  $\hat{b}$  is estimated consistently from a large observational dataset or a larger previous experiment with closely related covariates and potential outcomes. The large pilot asymptotics in Bai (2022) can be extended to show that the two-stage sampling and assignment design  $T_{1:n} \sim \operatorname{Loc}(\hat{c}, q)$  and  $D_{1:n} \sim \operatorname{Loc}((\hat{c}, \hat{b}), p)$  achieves the optimal variance  $V_1$  in Equation 3.7. Another natural idea is to robustify the Bai (2022) approach, setting  $T_{1:n} \sim \operatorname{Loc}((\hat{c}, \hat{b}, \psi'), q)$  and  $D_{1:n} \sim \operatorname{Loc}((\hat{c}, \hat{b}, \psi'), p)$  for stratification variables  $\psi'$  expected to be predictive of both treatment effects and outcomes ex-ante. This can then be combined with the methods in the previous section, setting  $\psi = (\hat{c}, \hat{b}, \psi')$  and proceeding exactly as in Section 6.1. The efficiency of such designs under fixed pilot asymptotics is described by Equation 3.6. Conditionally asymptotically exact inference, conditional on the pilot data, is available using the methods in Section 7.

**Remark 6.7** (Imbalance Term vs. Residual Variance). We noted earlier that under completely randomized sampling and assignment  $\sqrt{n_T}(\widehat{\theta} - ATE) \Rightarrow \mathcal{N}(0, V)$  with

$$V = \operatorname{Var}(c(X)) + \operatorname{Var}(b(X)) + E\left[\frac{\sigma_1^2(X)}{p} + \frac{\sigma_0^2(X)}{1-p}\right].$$

The middle term  $\operatorname{Var}(b(X))$  is the variance due to covariate imbalance, and the third term is the residual variance. We can think of  $\operatorname{Var}(b(X))$  as the "easier" term. We can make this term asymptotically negligible by any one of the following: (1) fine stratification on  $\psi(X) = X$  under very weak assumptions for  $\dim(X)$  small (2) ex-post propensity reweighting under a smoothness condition (3) ex-post regression adjustment under well-specification (4) the Bai (2022) design with a large enough pilot, or any combination of these methods. By contrast, after treatments have been assigned, neither regression adjustment nor propensity reweighting can help us further minimize the semiparametric variance bound

$$V_H(p) = \text{Var}(c(X)) + E\left[\frac{\sigma_1^2(X)}{p(X)} + \frac{\sigma_0^2(X)}{1 - p(X)}\right]$$

In this sense, the residual variance in this expression is the "harder" quantity. To affect it, we need to change the law of the data-generating process by changing the treatment and

sampling proportions at design-time, as we have implemented in the previous sections.

#### 7 Inference Methods

This section provides new methods for asymptotically exact inference on the ATE under two-stage locally randomized designs. To do so, we generalize pairs-of-pairs<sup>15</sup> type methods to accommodate designs with both finely stratified sampling and assignment, as well as varying propensities  $q(\psi), p(\psi)$ . Our inference methods enable applied researchers to report smaller confidence intervals that fully reflect the efficiency gains from all of our proposed designs.

For each assignment group  $g \in \mathcal{G}_n$ , define the centroid  $\bar{\psi}_g = |g|^{-1} \sum_{i \in g} \psi_i$ . Let  $\nu : \mathcal{G}_n \to \mathcal{G}_n$  be a bijective matching between groups satisfying  $\nu(g) \neq g$ ,  $\nu^2 = \operatorname{Id}$ , and the homogeneity condition  $\frac{1}{n} \sum_{g \in \mathcal{G}_n} |\bar{\psi}_g - \bar{\psi}_{\nu(g)}|_2^2 = o_p(1)$ . In practice,  $\nu$  is obtained by matching the group centroids  $\bar{\psi}_g$  into pairs using the algorithm in Section 2. Let  $\mathcal{G}_n^{\nu} = \{g \cup \nu(g) : g \in \mathcal{G}_n\}$  be the unions of paired groups formed by this matching. Define  $a(g) = \sum_{i \in g} D_i$  and k(g) = |g|. Define the propensity weights  $w_i^1 = (1 - p_i q_i)/(p_i q_i)^2$  and  $w_i^0 = (1 - q_i(1 - p_i))/(q_i(1 - p_i))^2$ . Finally, define the variance estimator components

$$\widehat{v}_{1} = n^{-1} \sum_{g \in \mathcal{G}_{n}^{\nu}} \frac{1}{a(g) - 1} \sum_{i \neq j \in g} Y_{i} Y_{j} D_{i} D_{j} (w_{i}^{1} w_{j}^{1})^{1/2}$$

$$\widehat{v}_{0} = n^{-1} \sum_{g \in \mathcal{G}_{n}^{\nu}} \frac{1}{(k - a)(g) - 1} \sum_{i \neq j \in g} Y_{i} Y_{j} (1 - D_{i}) (1 - D_{j}) (w_{i}^{0} w_{j}^{0})^{1/2}$$

$$\widehat{v}_{10} = n^{-1} \sum_{g \in \mathcal{G}_{n}} \frac{k}{a(k - a)} (g) \sum_{i, j \in g} Y_{i} Y_{j} D_{i} (1 - D_{j}) (q_{i} q_{j})^{-1/2}$$

Our inference strategy begins with the sample variance of the double-IPW estimator (Equation 3.5), which is consistent for the true asymptotic variance under an iid design, but too large under stratified designs. We correct this sample variance using the estimators above, which measure how well the stratification variables predict observed outcomes in local regions of the covariate space. Define the variance estimator

$$\widehat{V} = \operatorname{Var}_n \left( \frac{T_i(D_i - p(\psi_i))Y_i}{q(\psi_i)(p - p^2)(\psi_i)} \right) - \widehat{v}_1 - \widehat{v}_0 - 2\widehat{v}_{10}.$$

$$(7.1)$$

<sup>&</sup>lt;sup>15</sup>Also known as the method of collapsed strata, as in Hansen et al. (1953). See Abadie and Imbens (2008) and Bai et al. (2021) for recent analyses.

Our main result shows that  $\hat{V}$  is consistent for the limiting variance of Theorem 3.11, enabling asymptotically exact inference.

**Theorem 7.1** (Inference). Assume the conditions of Theorem 3.11. If sampling  $T_{1:n} \sim$  $Loc(\psi, q(\psi))$  and assignment  $D_{1:n} \sim Loc(\psi, p(\psi))$ , then  $\widehat{V} = V + o_p(1)$ .

By Theorem 7.1 and the CLT in Section 3, the confidence interval  $\widehat{C}=[\widehat{\theta}$   $\pm$  $\widehat{V}^{1/2}c_{1-\alpha/2}/\sqrt{n}$  with  $c_{\alpha}=\Phi^{-1}(\alpha)$  is asymptotically exact in the sense that  $P(\text{ATE}\in$  $\widehat{C}$ ) = 1 -  $\alpha$  + o(1). Importantly, note that the scaling is by number of eligible units n, not the smaller experiment size  $n_T = \sum_i T_i \leq n$ .

#### 8 **Empirical Results**

In this section, we quantify the performance of each of our designs on N=9 real DGP's from experimental papers covering a range of fields in applied economics. Our theoretical results showed separate variance reductions from each of the following: (a) finely stratified treatment assignment, (b) finely stratified sampling (c) the optimal propensities  $q^*(\psi)$  and  $p^*(\psi)$  (infeasible), and (d) consistent pilot estimates  $\widehat{q}(\psi)$  and  $\widehat{p}(\psi)$  of the optimal propensities (feasible). To quantify the marginal efficiency gain from each of our proposed methods in finite samples, we simulate unadjusted ATE estimation under the following designs:

**CR**: Complete randomization  $T_{1:n} \sim \operatorname{CR}(q_k^*)$  and  $D_{1:n} \sim \operatorname{CR}(p)$ , with  $q_k^*$  a discretization of the budget-exhausting sampling propensity  $q^* = \bar{B}/E_n[C(\psi_i)]$  and fixed assignment propensity  $p.^{16}$ 

**CR**, **Loc**: As in CR but with stratified assignment  $D_{1:n} \sim \text{Loc}(\psi, p)$ .

**Loc**: Stratified sampling and assignment  $T_{1:n} \sim \text{Loc}(\psi, q_k^*)$  and  $D_{1:n} \sim \text{Loc}(\psi, p)$ .

**Hom**: As in **Loc** but with sampling propensity  $q_{hom,k}^*(\psi)$  a discretization of  $q_{hom}^*(\psi) = \bar{B} \cdot C(\psi)^{-1/2}/E[C(\psi)^{1/2}],$  the optimal sampling propensity assuming homoskedasticity. This is feasible but may be misspecified.

**Pilot S/L**: As in **Loc**, but with  $T_{1:n} \sim \text{Loc}(\psi, \widehat{q}_k(\psi))$  and  $D_{1:n} \sim \text{Loc}(\psi, \widehat{p}_k)$ , where  $\widehat{q}_k(\psi)$  and  $\widehat{p}_k$  are pilot estimates of the optimal design as in Section 6. We consider pilots of size (S)  $n_{pilot} = 100$  or (L)  $n_{pilot} = 400.$ <sup>17</sup>

<sup>16</sup>In particular, we let  $q_k^* = a/k$ , using the minimal k such that  $q_k^* \cdot E_n[C(\psi_i)] \in [.95\bar{B}, 1.05\bar{B}]$ .

17Variance functions  $\sigma_d^2(\psi)$  are estimated using a modification of Fan and Yao (1998), see appendix section A.2 for details. The pilot data has p = 1/2, q = 1 and treatments assigned by matched pairs.

We evaluate each of these designs on data from experimental papers published in the AER between May 2021 and November 2022. We exclude papers for which data is unavailable or that do not fit into our framework for various reasons, e.g. having multiple interventions on the same unit with a time series structure. The included papers are Abebe et al. (2021), Baysan (2022), Casey et al. (2021), Dellavigna et al. (2022), Domurat et al. (2021), Hussam et al. (2022), and Lowe (2021). We additionally include data from Banerjee et al. (2021), a study with significant treatment effect heterogeneity as recently analyzed by Chernozhukov et al. (2023), as well as data from the Oregon health insurance experiment, reported in Finkelstein et al. (2012), for a total of N=9.

For each paper, we impute missing potential outcomes for all units, defining the imputation  $\tilde{Y}_i(d) = Y_i(d)\mathbb{1}(D_i = d) + \hat{Y}_i(d)\mathbb{1}(D_i \neq d)$ . Following the empirical exercise in Bai (2022), we use the matching-based imputation  $\widehat{Y}_i(d) = Y_{j(i)}(d)$  with j(i) = $\operatorname{argmin}_{j:D_j=d} |\psi_i - \psi_j|_2$ . Let  $N_0$  denote the size of the original experiment. Using this full panel of imputed potential outcomes, we do the following:

- (1) Draw  $(\tilde{Y}_i(0), \tilde{Y}_i(1), \psi_i)$  for  $i = 1, \ldots, n$  with replacement from  $(\tilde{Y}_i(0), \tilde{Y}_i(1), \psi_i)_{i=1}^{N_0}$ .
- (2) Randomize  $T_{1:n}$  and  $D_{1:n}$  according to one of the designs (a)  $\mathbf{CR}$  (b)  $\mathbf{CR}$ ,  $\mathbf{Loc}$  (c) Loc (d) Hom and (e) Pilot S/L.
- (3) Reveal outcomes  $\tilde{Y}_i = T_i D_i \tilde{Y}_i(1) + T_i (1 D_i) \tilde{Y}_i(0)$ , form the estimator  $\hat{\theta}$  and confidence interval  $\widehat{C} = [\widehat{\theta} \pm \widehat{V}^{1/2} c_{1-\alpha/2} / \sqrt{n}]$  for  $\alpha = 0.05$ .

Since the ATE for the imputed DGP  $(\tilde{Y}_i(0), \tilde{Y}_i(1), \psi_i)_{i=1}^N$  is known, we can compute the standard deviation (SD), 19 coverage probabilities, and percent reduction in confidence interval length for each DGP and design. The goal of this exercise is to quantify the marginal variance reduction from each of our methods on the type of DGP's that occur in applied economics research, isolating the separate efficiency gains from finely stratified assignment, finely stratified sampling, as well as implementation of the optimal propensities from Section 4.

Descriptions of each paper, including the treatment and outcome variables, our choice of stratification variables  $\psi$ , level of aggregation, and other parameters are provided in Section A.1 in the appendix. Experiment sizes n are as in the original papers, ranging from n = 91 for Casey et al. (2021) to n = 1903 for Finkelstein et al. (2012).

<sup>&</sup>lt;sup>18</sup>Model-based imputation of  $Y_i(d) = m_d(\psi_i) + \sigma_d^2(\psi_i)\epsilon_i^d$  with  $E[\epsilon_i^d|\psi_i] = 0$ ,  $Var(\epsilon_i^d|\psi_i) = 1$ , and  $\epsilon_i^d \sim \mathcal{N}(0,1)$  yields qualitatively similar results.

<sup>19</sup>All of our designs and estimators have  $E[\widehat{\theta} - ATE] = 0$ , so we do not report MSE.

	Design, Paper	A.	Ban.	Bay.	С.	De.	Do.	F.	Н.	L.
SD	CR	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
	CR, Loc	0.81	0.48	0.51	0.88	0.55	0.93	0.79	0.73	0.87
	$\operatorname{Loc}$	0.75	0.45	0.39	0.84	0.47	0.88	0.74	0.70	0.76
	Hom.	0.72	0.46	0.44	0.79	0.58	0.86	0.85	0.68	0.90
	Pilot S	0.72	0.45	0.55	0.81	0.57	1.01	0.75	0.71	0.75
	Pilot L	0.70	0.42	0.52	0.81	0.52	0.87	0.65	0.68	0.71
	CR	0	0	0	0	0	0	0	0	0
$\%\Delta { m CI}$	CR, Loc	-11	-49	-41	-6	-36	-4	-14	-10	-11
	Loc	-12	-48	-38	-5	-33	-4	-14	-15	-11
	Hom.	-21	-44	-47	-6	-40	-8	-8	-16	-10
	Pilot S	-19	-47	-23	-5	-23	3	-18	-15	-21
	Pilot L	-21	-52	-31	-5	-30	-9	-27	-18	-24
Cover	CR	0.95	0.95	0.95	0.94	0.96	0.95	0.94	0.94	0.96
	CR, Loc	0.96	0.96	0.99	0.96	0.98	0.96	0.96	0.98	0.96
	Loc	0.98	0.97	1.00	0.96	1.00	0.97	0.97	0.97	0.98
	Hom.	0.97	0.98	0.98	0.97	0.97	0.96	0.96	0.98	0.95
	Pilot S	0.97	0.98	0.99	0.96	0.99	0.95	0.97	0.98	0.97
	Pilot L	0.97	0.97	0.99	0.97	0.99	0.96	0.97	0.97	0.96
	$\overline{n}$	1451	903	550	91	446	1000	1903	116	770
	$\dim(\psi)$	8	6	3	3	3	4	6	4	3

Table 1: Empirical Results

The one exception is Domurat et al. (2021) ( $N_0 = 87394$ ), for which we set n = 1000 for Monte Carlo tractability. Baseline treatment proportions are set to p = 1/2, except for Lowe (2021) with p = 2/3 and Finkelstein et al. (2012) with p = 1/3. We use the large experiment version of our method with folds of size 200 (Section 2.1) and implement sampling subordinate assignment (Remark 3.14).

Costs and Discretization - Our theory showed that efficiency can be improved by (1) sourcing a large pool of units willing to participate in the experiment and (2) choosing a representative experimental subsample from this pool. If the marginal cost of including a unit is zero, step (2) is trivial, and we just take as many units as possible. The marginal cost  $C(\psi)$  of including different units is not reported in the papers in our sample. To understand the potential variance reduction from representative sampling with fixed q as well as the varying optimal propensity  $q^*(\psi)$  in the types of DGP's that occur in applied economics research, we specify non-zero costs  $C(\psi) = \mathbb{1}(|\psi|_2 \le \kappa) + 5\mathbb{1}(|\psi|_2 > \kappa)$  with  $\kappa = \mathrm{Median}_{i=1}^n |\psi_i|_2$  and  $\bar{B} = 1.5$ . This results in feasible constant sampling proportions  $q \approx 7/10$ . For example, if  $\psi_i$  were village location relative to an urban center, this would correspond to higher cost of collecting data in rural villages which, anecdotally, is a common feature of experiments in development economics. We discretize  $q_{hom}^*(\psi)$ and  $q^*(\psi)$  by choosing  $q_k(\cdot)$  to minimize discretization error  $E_n[(q_k - q^*)^2(\psi_i)]$  over the set  $\{q: q(\psi) \in a/10: a=1,\ldots,10\}$  subject to a constraint on the number of distinct propensity levels  $L_n = |\text{Image}(q_k)|$ , with  $L_n \le 2$  for n < 500,  $L_n \le 3$  for  $500 \le n < 1000$ and  $L_n \le 4$  for  $1000 \le n \le 2000$ .

Results. Our main results are presented in Table 1, with papers listed by initials of the first author. The largest change in standard deviation (SD) is in the contrast between complete randomization CR and finely stratified assignment CR, Loc, with an average of -27% across the papers in our sample. This improvement is particularly striking in papers like Baysan (2022) and Banerjee et al. (2021) with highly predictive baseline covariates. The average marginal change in SD attributable to finely stratified sampling (from CR, Loc to Loc) is smaller at -6%. Recall that stratified sampling reduces the variance component  $\operatorname{Var}(c(\psi)) \to q \operatorname{Var}(c(\psi))$ , with q = 7/10 in our simulations. Larger reductions may be expected for smaller q (more eligible units). Using the optimal sampling proportions  $q_{hom}^*(\psi)$ , which assume homoskedasticity, reduces the variance for some studies but increases it for others, resulting in +4% change on average. This is not surprising considering that many of these studies have considerable heteroskedasticity. The change in SD between Loc and Pilot S is +4% on average, while for the case with

a large pilot the change in SD from **Loc** to **Pilot L** is -5% on average. This shows that with a large pilot, closely related previous experiment, or observational data from the same population, the feasible estimates of the optimal designs in Section 4 can be used to increase efficiency. However, our empirical results suggest this may not be appropriate when only a small pilot study is available.

Next we discuss the performance of our inference methods (Section 7). Coverage is close to nominal, but somewhat conservative in finite samples. This is due to two different forces. First, match quality between groups g and  $\nu(g)$  in the collapsed-strata variance estimators  $\hat{v}_1$  and  $\hat{v}_0$  is worse than match quality within groups, which results in  $\hat{v}_1$  and  $\hat{v}_0$  in Section 7 being conservative. This effect is most severe for designs with highly predictive covariates. Second, match quality at the sampling stage  $T_{1:n} \sim \text{Loc}(\psi, q(\psi))$  is generally better than match quality at the assignment stage, since more units are available during sampling. However, our variance estimators can only only use the "thinned out" outcome data available for the units  $T_i = 1$  included in the experiment, which underestimates match quality during sampling. This effect will be most severe for small sampling proportions  $q \to 0$  and in DGP's with significant treatment effect heterogeneity.

The change in confidence interval length  $\%\Delta CI$  is slightly conservative but broadly reflects the efficiency gains in the first panel. This shows that our inference methods are able to take advantage of the reduction in variance from both finely stratified sampling and assignment, as well as designs with varying sampling proportions.

## 9 Recommendations for Practice

Our empirical results show robust variance reductions from fine stratification at both the sampling and assignment stages. When choosing stratification variables  $\psi$ , we recommend including baseline outcomes, if available, and a small set of other variables suspected to be predictive of outcomes and treatment effect heterogeneity. In particular, if experimenters have pre-registered measuring treatment effect heterogeneity with respect to a certain variable, then it is natural to include this variable in  $\psi$ . Fine stratification methods increase the value of collecting baseline survey data, insofar as extra investment in the baseline survey process allows us to measure variables expected to be most predictive of outcomes and treatment effect heterogeneity. Our theory in Section 3 showed that the efficiency gains from stratified sampling are larger the more eligible

units we have, since this helps sample more representative experimental units. Because of this, sourcing a large pool of candidate units for the experiment can improve precision, even if the experimental budget constraints do not allow all of these units to ultimately be included in the experiment.

The feasible sampling design  $q_{hom}^*(\psi)$  (assuming homoskedasticity) had mixed effects in the empirical application. Relative to the simpler  $\mathbf{Loc}$  design with constant propensity q, the  $q_{hom}^*(\psi)$  design reduced variance for some DGP's but increased it for others. Aside from potential misspecification, there is a finite sample tradeoff between (R) better optimization of the residual variance by using varying sampling propensity  $q(\psi)$  and (M) worse sampling and assignment matches due to having many different  $q(\psi)$  strata. For experiments with highly predictive covariates, effect (M) may dominate, so that a design with constant  $q(\psi) = q$  may be preferable. However, if costs are very heterogeneous, then the residual variance effect (R) will dominate, and  $q_{hom}^*(\psi)$  can produce significant efficiency gains. The estimated optimal designs from Section 6 performed well in our empirical application for  $n_{pilot} = 400$ , but were generally too noisy for  $n_{pilot} = 100$ . In the absence of a very large pilot or related previous experiment, one alternative is to use observational data to calibrate the ex-ante variance function  $\bar{\sigma}^2(\psi)$  appearing in the optimal design  $q^*(\psi)$ . This could improve on the design  $q^*_{hom}(\psi)$ , which unrealistically assumes perfect homoskedasticity, without the added noise associated with estimating the ex-ante variance  $\bar{\sigma}^2(\psi)$  from a small pilot.

Finally, the inference methods in Section 7 were slightly conservative in finite samples, but still allow researchers to report smaller confidence intervals that reflect the efficiency gains from finely stratified sampling and assignment.

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## 10 Appendix

#### 10.1 Finite Population Estimands

If the eligible units  $\{1, \ldots, n\}$  comprise the entire population of interest, then we may be interested in estimation and inference on the sample average treatment effect SATE =  $E_n[Y_i(1) - Y_i(0)]$ , or the average conditional treatment effect (ACTE)  $E_n[c(\psi_i)]$ , studied in Armstrong and Kolesár (2021). Note that both estimands are defined over the full population of eligible units, not just the smaller set of experiment participants  $\{i: T_i = 1\}$ . For the SATE, suppose  $T_{1:n} \sim \text{Loc}(\psi, q)$  and  $D_{1:n} \sim \text{Loc}(\psi, p)$  and define the residual treatment effect variance  $\sigma_{\tau}^2(\psi) = \text{Var}(Y(1) - Y(0)|\psi)$ . Under the same conditions as Theorem 3.2, we have  $\sqrt{n_T}(\hat{\theta} - \text{SATE}) \Rightarrow \mathcal{N}(0, V_{\text{SATE}})$  with

$$V_{\text{SATE}} = E \left[ \frac{\sigma_1^2(\psi)}{p} + \frac{\sigma_0^2(\psi)}{1 - p} - q\sigma_\tau^2(\psi) \right].$$
 (10.1)

The final variance component  $E[\sigma_{\tau}^2(\psi)]$  is not identified, as in the case of SATE estimation under complete randomization. Setting  $\psi=1$  and q=1 recovers the classical results in that setting. Observe that  $V_{\text{SATE}}$  decreases as the residual treatment effect heterogeneity  $\sigma_{\tau}^2(\psi)$  increases. The negative sign reflects a competition between two opposing forces. To see this, let  $\bar{Y}_i = Y_i(1)/p + Y_i(0)/(1-p)$  and consider the error decomposition

$$\widehat{\theta} - \text{SATE} = \text{Cov}_n(T_i, Y_i(1) - Y_i(0))/q + \text{Cov}_n(D_i, \bar{Y}_i | T_i = 1).$$

The first term parameterizes the errors due to correlation between the sampling variables and treatment effects, and naturally increases with  $\sigma_{\tau}^2(\psi) = \text{Var}(Y(1) - Y(0)|\psi)$ . The second term is increasing in  $\text{Cov}(Y(1), Y(0)|\psi)$ , or equivalently decreasing in  $\sigma_{\tau}^2(\psi)$ , and larger in mean square, resulting in a net negative dependence on  $\sigma_{\tau}^2(\psi)$ . As  $q \to 0$ , the relative variance<sup>20</sup> due to sampling increases, exactly cancelling the  $E[\sigma_{\tau}^2(\psi)]$  fac-

The normalization  $\sqrt{n_T(\hat{\theta} - \text{SATE})}$  by experiment size  $n_T = \sum_i T_i$  holds the number of sampled units fixed.

tor due to assignment in the limit. Conservative inference for the SATE under stratified sampling and assignment can be based on either of the lower bounds  $\sigma_{\tau}^{2}(\psi) \geq \sigma_{1}^{2}(\psi) + \sigma_{0}^{2}(\psi) - 2\sigma_{1}(\psi)\sigma_{0}(\psi) \geq 0$ .

The average conditional treatment effect ACTE =  $E_n[c(\psi)]$  is more difficult to motivate from a policy perspective. One potential application is a structural model of the form  $Y_{it}(1) - Y_{it}(0) = c(\psi_i) + \epsilon_{it}$ , with systematic component  $c(\psi_i)$  mediated solely through observables  $\psi$  and transitory shock component  $\epsilon_{it}$ . Intuitively, in this model the ACTE acts like a "denoised" version of the SATE. If the  $\epsilon_{it}$  are uncorrelated, the ACTE estimated at time t is the best predictor of the SATE for a policy implemented at time t+1. The proof of Theorem 3.2 shows that  $\sqrt{n_T}(\widehat{\theta} - E_n[c(\psi_i)]) \Rightarrow \mathcal{N}(0, V_c)$  with identified variance  $V_c = E[\sigma_1^2(\psi)/p + \sigma_0^2(\psi)/(1-p)] \geq V_{\text{SATE}}$ .

#### 10.2 Details of Matching Algorithm

Write  $n = lk + \delta$  for some integer l and  $0 \le \delta < k$ . First, match a remainder group of size  $\delta$  and set it aside. Then suppose without loss that n = lk. Let J be the minimal positive integer such that  $2^J \ge k$  and let  $\sum_{j=0}^{J-1} a_j 2^j$  with  $a_j \in \{0,1\}$  be the binary representation of  $2^J - k \ge 0$ . Before the jth call of Derigs' algorithm, add l singleton groups of fake units  $g = \{F_j\}$  of type j to the dataset if and only if  $a_j = 1$ . Let R(g) denote the real units in a group  $R(g) \subseteq [n]$  and F(g) the fake units so that  $g = R(g) \cup F(g)$ . Before the jth call to Derig's algorithm, set  $d(g,g') = +\infty$  if either of the following occur: (1)  $F(g) \cap F(g') \ne \emptyset$  or (2)  $|F(g) \cup F(g')| > 0$  but  $|F(g) \cup F(g')| \ne \sum_{i=0}^{j} a_i$ . Otherwise, set the distance  $d(g,g') = |\bar{\psi}_{R(g)} - \bar{\psi}_{R(g')}|_2^2$ . Compute the optimal pairing at each step. After J steps, remove all the fake units by setting g = R(g). The binary representation trick is inspired by Karmakar (2022), who studies a related matching problem. However, the algorithm in his paper does not seem to guarantee groups of the correct cardinality for larger k.

Figure 4 shows PCA Folds for the "large experiment" version of our algorithm. We use the data from Finkelstein et al. (2012), with K = 4 folds and n = 1903 samples.

<sup>&</sup>lt;sup>21</sup>Inference on a more general denoised SATE parameter in a model with transitory shocks is studied in Deeb and de Chaisemartin (2022).

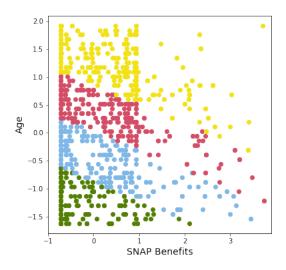


Figure 4: PCA Folds

#### 10.3 Remarks

Remark 10.1 (Increasing Stratification Condition). At a high level, the condition  $\psi_1 \subseteq \psi_2$  allows us to ignore the complicated effect of first-stage sampling on the joint distribution of sampled stratification variables  $(\psi_{1,i})_{i:T_i=1}$ . To see the problem, observe that if q = 1/k then  $T_i = T_j = 1$  implies that i, j cannot have been matched together during sampling, since otherwise only one of them would have T = 1. Then, for instance, we expect these units to be some distance from each other, so that

$$P(|\psi_{1,i} - \psi_{1,j}| < \epsilon) > P(|\psi_{1,i} - \psi_{1,j}| < \epsilon \,|\, T_i = T_j = 1). \tag{10.2}$$

If  $E[Y_i(d)|\psi_{1,i}] \neq 0$ , such changes to the joint distribution will show up in the conditional variance  $\operatorname{Var}(\widehat{\theta}|\psi_{1:n},T_{1:n})$  in complicated ways that depend on the details of the matching algorithm. However, we can use the fact that the assignment stratification "partials out"  $Y_i(d)$  so that, to first order, only the residuals  $u_i = Y_i - E[Y_i(d)|\psi_{2,i}]$  enter this conditional variance. If  $\psi_1 \subseteq \psi_2$  the residuals  $u_i$  are less affected by selection on  $\psi_{1,i}$ . For example, under this condition we can show that  $E[u_iu_j|T_i=T_j=1]=E[u_iu_j]=0$ . We conjecture the theorem may be true without this condition if the effects in Equation 10.2 are lower order, but leave the detailed study of this issue for specific matching procedures to future work.

# Online Appendix to "Optimal Stratification of Survey Experiments"

#### Max Cytrynbaum

#### A.1 Empirical Application Details

This section provides descriptions of each paper and implementation details for our empirical application in Section 8. In all cases, we normalize the stratification variables so that  $Var(\psi_{ij}) = 1$  for  $j = 1, ..., dim(\psi)$ .

- (1) Abebe et al. (2021) estimates the effect of an application incentive on the ability of applicants for clerical employment in Ethiopia. We let Y be the authors' index of cognitive ability, D be the application incentive, and  $\psi(X)$  be gender, age, work experience in years, self-reported gpa and previous wage, and indicators for being born in Addis Ababa, speaking Amharic, and studying engineering.
- (2) Banerjee et al. (2021) estimates the effect of various strategies to promote child-vaccination on the number of children completing the full vaccination sequence. We let  $Y_i$  be the number of children receiving the measles shot over the full trial period in village i and  $D_i$  whether the village received the SMS reminder intervention. We let  $\psi$  include village population, the proportion of individuals in the baseline survey of that village who were in a "scheduled caste", a "backward class", who received nursery education or less, the proportion of vaccine completions among older children, and proportion who had a vaccine card.
- (3) Baysan (2022) estimates the effect of political information campaigns about concentration of executive power in Turkey on voter polarization. Data is at the ballot box level, while assignment to information campaigns is at the neighborhood level. We let  $Y_i$  be the vote share of "No" votes, averaged over ballot boxes in a neighborhood, in the 2017 referendum. We let D be whether the village was exposed to any information campaign, and  $\psi$  include the village-level average vote share for the CHP in the 2015 election, a measure of turnout, and the number of ballots collected.
- (4) Casey et al. (2021) estimates the effect of increased information given to political parties about voter preferences over candidates on whether the most voter-

preferred candidate was selected to run by the party. We let D be assignment to the treatment package at the party-constituency level, Y whether the most preferred candidate was selected, and let  $\psi$  include competitiveness of the race, candidate professional qualifications index, and candidate public service motivation index.

- (5) Dellavigna et al. (2022) estimates the effect of employer gifts and other "social preference" related interventions on worker productivity. We study the first experiment in the paper and let D=1 if the worker received either a positive gift or an in-kind gift and D=0 for no gift or a negative gift. We let Y be worker output in the last working period. We let  $\psi$  be total productivity during the first 8 periods of the trial (excluding the final gift period), gender, and age.
- (6) Domurat et al. (2021) estimates the effect of informational interventions about Covered California insurance policies on takeup of insurance. We let D=0 for the control group and D=1 if assigned to any of the letter campaigns in arms 3, 4, or 5. Y is an indicator for insurance takeup.  $\psi$  includes a measure of household income, mean age, household subsidy size, and an indicator for being Latino.
- (7) Finkelstein et al. (2012) reports the effect of winning the 2008 Oregon Medicaid lottery on various health and public service utilization outcomes. We use data from wave one, restricting to single person households. We estimate an ITT effect with Y the number of emergency department (ED) visits in the post-period and D an indicator for winning the lottery. We let  $\psi$  include gender, age, any visits to the ED in the pre-period, number of visits in the pre-period, total SNAP benefits in the pre-period, and indicators for ever being on SNAP or having a chronic condition.
- (8) Hussam et al. (2022) estimates the value of employment on measures of psychosocial wellbeing. Treatment assignment is at the block level in the refugee camp, with a sample of five individuals chosen in each block. We aggregate by taking the mean of outcomes and covariates in each block. We let D=0 if the block was randomized to cash only and D=1 if it was randomized to employment. Y is the endline mental health index, and  $\psi$  includes the baseline mental health index, average gender (in [0,1]), proportion who had a family member killed, and a measure of sociability.
- (9) Lowe (2021) estimates the effect of collaborative and adversarial intergroup contact on cross-caste friendships using randomization to different teams in a cricket league in India. We let Y be number of other caste friends at endline, D be whether the

person is assigned to a mixed caste team, and  $\psi$  include number of other caste friends at baseline, age, and a measure of cricket ability.

#### A.2 Heteroskedasticity Function Estimation

The theory in Section 6 requires heteroskedasticity function estimates  $\hat{\sigma}_d^2(\psi)$ . Our simulations and empirical application using a modification of Fan and Yao (1998). In a setting without outcomes  $Y = m(X) + \sigma^2(X)\epsilon$ , they propose (1) use local linear regression to estimate m(X) and (2) use local linear regression to project estimated residuals  $(Y - \hat{m}(X))^2$  on X. In our setting, we let  $\tilde{Y}_i(1) = Y_i D_i T_i/p_i q_i$  and (1) project  $\tilde{Y}_i(1) \sim \psi_i$  to estimate  $m_1(\psi_i)$ . Next, we (2) project weighted residuals  $\tilde{\epsilon}_i(1)^2 = (Y_i - \hat{m}(\psi_i))^2 D_i T_i/p_i q_i \sim \psi_i$  to estimate  $\hat{\sigma}_1^2(\psi_i)$ , and similarly for d = 0. We tested linear ridge regression, RBF-kernel ridge regression, and random forests for each regression step, with hyperparameters chosen by cross-validation in all cases. Kernel ridge estimated  $\sigma_d^2(\psi)$  the most precisely in dimensions  $\dim(\psi) = 1, 2$ , while forests were superior in higher dimensions. Our simulation and empirical results are presented using random forest regression. Pilot data is drawn from a stratified experiment of the specified size with p = 1/2.

## A Proofs

## A.1 Matching

**Theorem A.1** (Matching). Consider triangular arrays  $(\psi_{i,n})_{i=1}^n \subseteq \mathbb{R}^d$  and  $(p_{i,n})_{i=1}^n \subseteq \mathbb{Q}$  with levels  $p_{i,n} \in L_n = \{a_l/k_l\}$  and  $\overline{k}_n = \max\{k_l : a_l/k_l \in L_n\}$ . For any sequence of subsets  $S_n \subseteq [n]$ , there exists a sequence of partitions  $(\mathcal{G}_n)_{n\geq 1}$  of  $S_n$  such that  $\mathcal{G}_n = \bigcup_l \mathcal{G}_{nl}$  and  $\mathcal{G}_{nl}$  partitions  $S_n \cap \{i : p_{i,n} = a_l/k_l\}$  with  $|g| = k_l$  for all but one non-empty group  $g \in \mathcal{G}_{nl}$ . The partition  $\mathcal{G}_n$  satisfies the homogeneity rate

$$n^{-1} \sum_{g \in \mathcal{G}_n} \frac{1}{|g|} \sum_{i,j \in g} |\psi_{i,n} - \psi_{j,n}|_2^2 \le (1 \vee \max_{i=1}^n |\psi_{i,n}|_2^2) \cdot O((n/\overline{k}_n |L_n|)^{-2/(d+1)}). \tag{A.1}$$

Let  $\mathcal{G}_{nl}^*$  be the optimal partition of  $S_n \cap \{i : p_{i,n} = a_l/k_l\}$ , solving the minimization

$$\mathcal{G}_{nl}^* = \underset{\mathcal{G}_{nl}}{\operatorname{argmin}} \left[ n^{-1} \sum_{g \in \mathcal{G}_{nl}} \sum_{i,j \in g} |\psi_{i,n} - \psi_{j,n}|_2^2 \right]$$

subject to the group size constraint  $|g| = k_l$ . Then  $\mathcal{G}_n^* = \bigcup_l \mathcal{G}_{nl}^*$  satisfies the homogeneity rate in Equation A.1.

*Proof.* First, note that for any partition  $\mathcal{G}_n$ 

$$\frac{1}{n} \sum_{q \in \mathcal{G}_n} \frac{1}{|g|} \sum_{i,j \in g} |\psi_{i,n} - \psi_{j,n}|_2^2 \le (1 \vee \max_{i=1}^n |\psi_{i,n}|_2^2) \cdot \frac{1}{n} \sum_{q \in \mathcal{G}_n} \frac{1}{|g|} \sum_{i,j \in g} \left| \frac{\psi_{i,n} - \psi_{j,n}}{1 \vee \max_{i=1}^n |\psi_{i,n}|_2} \right|_2^2$$

Clearly,  $|\psi_{i,n}/(1 \vee \max_{i=1}^n |\psi_{i,n}|_2)|_2 \leq 1$  for all  $1 \leq i \leq n$ . Then by recentering, it suffices to show the claim for  $\psi_{i,n} \in [0,1]^d$  for all  $1 \leq i \leq n$  as  $n \to \infty$ . Consider blocks of the form  $B = \{\sum_{k=1}^d x_k e_k : x_k \in [s_k/m, (s_k+1)/m]\}$  for indices  $\{s_k\}_{k=1}^d \subseteq \{0, \ldots, m-1\}$ . Fix an ordering of these blocks  $(B_l)_{l=1}^{m^d}$  such that  $B_l$  and  $B_{l+1}$  are adjacent for all l. Intuitively, this forms a "block path" through  $[0,1]^d$ , see Bai et al. (2021) for a picture. Define  $l(i) = \min_{l=1}^{m^d} \{l : \psi_{i,n} \in B_l\}$ .

Algorithm - Fix  $p_a \in L_n$  and form groups  $(g_{a,s})_{s=1}^n$  of units  $g_{a,s} \subseteq \{i : p_{i,n} = p_a = f_a/k_a\}$  by induction as follows. (1) Form groups of size  $k_a$  arbitrarily among  $\{i : l(i) = 1, and p_n(X_i, \xi_n) = p_a$ , possibly using external randomness  $\pi_n$ . This process results in at most one partially completed group with  $|g_{a,s'}| < k_a$ . While  $|g_{a,s'}| < k_a$ , do the following: (2) increment  $l \to l+1$  and (3) add an unmatched unit i with l(i) = l+1 to this group. If  $|g_{a,s'}| = k_a$ , stop. If  $|g_{a,s'}| < k_a$  and there are unmatched units in  $B_{l+1}$ , goto (3). If  $|g_{a,s'}| < k_a$  and there are no unmatched units in  $B_{l+1}$ , increment l and go to (1). Suppose that  $g_{a,s'}$  is completed with a unit from  $B_{l'}$ . Then repeat the process above starting with the next group  $g_{a,s'+1}$  and the units in block  $B_{l'}$ . Since there are  $n < \infty$  units, this process terminates. Repeat this for each  $a = 1, \ldots, |L_n|$ . By construction, this creates groups  $\mathcal{G}_n = \{g_{a,s} : 1 \le a \le |L_n|, 1 \le s \le n\}$  with the ordering property

$$l(i) \le l(j) \quad \forall i \in g_{a,s}, j \in g_{a,s'} \quad s < s' \quad a = 1, \dots, |L_n|$$
 (A.2)

Fix an indexing of all within-group pairs  $(\mathfrak{p}_{a,s,t})_{t=1}^{k_a^2-k_a} \equiv \{(i,j): i \neq j; i,j \in g_{a,s}\},$  and denote  $\mathfrak{p}_{a,s,t} = (i_{a,s,t},j_{a,s,t})$ . Define  $E_{a,s,t} = \{l(i_{a,s,t}) = l(j_{a,s,t})\},$  the event that a pair

is in the same element of the block partition. With this notation, we have

$$n^{-1} \sum_{g \in \mathcal{G}_n} \frac{1}{|g|} \sum_{i,j \in g} |\psi_{i,n} - \psi_{j,n}|_2^2 = n^{-1} \sum_{a=1}^{|L_n|} \sum_{s=1}^n k_a^{-1} \sum_{i,j \in g_{a,s}} |\psi_{i,n} - \psi_{j,n}|_2^2$$

$$\leq n^{-1} \sum_{a=1}^{|L_n|} \sum_{s=1}^n k_a^{-1} \sum_{t=1}^{k_a^2 - k_a} |\psi_{i_{a,s,t},n} - \psi_{j_{a,s,t},n}|_2^2 \mathbb{1}(g_{a,s} \neq \emptyset)$$

(1) Suppose  $E_{a,s,t}$  occurs. Then  $d_{a,s,t} \equiv |\psi_{i_{a,s,t},n} - \psi_{j_{a,s,t},n}|_2 \leq \max_{l=1}^{m^d} \operatorname{diam}(B_l, |\cdot|_2) \leq \sqrt{d}/m$  on this event. Then we may bound

$$n^{-1} \sum_{a=1}^{|L_n|} \sum_{s=1}^n k_a^{-1} \sum_{t=1}^{k_a^2 - k_a} d_{a,s,t}^2 \mathbb{1}(E_{a,s,t}) \mathbb{1}(g_{a,s} \neq \emptyset) \le \frac{d}{nm^2} \sum_{a=1}^{|L_n|} \sum_{s=1}^n k_a^{-1} \sum_{t=1}^{k_a^2 - k_a} \mathbb{1}(g_{a,s} \neq \emptyset)$$

$$\le \frac{d}{nm^2} \sum_{a=1}^{|L_n|} \sum_{s=1}^n k_a \mathbb{1}(g_{a,s} \neq \emptyset) \le \frac{d}{m^2}$$

The final inequality since the double sum exactly counts the number of units in the sample (by group)  $\sum_{a=1}^{|L_n|} \sum_{s=1}^n k_a \mathbb{1}(g_{a,s} \neq \emptyset) = |S_n| \leq n$ .

(2) Now consider the terms where  $E_{a,s,t}$  does not occur. Fix any such pair  $(i_{a,s,t}, j_{a,s,t})$ . Without loss, suppose the block membership  $l(i_{a,s,t}) < l(j_{a,s,t})$ . For  $l(i_{a,s,t}) \le l \le l(j_{a,s,t})$ , define a sequence  $z_l$  as follows.  $z_{l(i_{a,s,t})} = \psi_{i_{a,s,t},n}$ ,  $z_{l(j_{a,s,t})} = \psi_{j_{a,s,t},n}$  and  $z_l \in B_l$  chosen arbitrarily otherwise. Note that for  $x \in B_l$  and  $y \in B_{l+1}$ , by construction of the contiguous blocks  $|x - y|_2 \le 2\sqrt{d}/m$ . Then by telescoping and triangle inequality, on the event  $E_{a,s,t}^c$ 

$$d_{a,s,t} = |\psi_{i_{a,s,t},n} - \psi_{j_{a,s,t},n}|_2 \le \sum_{l=l(i_{a,s,t})}^{l(j_{a,s,t})-1} |z_{l+1} - z_l|_2 \le \frac{2\sqrt{d}}{m} \cdot [l(j_{a,s,t}) - l(i_{a,s,t})]$$

Note also that if  $x, y \in [0, 1]^d$  then  $|x - y|_2^2 = d(|x - y|_2/\sqrt{d})^2 \le \sqrt{d}|x - y|_2$ , using  $c^2 \le c$ 

for  $0 \le c \le 1$ . In particular, we have  $d_{a,s,t}^2 \le \sqrt{d} \cdot d_{a,s,t}$ .

$$n^{-1} \sum_{a=1}^{|L_n|} \sum_{s=1}^n k_a^{-1} \sum_{t=1}^{k_a^2 - k_a} d_{a,s,t}^2 \mathbb{1}(E_{a,s,t}^c) \le \sqrt{d} n^{-1} \sum_{a=1}^{|L_n|} \sum_{s=1}^n k_a^{-1} \sum_{t=1}^{k_a^2 - k_a} d_{a,s,t} \mathbb{1}(E_{a,s,t}^c)$$

$$\sum_{a=1}^{|L_n|} \frac{2d}{mnk_a} \sum_{t=1}^{k_a^2 - k_a} \sum_{s=1}^n [l(i_{a,s,t}) - l(j_{a,s,t})] \mathbb{1}(E_{a,s,t}^c) \le \sum_{a=1}^{|L_n|} \frac{2\sqrt{d}}{mnk_a} \sum_{t=1}^{k_a^2 - k_a} m^d$$

$$\le \sum_{a=1}^{|L_n|} \frac{2\sqrt{d}m^d}{mn} k_a \le 2\sqrt{d} |L_n| \overline{k}_n n^{-1} m^{d-1}$$

The second inequality follows by the ordering property in equation A.2 above, since for each  $t = 1, ..., k_a^2 - k_a$ , the intervals  $([l(i_{a,s,t}), l(j_{a,s,t})])_{s=1}^n$  are non-overlapping, and there are at most  $m^d$  blocks. Summarizing the above work, we have shown that

$$n^{-1} \sum_{a=1}^{|L_n|} \sum_{s=1}^n k_a^{-1} \sum_{i,j \in g_{a,s}} |\psi_{i,n} - \psi_{j,n}|_2^2 \le n^{-1} \sum_{a=1}^{|L_n|} \sum_{s=1}^n k_a^{-1} \sum_{t=1}^{k_a^2 - k_a} d_{a,s,t}^2 \mathbb{1}(E_{a,s,t}) + d_{a,s,t}^2 \mathbb{1}(E_{a,s,t})$$

$$\le \frac{d}{m^2} + \frac{2\sqrt{d}|L_n|\overline{k}_n m^{d-1}}{n}$$

Setting  $m \simeq (n/(|L_n|\overline{k}_n))^{1/(d+1)}$  gives the rate

$$n^{-1} \sum_{a=1}^{|L_n|} \sum_{s=1}^n k_a^{-1} \sum_{i,j \in q_{a,s}} |\psi_{i,n} - \psi_{j,n}|_2^2 = O\left(\left(n/(|L_n|\overline{k}_n)\right)^{-2/(d+1)}\right)$$

This finishes the proof of the first statement. The second statement follows by optimality of  $\mathcal{G}_{nl}^*$  and comparison with the groups just constructed.

#### A.2 Balance

**Lemma A.2** (Stochastic Balance). Let  $(\mathcal{F}_n)_{n\geq 1}$  such that treatment groups  $\mathcal{G}_n$ ,  $(h_n(W_i))_{i=1}^n \in \mathcal{F}_n$  for a sequence of functions  $(h_n)_{n\geq 1}$  and  $\mathcal{F}_n \perp t$ . Let  $D_{1:n} \sim \operatorname{Loc}(\psi_n, p_n)$  and  $T_{1:n} \in \{0,1\}^n$  such that  $\{i: T_i = 1\} = \sqcup_{g \in \mathcal{G}_n} g$ . The following hold

- (1)  $E[E_n[T_i(D_i p_n(X_i))h_n(W_i)]|\mathcal{F}_n] = 0$
- (2)  $\operatorname{Var}(E_n[T_i(D_i p_n(X_i)))h_n(W_i)]|\mathcal{F}_n) \le 2n^{-1}E_n[T_ih_n(W_i)^2] \le 2n^{-1}E_n[h_n(W_i)^2]$
- (3) Suppose  $\exists (\mathcal{F}_n)_{n\geq 1}$  satisfying the conditions above. If  $\sup_{n\geq 1} E[h_n(W)^2] < \infty$  then

 $E_n[T_i(D_i - p_n(X_i))h_n(W_i)] = O_p(n^{-1/2})$ . If  $(h_n(W))_{n\geq 1}$  is uniformly integrable then  $E_n[T_i(D_i - p_n(X_i))h_n(W_i)] = o_p(1)$ .

(4) The variance  $Var(\sqrt{n}E_n[T_i(D_i - p_n(X_i)))h_n(W_i)]|\mathcal{F}_n)$  is bounded above by

$$n^{-1} \sum_{g \in \mathcal{G}_n} |g|^{-1} \sum_{i,j \in g} (h_n(W_i) - h_n(W_j))^2 + n^{-1} \overline{k}_n |L_n| \cdot \max_{i=1}^n h_n(W_i)^2$$

*Proof.* First, by assumption  $\{i: T_i = 1\} = \bigsqcup_{g \in \mathcal{G}} g$ , so  $E_n[T_i(D_i - p_{i,n})h_n(W_i)]$  is

$$n^{-1} \sum_{g \in \mathcal{G}_n} \sum_{i \in g} (D_i - p_{i,n}) h_n(W_i) = n^{-1} \sum_{a=1}^{|L_n|} \sum_{s=1}^n \sum_{i=1}^n (D_i - p_a) h_n(W_i) \mathbb{1}(i \in g_{a,s})$$

By Lemma C.10 and our measurability assumptions

$$E[(D_i - p_a)h_n(W_i)\mathbb{1}(i \in g_{a,s})|\mathcal{F}_n] = h_n(W_i)E[(D_i - p_a)\mathbb{1}(i \in g_{a,s})|\mathcal{F}_n] = 0$$

By linearity, this shows the claim. By Lemma C.10,  $Var(E_n[(D_i - p_{i,n})h_n(W_i)]|\mathcal{F}_n)$  is

$$n^{-2} \sum_{a,a'}^{|L_n|} \sum_{s,s'=1}^{n} \sum_{i,j}^{n} \operatorname{Cov}((D_i - p_a)h_n(W_i)\mathbb{1}(i \in g_{a,s}), (D_j - p_{a'})h_n(W_j)\mathbb{1}(j \in g_{a',s'})|\mathcal{F}_n)$$

$$= n^{-2} \sum_{a,a'}^{|L_n|} \sum_{s,s'=1}^{n} \sum_{i,j}^{n} h_n(W_i)h_n(W_j)\mathbb{1}(i \in g_{a,s})\mathbb{1}(j \in g_{a',s'}) \operatorname{Cov}(D_i, D_j|\mathcal{F}_n)$$

$$= n^{-2} \sum_{a=1}^{|L_n|} \sum_{s=1}^{n} \sum_{i,j}^{n} h_n(W_i)h_n(W_j)\mathbb{1}(i,j \in g_{a,s}) \operatorname{Cov}(D_i, D_j|\mathcal{F}_n)$$

The final equality follows from Lemma C.10. By triangle inequality and the covariance bound in Lemma C.10, this is bounded above by

$$n^{-2} \sum_{a=1}^{|L_n|} \sum_{s=1}^n \left[ \sum_{i=1}^n h_n(W_i)^2 \mathbb{1}(i \in g_{a,s}) + \sum_{i \neq j}^n |h_n(W_i)| |h_n(W_j)| \mathbb{1}(i, j \in g_{a,s}) k_a^{-1} \mathbb{1}(s \neq n) \right]$$

$$\leq n^{-1} E_n [T_i h_n(W_i)^2] + \sum_{a=1}^{|L_n|} k_a^{-1} \sum_{s=1}^n \sum_{i \neq j}^n |h_n(W_i)| |h_n(W_j)| \mathbb{1}(i, j \in g_{a,s})$$

$$\leq n^{-1} E_n [T_i h_n(W_i)^2] + n^{-2} \sum_{a=1}^{|L_n|} k_a^{-1} \sum_{s=1}^n \left( \sum_{i=1}^n |h_n(W_i)| \mathbb{1}(i \in g_{a,s}) \right)^2$$

Continuing the calculation, by Jensen's inequality the second term is equal to

$$n^{-2} \sum_{a=1}^{|L_n|} k_a \sum_{s=1}^n \left( k_a^{-1} \sum_{i \in g_{a,s}} |h_n(W_i)| \right)^2 \le n^{-2} \sum_{a=1}^{|L_n|} \sum_{s=1}^n k_a k_a^{-1} \sum_{i \in g_{a,s}} |h_n(W_i)|^2 = n^{-1} E_n[T_i h_n(W_i)^2]$$

This completes the proof of (2). Claim (3) follows by applying (1), (2) with  $(\mathcal{F}_n)_{n\geq 1}$  any sequence satisfying the conditions, followed by Markov inequality (Lemma C.2). For the final part of (3), let  $c_n \to \infty$  with  $c_n = o(\sqrt{n})$  and define  $\bar{h}_{in} = h_n(W_i)\mathbb{1}(|h_n(W_i)| \leq c_n)$ . Consider the expansion  $E_n[T_i(D_i - p_{i,n})h_n(W_i)] = E_n[T_i(D_i - p_{i,n})(h_n(W_i) - \bar{h}_n(W_i))] + E_n[T_i(D_i - p_{i,n})\bar{h}_n(W_i)] \equiv A_n + B_n$ . We may write  $|A_n| \leq E_n[|h_n(W_i) - \bar{h}_n(W_i)|] = E_n[|h_n(W_i)|\mathbb{1}(|h_n(W_i)| > c_n)]$ . Then we have  $E[|A_n|] \leq E[|h_n(W_i)|\mathbb{1}(|h_n(W_i)| > c_n)] \to 0$  as  $n \to \infty$  by uniform integrability. Then  $A_n = o_p(1)$  by Markov inequality. By the first part of (3),  $Var(B_n|\mathcal{F}_n) \leq 2n^{-1}E_n[\bar{h}_n(W_i)^2] \leq 2n^{-1}c_n^2 = o(1)$ . Then  $B_n = o_p(1)$  by conditional Chebyshev.

For the final identity (5), note that from Lemma C.10 for  $s \neq n$  and  $p_a = q_a/k_a$ 

$$\sum_{i,j \in g_{a,s}} h_n(W_i) h_n(W_j) \operatorname{Cov}(D_i, D_j | \mathcal{F}_n) = \frac{q_a(k_a - q_a)}{k_a^2} \sum_{i \in g_{a,s}} h_n(W_i)^2 + \frac{q_a(k_a - q_a)}{k_a^2(k_a - 1)} \sum_{i,j \in q_{a,s}} (-2) h_n(W_i) h_n(W_j)$$

Note that  $-2ab = (a-b)^2 - a^2 - b^2$ . Then the second sum is

$$\sum_{i,j \in g_{a,s}} (-2)h_n(W_i)h_n(W_j) = \sum_{i,j \in g_{a,s}} [(h_n(W_i) - h_n(W_j))^2 - h_n(W_i)^2 - h_n(W_j)^2]$$

$$= \sum_{i,j \in g_{a,s}} (h_n(W_i) - h_n(W_j))^2 - (k_a - 1) \sum_{i \in g_{a,s}} h_n(W_i)^2$$

Substituting in the first display above, the diagonal terms cancel. For the claimed constant, note that  $\max_{p \in (0,1)} p(1-p) \le 1/4$  and  $\max_{k \ge 2} \frac{k}{k-1} \le 2$ , so  $\frac{q_a(k_a-q_a)}{k_a^2(k_a-1)} \le k_a^{-1}$ . Aggregating over (a,s) gives

$$n^{-1} \sum_{a=1}^{|L_n|} \left[ \sum_{s=1}^{n-1} \sum_{i,j \in g_{a,s}}^{n} (h_n(W_i) - h_n(W_j))^2 + \sum_{i=1}^{n} h_n(W_i)^2 \mathbb{1}(i \in g_{a,n}) \right]$$

The second term is

$$n^{-1} \sum_{a=1}^{|L_n|} \sum_{i=1}^n h_n(W_i)^2 \mathbb{1}(i \in g_{a,n}) \le n^{-1} \max_{i=1}^n h_n(W_i)^2 \sum_{a=1}^{|L_n|} \sum_{i=1}^n \mathbb{1}(i \in g_{a,n})$$

$$\le n^{-1} \overline{k}_n |L_n| \cdot \max_{i=1}^n h_n(W_i)^2$$

This finishes the proof.

**Lemma A.3** (Balancing). Suppose  $T_{1:n} \sim \text{Loc}(\psi_1, q(x))$  and  $D_{1:n} \sim \text{Loc}(\psi_2, p(x))$  with  $(\psi_1(X), q(X)) \in \sigma(\psi_2(X))$ , and  $\psi_1, \psi_2, q$ , and p possibly dependent on  $\xi \perp W_{1:n}$ . Suppose  $E[|\psi_1(X)|^{\alpha_1}] < \infty$  for  $\alpha_1 > d(\psi_2) + 1$  and  $E[|\psi_2(X)|^{\alpha_1}] < \infty$  for  $\alpha_2 > d(\psi_2) + 1$ . If  $E[f(\psi_2(X), p(X), \xi)^2 | \xi] < \infty$   $\xi$ -a.s. then

$$E_n[T_i(D_i - p(X_i))f(\psi_2(X_i), p(X_i), \xi)] = o_p(n^{-1/2})$$

If  $E[g(\psi_1(X), q(X), \xi)^2 | \xi] < \infty \xi$ -a.s. then  $E_n[(T_i - q(X_i))g(\psi_1(X_i), q(X_i), \xi)] = o_p(n^{-1/2})$ . Suppose further that  $\overline{k}_n | L_n | = o(n^{1-(d+1)/(\alpha_1 \wedge \alpha_2)})$ . Then  $E_n[T_i(D_i - p_n(X_i))f(\psi_2(X_i), \xi)] = o_p(n^{-1/2})$  and  $E_n[(T_i - q_n(X_i))g(\psi_1(X_i), \xi)] = o_p(n^{-1/2})$  under the same conditions.

Proof. We begin with the first claim. Fix a sequence  $c_n$  with  $c_n \to \infty$  and  $c_n^2 = o((\overline{k}_n|L_n|)^{-2/(d+1)}n^{2/(d+1)-2/\alpha_2})$ . Work on the assumed almost sure event and fix  $\xi$ . Denote  $Z = (\psi_2(X), p(X))$ . Define  $L_2(Z) = \{g(Z) : E[g(Z)^2|\xi] < \infty\}$ . By assumption,  $f(Z,\xi) \in L_2(Z)$ . Our strategy is to approximate  $f(Z,\xi)$  by Lipschitz functions. Define the spaces  $\mathcal{L}_n = \{g(Z) \in L_2(Z) : |g|_{lip} \lor |g|_{\infty} \le c_n\}$  and let  $g_n \in \mathcal{L}_n$  be such that  $E[(g_n(Z) - f(Z))^2] \le 2\inf_{g \in \mathcal{L}_n} E[(g(Z) - f(Z))^2]$ . We claim that  $|g_n - f|_{2,Z}^2 \to 0$ . Let  $\epsilon > 0$  and note that by Lemma C.5 there exists a function  $|h|_{lip} \lor |h|_{\infty} < \infty$  with  $|h - f|_{2,Z}^2 < \epsilon$ . Since  $c_n \to \infty$ , there exists N such that  $c_n \ge |h|_{lip} \lor |h|_{\infty}$  for all  $n \ge N$ . Then for  $n \ge N$  we have  $|g_n - f|_{2,Z}^2 \le 2\inf_{g \in \mathcal{L}_n} |g - f|_{2,Z}^2 \le 2|h - f|_{2,Z}^2 < 2\epsilon$  since  $h \in \mathcal{L}_n$ . Since  $\epsilon$  was arbitrary, this shows the claim. Summarizing our work so far, we found  $g_n(Z,\xi)$  such that  $E[(f(Z,\xi) - g_n(Z,\xi))^2|\xi] = o(1)$ ,  $|g_n(Z,\xi) - g_n(Z',\xi)| \le c_n |Z - Z'|_2$ , and  $|g_n(\cdot,\xi)|_{\infty} \le c_n |\xi$ -a.s. Now we expand

$$E_n[T_i(D_i - p_i)f(Z_i, \xi)] = E_n[T_i(D_i - p_i)(f(Z_i, \xi) - g_n(Z_i, \xi))] + E_n[T_i(D_i - p_i)g_n(Z_i, \xi)]$$

Denote these terms  $A_n, B_n$ . Let  $\mathcal{F}_n = \sigma((\psi_2)_{1:n}, (p_i)_{1:n}, \pi_n, \tau^t, \xi)$ . Since  $(\psi_1, q) \in \sigma(\psi_2)$ ,

we have  $\mathcal{G}_n$ ,  $f(Z_i)_{1:n}$ ,  $g_n(Z_i)_{1:n} \in \mathcal{F}_n$ . Then by Lemma A.2  $E[A_n|\mathcal{F}_n] = 0$  and

$$Var(\sqrt{n}E_n[T_i(D_i - p_i)(f(Z_i, \xi) - g_n(Z_i, \xi))]|\mathcal{F}_n) \le 2E_n[(f(Z_i, \xi) - g_n(Z_i, \xi))^2] = o_p(1)$$

The equality by conditional Markov (Lemma C.2) since  $E[E_n[(f(Z_i,\xi)-g_n(Z_i,\xi))^2]|\xi] = |f-g_n|_{2,Z}^2 = o(1) \xi$ -a.s. as shown above. Then  $A_n = o_p(n^{-1/2})$ , again by conditional Markov. Next consider  $B_n$ . By Lemma A.2, we have  $E[B_n|\mathcal{F}_n] = 0$ . Using the claim and Lemma A.2, we calculate

$$\operatorname{Var}(\sqrt{n}B_{n}|\mathcal{F}_{n}) \leq n^{-1} \sum_{g} \frac{1}{|g|} \sum_{i,j \in g} (g_{n}(Z_{i},\xi) - g_{n}(Z_{j},\xi))^{2} + n^{-1}\overline{k}_{n}|L_{n}| \max_{i=1}^{n} g_{n}(Z_{i},\xi)^{2}$$

$$\leq c_{n}^{2}n^{-1} \sum_{g} \frac{1}{|g|} \sum_{i,j \in g} |Z_{i} - Z_{j}|_{2}^{2} + n^{-1}\overline{k}_{n}|L_{n}|c_{n}^{2}$$

$$= c_{n}^{2}n^{-1} \sum_{g} \frac{1}{|g|} \sum_{i,j \in g} (|\psi_{2,i} - \psi_{2,j}|_{2}^{2} + |p_{i} - p_{j}|^{2}) + n^{-1}\overline{k}_{n}|L_{n}|c_{n}^{2}$$

$$= c_{n}^{2}o_{p}(n^{2/\alpha_{2}}(n/(\overline{k}_{n}|L_{n}|)^{-2/(d+1)}) + n^{-1}\overline{k}_{n}|L_{n}|c_{n}^{2} = o_{p}(1)$$

The second to last equality since  $p_i = p_j$  for any  $i, j \in g$ ,  $\forall g$  and by Theorem A.1, using the fact that  $\max_{i=1}^n |\psi_{2,i}|^2 = o_p(n^{2/\alpha_2})$  by Lemma C.8. The final equality follows by our choice of  $c_n$ . Then  $B_n = o_p(n^{-1/2})$ , again by conditional Markov. This finishes the proof. The conclusion for sampling variables follows by the same proof, setting  $T_i, q_i \to 1$ ,  $D_i \to T_i$  and  $p_i \to q_i$  and  $\psi_2 \to \psi_1$ . The second set of claims follows by setting  $Z = \psi_2(X)$  and  $p_i \to p_{i,n}$  in the above proof.

#### A.3 CLT

**Assumption A.4.** Consider the following assumptions

- (A1)  $E[Y(d)^2] < \infty$  and  $\psi_1, \psi_2, q, p$  as in Theorem 3.11 with  $q_i, p_i \in [\delta, 1 \delta] \subseteq (0, 1)$ .
- (A2)  $E[Y(d)^4] < \infty$  and propensities  $\widehat{p}_{i,n} = \widehat{p}_{i,n}(X_i, \xi_n)$ ,  $\widehat{q}_{i,n} = \widehat{q}_{i,n}(X_i, \xi_n)$ ,  $p_i = p(X_i)$ , and  $q_i = q(X_i)$  for  $\xi_n \perp \!\!\! \perp \sigma(W_{1:n}, \tau^t, \tau^d, \pi_n)$ .  $\widehat{p}_{i,n}, p_i \in [\delta, 1 \delta] \subseteq (0, 1)$  and  $\widehat{q}_{i,n}, q_i \geq \delta$ . Also  $E_n[(\widehat{p}_{i,n} p_i)^2] = o_p(1)$  and  $E_n[(\widehat{q}_{i,n} q_i)^2] = o_p(1)$ .

**Theorem A.5** (CLT). (1) Suppose Assumption A.4 (A1) holds. Let  $T_{1:n} \sim \text{Loc}(\psi_1, q(x))$  and  $D_{1:n} \sim \text{Loc}(\psi_2, p(x))$ . Define  $c_{1,i} = E[Y_i(1) - Y_i(0)|\psi_{1,i}, q_i, \xi]$ . Then  $\sqrt{n}(E_n[c_{1,i}] - V_n[c_{1,i}])$ 

ATE) $|\xi \Rightarrow \mathcal{N}(0, V_1)$  with  $V_1 = \text{Var}(c_{1,i}|\xi)$ . Define

$$u_i = q_i^{-1}(E[Y_i(1) - Y_i(0)|\psi_{1,i}, q_i, \xi] - E[Y_i(1) - Y_i(0)|\psi_{2,i}, p_i, \xi])$$

and  $\mathcal{F}_{0,n} = \sigma(\xi, \pi_n, (\psi_{1,i})_{1:n}, (q_i)_{1:n}, \tau^t)$ . Then  $\sqrt{n}E_n[T_iu_i]|\mathcal{F}_{0,n} \Rightarrow \mathcal{N}(0, V_1)$  with asymptotic variance

$$V_2 = E[q_i^{-1} \operatorname{Var}(E[Y_i(1) - Y_i(0) | \psi_{2,i}, p_i, \xi] | \psi_{1,i}, q_i, \xi) | \xi].$$

Define the residuals  $\epsilon_i^d = Y_i(d) - E[Y_i(d)|\psi_{2,i}, p_i, \xi]$  and  $\mathcal{G}_n = \sigma(\xi, \pi_n, \tau^t, \tau^d, (\psi_{2,i})_{1:n}, (p_i)_{1:n}, )$ . Then  $\sqrt{n}E_n[T_iD_i\epsilon_i^1/(p_iq_i) + T_i(1-D_i)\epsilon_i^0/((1-p_i)q_i)]|\mathcal{G}_{0,n} \Rightarrow \mathcal{N}(0, V_3)$  with variance

$$V_3 = E\left[\frac{\text{Var}(Y_i(1)|\psi_{2,i}, p_i, \xi)}{q_i p_i} + \frac{\text{Var}(Y_i(0)|\psi_{2,i}, p_i, \xi)}{q_i (1 - p_i)} \middle| \xi\right].$$

(2) Alternatively, suppose Assumption A.4 (A2) holds. Define the residuals  $\epsilon_i^d = Y_i(d) - E[Y_i(d)|X]$ . Let  $\psi_{k,n} = \psi_{k,n}(X)$  for k = 1, 2. Let  $T_{1:n} \sim \text{Loc}(\psi_{1,n}, \widehat{q}_n(x))$  and  $D_{1:n} \sim \text{Loc}(\psi_{2,n}, \widehat{p}_n(x))$  and define  $\mathcal{G}_{0,n} = \sigma(\pi_n, \xi_n, X_{1:n}, \tau^t, \tau^d)$ . Then  $\sqrt{n}E_n[T_iD_i\epsilon_i^1/(\widehat{p}_{i,n}\widehat{q}_{i,n}) + T_i(1-D_i)\epsilon_i^0/((1-\widehat{p}_{i,n})\widehat{q}_{i,n})]|\mathcal{G}_{0,n} \Rightarrow \mathcal{N}(0, V_3)$  with variance

$$V_3 = E \left[ \frac{1}{q(X_i)} \left( \frac{\sigma_1^2(X_i)}{p(X_i)} + \frac{\sigma_0^2(X_i)}{1 - p(X_i)} \right) \right].$$

Proof. First consider (1). Define  $\mathcal{H}_{0,n} = \sigma(\xi)$  and  $\mathcal{H}_{k,n} = \sigma(\xi, (c_{1,i})_{i=1:k})$  for  $k \geq 1$ . Claim that  $(\mathcal{H}_{k,n}, c_{1,k} - \text{ATE})_{k\geq 1}$  is an MDS. Adaptation is clear. For the MDS property,  $E[c_{1,i}|\mathcal{F}_{i-1,n}] = E[c_{1,i}|\xi, (c_{1,k})_{k=1:i-1}] = E[c_{1,i}|\xi] = E[Y_i(1) - Y_i(0)|\xi] = \text{ATE by tower}$  law and independence. Similarly,  $E[(c_{1,i} - \theta)^2|\mathcal{F}_{i-1,n}] = E[(c_{1,i} - \theta)^2|\xi] = \text{Var}(c_{1,i}|\xi)$ . To finish, we show the Lindeberg condition. Note that by conditional Jensen inequality  $Var(c_{1,i}|\xi) \leq E[c_{1,i}^2|\xi] \leq E[(Y_1 - Y_0)^2] < \infty$ . Then we have  $(c_{1,i} - \theta)^2\mathbb{1}((c_{1,i} - \theta)^2 > n\epsilon) \to 0$   $\xi$ -a.s., so by dominated convergence as  $n \to \infty$ 

$$E_n[E[(c_{1,i}-\theta)^2\mathbb{1}((c_{1,i}-\theta)^2>n\epsilon^2)|\xi]] = E[(c_{1,i}-\theta)^2\mathbb{1}((c_{1,i}-\theta)^2>n\epsilon^2)|\xi] \to 0$$

Then the Lindberg condition is satisfed, so by Theorem C.4  $\sqrt{n}(E_n[c_{1,i}] - \text{ATE})|\xi \Rightarrow \mathcal{N}(0, V_1)$  with the claimed limiting variance. Consider the second claim. Define  $\mathcal{F}_{k,n} = \sigma(\mathcal{F}_{0,n}, (\psi_{2,i})_{i=1:k}, (p_i)_{i=1:k})$  for  $k \geq 1$ . Claim that  $(T_k u_k, \mathcal{F}_{k,n})_{k\geq 1}$  is an MDS. Adaptation is clear from the definitions. Next we show the MDS property. Note that  $T_{1:n} \in \mathcal{F}_{0,n}$  since  $T_{1:n} = G(\tau^t, (\psi_{1,i})_{1:n}, (q_i)_{1:n}, \pi_n)$ . Note the crucial fact that  $(A, B) \perp \!\!\!\perp C \implies$ 

 $A \perp \!\!\!\perp C \mid B$ . By randomization we have  $(u_{k+1}, (\psi_{1,i})_{1:n}, (q_i)_{1:n}, \xi, (\psi_{2,i})_{i=1:k}, (p_i)_{i=1:k}) \perp \!\!\!\!\perp (\tau^t, \pi_n)$ . Combining this with the crucial fact, gives conditional independence from  $(\pi_n, \tau^t)$ 

$$E[T_{k+1}u_{k+1}|\mathcal{F}_{k,n}] = T_{k+1}E[u_{k+1}|\tau^t, (\psi_{1,i})_{1:n}, (q_i)_{1:n}, \pi_n, (\psi_{2,i})_{i=1:k}, (p_i)_{i=1:k}, \xi]$$
  
=  $T_{k+1}E[u_{k+1}|(\psi_{1,i})_{1:n}, (q_i)_{1:n}, (\psi_{2,i})_{i=1:k}, (p_i)_{i=1:k}, \xi]$ 

Next, note that since  $(X_i)_{i=1}^n$  are iid and  $\xi \perp \!\!\! \perp X_{1:n}$ , we have  $f(X_{k+1}, \xi) \perp \!\!\! \perp g(X_{-(k+1)}, \xi) | \xi$  for any functions f, g. Let  $g(X_{-(k+1)}, \xi) = ((\psi_{1,i})_{i \neq k+1}, (q_i)_{i \neq k+1}, \xi, (\psi_{2,i})_{i=1:k}, (p_i)_{i=1:k})$  and  $f(X_{k+1}, \xi) = u_{k+1}$ , giving conditional independence

$$E[u_{k+1}|(\psi_{1,i})_{1:n}, (q_i)_{1:n}, (\psi_{2,i})_{i=1:k}, (p_i)_{i=1:k}, \xi] = E[u_{k+1}|\psi_{1,k+1}, q_{k+1}, \xi]$$

$$= q_{k+1}^{-1} E[Y_{k+1}(1) - Y_{k+1}(0)|\psi_{1,k+1}, q_{k+1}, \xi]$$

$$- q_{k+1}^{-1} E[E[Y_{k+1}(1) - Y_{k+1}(0)|\psi_{2,k+1}, p_{k+1}, \xi]|\xi, \psi_{1,k+1}, q_{k+1}] = 0$$

The final equality by tower law since  $\sigma(\xi, \psi_{1,k+1}, q_{k+1}) \subseteq \sigma(\psi_{2,k+1}, p_{k+1}, \xi)$  by the increasing stratification assumption. This shows the MDS property. Next, we compute the variance process  $\Sigma_{k,n} = \sum_{i=1}^k E[(T_i u_i)^2 | \mathcal{F}_{i-1,n}]$ . By the exact argument above  $E[T_i u_i^2 | \mathcal{F}_{i-1,n}] = T_i E[u_i^2 | \psi_{1,i}, q_i, \xi]$ , so that  $E[T_i u_i^2 | \mathcal{F}_{i-1,n}] = T_i E[E[u_i^2 | \mathcal{F}_{i-1,n}] | \mathcal{F}_{i-1,n}] = T_i E[u_i^2 | \psi_{1,i}, q_i, \xi]$ , since  $(\psi_{1,i}, q_i, \xi) \in \mathcal{F}_{0,n} \subseteq \mathcal{F}_{i-1,n}$ . In particular, we have shown that  $\Sigma_{k,n} \in \mathcal{F}_{0,n}$  for all k, n, satisfying the variance condition of Proposition C.4. We have

$$\Sigma_n = E_n[T_i E[u_i^2 | \psi_{1,i}, q_i, \xi]] = E_n[(T_i - q_i) E[u_i^2 | \psi_{1,i}, q_i, \xi]] + E_n[q_i E[u_i^2 | \psi_{1,i}, q_i, \xi]]$$

Call these terms  $A_n$ ,  $B_n$ . By conditional Jensen and Young's, we have  $E[|E[u_i^2|\psi_{1,i},q_i,\xi]|] \le E[u_i^2] \lesssim E[(Y_i(1) - Y_i(0))^2] \lesssim \sum_{d=0,1} E[Y_i(d)^2] < \infty$ . Then  $A_n = o_p(1)$  by Lemma A.2. For the second term  $B_n$ , we have

$$E[B_n|\xi] = E[E_n[q_i E[u_i^2|\psi_{1,i}, q_i, \xi]]|\xi] = E[q_i E[u_i^2|\psi_{1,i}, q_i, \xi]|\xi]$$
$$= E[q_i^{-1} \operatorname{Var}(E[Y_i(1) - Y_i(0)|\psi_{2,i}, p_i, \xi]|\psi_{1,i}, q_i, \xi)|\xi]$$

Moreover, similar to the calculation for  $A_n$ , conditional Jensen and Young's show that  $E[|E[u_i^2|\psi_{1,i},q_i,\xi]|\xi] \lesssim \sum_{d=0,1} E[Y_i(d)^2] < \infty$ , so  $B_n - E[B_n|\xi] = o_p(1)$  by conditional WLLN. Then we have shown  $\Sigma_n - E[B_n|\xi] = o_p(1)$ , with the claimed limit. Finally, we show the Lindberg condition in Equation C.1. Let  $\Delta_i = Y_i(1) - Y_i(0)$ . By the propensity

lower bound and Young's inequality  $T_i^2 u_i^2 \leq 2\delta^{-2}(E[\Delta_i|\psi_{1,i},q_i,\xi]^2 + E[\Delta_i|\psi_{2,i},p_i,\xi]^2) \equiv v_i$ . Note also that  $E[v_i] \lesssim E[E[\Delta_i|\psi_{1,i},q_i,\xi]^2 + E[\Delta_i|\psi_{2,i},p_i,\xi]^2] \leq 2E[\Delta_i^2] \lesssim E[Y(1)^2 + Y(0)^2] < \infty$ . The second inequality is conditional Jensen. Then for  $\epsilon > 0$ 

$$n^{-1} \sum_{i=1}^{n} E[T_i^2 u_i^2 \mathbb{1}(T_i^2 u_i^2 > n\epsilon^2) | \mathcal{F}_{0,n}] \le n^{-1} \sum_{i=1}^{n} E[v_i \mathbb{1}(v_i > n\epsilon^2) | \mathcal{F}_{0,n}] \equiv C_n$$

As in the conditional independence arguments above, we have

$$n^{-1} \sum_{i=1}^{n} E[v_{i} \mathbb{1}(v_{i} > n\epsilon^{2}) | \mathcal{F}_{0,n}] = n^{-1} \sum_{i=1}^{n} E[v_{i} \mathbb{1}(v_{i} > n\epsilon^{2}) | \tau^{t}, \pi_{n}, (\psi_{1,i})_{1:n}, (q_{i})_{1:n}, \xi]$$

$$= n^{-1} \sum_{i=1}^{n} E[v_{i} \mathbb{1}(v_{i} > n\epsilon^{2}) | (\psi_{1,i})_{1:n}, (q_{i})_{1:n}, \xi] = n^{-1} \sum_{i=1}^{n} E[v_{i} \mathbb{1}(v_{i} > n\epsilon^{2}) | \psi_{1,i}, q_{i}, \xi]$$

Then  $E[C_n] = E[E[C_n|\xi]] = E[v_i\mathbb{1}(v_i > n\epsilon^2)] \to 0$  as  $n \to \infty$  since  $v_i \ge 0$  and  $E[v_i] < \infty$ . Then  $C_n \stackrel{p}{\to} 0$  by Markov inequality. This finishes the proof of the Lindberg condition. We skip the proof of the final claim, since it is similar to the proof of claim (2).

Next we show claim (2). Define  $\mathcal{G}_{k,n} = \sigma(\mathcal{G}_{0,n}, (\epsilon_i^0, \epsilon_i^1)_{i=1:k})$ . Then claim that  $(z_{i,n}, \mathcal{G}_{i,n})_{i\geq 1}$  is an MDS with  $z_{i,n} = T_i D_i \epsilon_i^1/(\widehat{p}_{i,n} \widehat{q}_{i,n}) + T_i (1-D_i) \epsilon_i^0/((1-\widehat{p}_{i,n})\widehat{q}_{i,n})$ . Adaptation is clear. Next we show the MDS property. It suffices to show  $E[\epsilon_i^d | \mathcal{G}_{i-1,n}] = 0$ . Again we use the fact  $(A, B) \perp \!\!\!\perp C \implies A \perp \!\!\!\perp C \mid B$ . Then note that  $E[\epsilon_i^d | \mathcal{G}_{i-1,n}]$  is equal to

$$E[\epsilon_i^d | \pi_n, \xi_n, X_{1:n}, \tau^t, \tau^d, (\epsilon_i^0, \epsilon_i^1)_{i=1:i-1}] = E[\epsilon_i^d | X_{1:n}, (\epsilon_i^0, \epsilon_i^1)_{i=1:i-1}] = E[\epsilon_i^d | X_i] = 0.$$

The second equality by the fact with  $A = \epsilon_i^d$ ,  $B = (X_{1:n}, (\epsilon_i^0, \epsilon_i^1)_{i=1:i-1})$ , and  $C = (\pi_n, \xi_n, \tau^t, \tau^d)$ . The third equality by setting  $A = \epsilon_i^d$ ,  $B = X_i$ , and  $C = (X_{-i}, (\epsilon_i^0, \epsilon_i^1)_{i=1:i-1})$ . This proves the MDS property. Next we analyze  $\Sigma_{k,n} = n^{-1} \sum_{i=1}^k E[z_{i,n}^2 | \mathcal{G}_{i-1,n}]$ , the variance process. By the exact reasoning above,  $E[(\epsilon_i^d)^2 | \mathcal{G}_{i-1,n}] = E[(\epsilon_i^d)^2 | X_i] = \sigma_d^2(X_i)$ .

$$\Sigma_{k,n} = n^{-1} \sum_{i=1}^{k} T_i D_i \sigma_1^2(X_i) / (\widehat{p}_{i,n} \widehat{q}_{i,n})^2 + T_i (1 - D_i) \sigma_0^2(X_i) / ((1 - \widehat{p}_{i,n}) \widehat{q}_{i,n})^2$$

so that  $\Sigma_{k,n} \in \mathcal{G}_{0,n}$  for all k, n, satisfying the variance condition of Proposition C.4.

$$E_n[T_iD_i\sigma_1^2(X_i)/(\widehat{p}_{i,n}\widehat{q}_{i,n})^2] = E_n[((T_i - \widehat{q}_{i,n}) + \widehat{q}_{i,n})D_i\sigma_1^2(X_i)/(\widehat{p}_{i,n}\widehat{q}_{i,n})^2] = R_n^1 + R_n^2$$

By our propensity lower bounds we have  $D_i \sigma_1^2(X_i)/(\widehat{p}_{i,n}\widehat{q}_{i,n})^2 \leq \delta^{-4}\sigma_1^2(X_i)$  with  $E[\sigma_1^2(X)] < \infty$ , so  $D_i \sigma_1^2(X_i)/(\widehat{p}_{i,n}\widehat{q}_{i,n})^2$  is uniformly integrable. Then  $R_n^1 = o_p(1)$  by Lemma A.2. Similarly,  $R_n^2 = E_n[((D_i - \widehat{p}_{i,n}) + \widehat{p}_{i,n})\sigma_1^2(X_i)/\widehat{p}_{i,n}^2\widehat{q}_{i,n}] = R_n^3 + R_n^4$  and  $R_n^3 = o_p(1)$  by the same argument. Then  $\Sigma_n = E_n[\sigma_1^2(X_i)/\widehat{p}_{i,n}\widehat{q}_{i,n}] + o_p(1)$ .

$$|E_n[\sigma_1^2(X_i)/\widehat{p}_{i,n}\widehat{q}_{i,n} - \sigma_1^2(X_i)/p_iq_i]| \le \delta^{-4}|E_n[\sigma_1^2(X_i)((q_i - \widehat{q}_{i,n})p_i + \widehat{q}_{i,n}(p_i - \widehat{p}_{i,n}))]|$$

$$\le E_n[\sigma_1^2(X_i)^2]^{1/2} \left( E_n[(q_i - \widehat{q}_{i,n})^2]^{1/2} + E_n[(p_i - \widehat{p}_{i,n})^2]^{1/2} \right) = O_p(1)o_p(1) = o_p(1)$$

Then  $E_n[T_iD_i\sigma_1^2(X_i)/(\widehat{p}_{i,n}\widehat{q}_{i,n})^2] = E_n[\sigma_1^2(X_i)/p_iq_i] + o_p(1) = E[\sigma_1^2(X_i)/p_iq_i] + O_p(n^{-1/2})$  by Chebyshev inequality. By symmetry, the same holds for the D=0 term. Putting this together, we have shown that  $\Sigma_n \stackrel{p}{\to} E[\sigma_1^2(X_i)/(p_iq_i) + \sigma_0^2(X_i)/(1-p_i)q_i]$  as claimed. Finally, we show the Lindberg condition. Note the bound  $|z_{i,n}|^2 \leq 2\delta^{-4}((\epsilon_i^1)^2 + (\epsilon_i^0)^2) \equiv v_i$ , with  $E[v_i] \lesssim \operatorname{Var}(Y(1)) + \operatorname{Var}(Y(0)) < \infty$ . Then for  $\epsilon > 0$  we have

$$L_{n} = n^{-1} \sum_{i=1}^{n} E[z_{i,n}^{2} \mathbb{1}(z_{i,n}^{2} > n\epsilon^{2}) | \mathcal{G}_{0,n}] \leq n^{-1} \sum_{i=1}^{n} E[v_{i} \mathbb{1}(v_{i} > n\epsilon^{2}) | \mathcal{F}_{0,n}]$$

$$= n^{-1} \sum_{i=1}^{n} E[v_{i} \mathbb{1}(v_{i} > n\epsilon^{2}) | \pi_{n}, \xi_{n}, X_{1:n}, \tau^{t}, \tau^{d}] = n^{-1} \sum_{i=1}^{n} E[v_{i} \mathbb{1}(v_{i} > n\epsilon^{2}) | X_{i}]$$

The inequality from the upper bound just stated. The second equality from the conditional independence reasoning above. Then  $E[L_n] = E[v_i \mathbb{1}(v_i > n\epsilon^2)] \to 0$  as  $n \to \infty$  since  $E[v_i] < \infty$ . Then by Markov inequality  $L_n \stackrel{p}{\to} 0$ , which finishes the proof.

Proof of Theorem 3.11. Define  $c_{1,i} = E[Y(1) - Y(0)|\psi_{1,i}, q_i, \xi]$  and  $c_{2,i} = E[Y(1) - Y(0)|\psi_{2,i}, p_i, \xi]$ . Define  $b_{2,i} = E[Y(1)|\psi_{2,i}, p_i, \xi]((1-p_i)/p_i)^{1/2} + E[Y(0)|\psi_{2,i}, p_i, \xi](p_i/(1-p_i))^{1/2}$  and  $\epsilon_i^d = Y_i(d) - E[Y_i(d)|\psi_{2,i}, p_i, \xi]$ . Define the  $\sigma$ -algebras  $\mathcal{F}_{k,n}$  for  $1 \le k \le 4$ 

$$\mathcal{F}_{1,n} = \sigma(\psi_{1,1:n}, q_{1:n}, \xi, \pi_n)$$
  $\mathcal{F}_{2,n} = \sigma(\mathcal{F}_{1,n}, T_{1:n})$   $\mathcal{F}_{3,n} = \sigma(\mathcal{F}_{2,n}, \psi_{2,1:n}, p_{1:n})$ 

and  $\mathcal{F}_{4,n} = \sigma(\mathcal{F}_{3,n}, D_{1:n})$ . We expand our estimator by projection

$$\theta - \widehat{\theta} = (\theta - E[\widehat{\theta}|\mathcal{F}_{1,n}]) + (E[\widehat{\theta}|\mathcal{F}_{1,n}] - E[\widehat{\theta}|\mathcal{F}_{2,n}]) + (E[\widehat{\theta}|\mathcal{F}_{2,n}] - E[\widehat{\theta}|\mathcal{F}_{3,n}])$$

$$+ (E[\widehat{\theta}|\mathcal{F}_{3,n}] - E[\widehat{\theta}|\mathcal{F}_{4,n}]) + (E[\widehat{\theta}|\mathcal{F}_{4,n}] - \widehat{\theta})$$

$$= E_n[c_{1,i} - \theta] + E_n\left[\frac{T_i - q_i}{q_i}c_{1,i}\right] + E_n\left[\frac{T_i}{q_i}(c_{2,i} - c_{1,i})\right] + E_n\left[\frac{(D_i - p_i)T_i}{q_i\sqrt{p_i - p_i^2}}b_{2,i}\right]$$

$$+ E_n\left[\frac{D_iT_i\epsilon_i^1}{p_iq_i} + \frac{(1 - D_i)T_i\epsilon_i^0}{(1 - p_i)q_i}\right] \equiv A_n + B_n + C_n + S_n + R_n$$

We wish to apply Lemma A.3 to show that  $\sqrt{n}B_n$ ,  $\sqrt{n}S_n = o_p(1)$ . It suffices to check integrability. In the notation of the lemma, define  $g(\psi_{1,i}, q_i, \xi) = c_{1,i}/q_i$ , and note that by our propensity bound, Young's inequality, and contraction

$$E[E[c_{1,i}^2/q_i^2|\xi]] \le \delta^{-2}E[c_{1,i}^2] \lesssim E[\sum_{d=0,1} E[Y(d)|\psi_{1,i}, q_i, \xi]^2] \le \sum_{d=0,1} E[Y(d)^2]$$

This shows  $E[c_{1,i}^2/q_i^2|\xi] < \infty \xi$ -a.s. Similarly,  $E[b_{2,i}^2q_i^{-2}(p_i(1-p_i))^{-1}|\xi] < \infty \xi$ -a.s. Then  $\sqrt{n}B_n, \sqrt{n}S_n = o_p(1)$  by the lemma.

The conditions of Theorem A.5 are satisfied by assumption. Then  $\sqrt{n}A_n|\xi \Rightarrow \mathcal{N}(0,V_1)$  with  $V_1 = \operatorname{Var}(c_{1,i}|\xi), \sqrt{n}C_n|\mathcal{F}_{2,n} \Rightarrow \mathcal{N}(0,V_2)$  with  $V_2 = E[q_i^{-1}\operatorname{Var}(c_{2,i}|\psi_{1,i},q_i,\xi)|\xi],$  and  $\sqrt{n}R_n|\mathcal{F}_{4,n} \Rightarrow \mathcal{N}(0,V_3)$  with  $V_3 = E[q_i^{-1}(\sigma_{1,i}^2p_i^{-1} + \sigma_{0,i}^2(1-p_i)^{-1})|\xi]$  for  $\sigma_{d,i}^2 = \operatorname{Var}(Y(d)|\psi_{2,i},p_i,\xi)$ . Then by Slutsky and Lemma C.6, we have  $\sqrt{n}(\widehat{\theta} - \operatorname{ATE})|\xi \Rightarrow \mathcal{N}(0,V_1+V_2+V_3)$ .

To finish the proof, we use algebra to reformulate the variance  $V = V_1 + V_2 + V_3$ . By the law of total variance  $\operatorname{Var}(c(X)|\xi) = \operatorname{Var}(E[c(X)|\psi_1,q,\xi]|\xi) + E[\operatorname{Var}(c(X)|\psi_1,q,\xi)|\xi]$ , with  $E[c(X_i)|\psi_{1,i},q_i,\xi] = c_{1,i}$ . Then since  $\xi \perp W_{1:n}$ 

$$V_1 = \operatorname{Var}(c(X)) - E[\operatorname{Var}(c(X)|\psi_1, q, \xi)|\xi].$$

Next, by the law of total variance

$$Var(c(X_i)|\psi_{1,i}, q_i, \xi) = E[Var(c(X)|\psi_{2,i}, p_i, \xi)|\psi_{1,i}, q_i, \xi] + Var(E[c(X)|\psi_{2,i}, p_i, \xi)|\psi_{1,i}, q_i, \xi)$$

Using this equality and applying tower law gives

$$V_{2} = E[q_{i}^{-1} \operatorname{Var}(c_{2,i}|\psi_{1,i}, q_{i}, \xi)|\xi] = E[q_{i}^{-1} \operatorname{Var}(E[c(X)|\psi_{2,i}, p_{i}, \xi]|\psi_{1,i}, q_{i}, \xi)|\xi]$$

$$= E[q_{i}^{-1} \operatorname{Var}(c(X_{i})|\psi_{1,i}, q_{i}, \xi)|\xi] - E[q_{i}^{-1} E[\operatorname{Var}(c(X)|\psi_{2,i}, p_{i}, \xi)|\psi_{1,i}, q_{i}, \xi]|\xi]$$

$$= E[q_{i}^{-1} \operatorname{Var}(c(X_{i})|\psi_{1,i}, q_{i}, \xi)|\xi] - E[q_{i}^{-1} \operatorname{Var}(c(X)|\psi_{2,i}, p_{i}, \xi)|\xi]$$

Also,  $\operatorname{Var}(Y_i(d)|\psi_{2,i}, p_i, \xi) = \operatorname{Var}(E[Y_i(d)|X_i, \xi]|\psi_{2,i}, p_i, \xi)] + E[\operatorname{Var}(Y_i(d)|X_i, \xi)|\psi_{2,i}, p_i, \xi].$  Using this fact gives

$$V_{3} = E[(q_{i}p_{i})^{-1}\sigma_{1,i}^{2}|\xi] + E[(q_{i}(1-p_{i}))^{-1}\sigma_{0,i}^{2}|\xi]$$

$$= E[(q_{i}p_{i})^{-1}\operatorname{Var}(m_{1}(X_{i})|\psi_{2,i},p_{i},\xi)|\xi] + E[(q_{i}p_{i})^{-1}E[\sigma_{1}^{2}(X_{i})|\psi_{2,i},p_{i},\xi]|\xi]$$

$$+ E[(q_{i}(1-p_{i}))^{-1}\operatorname{Var}(m_{0}(X_{i})|\psi_{2,i},p_{i},\xi)|\xi] + E[(q_{i}(1-p_{i}))^{-1}E[\sigma_{0}^{2}(X_{i})|\psi_{2,i},p_{i},\xi]|\xi]$$

$$= E[(q_{i}p_{i})^{-1}\operatorname{Var}(m_{1}(X_{i})|\psi_{2,i},p_{i},\xi)|\xi] + E[(q_{i}(1-p_{i}))^{-1}\operatorname{Var}(m_{0}(X_{i})|\psi_{2,i},p_{i},\xi)|\xi]$$

$$+ E[(q_{i}p_{i})^{-1}\sigma_{1}^{2}(X_{i})|\xi] + E[(q_{i}(1-p_{i}))^{-1}\sigma_{0}^{2}(X_{i})|\xi]$$

The final equality by tower law and since  $q_i \in \sigma(\psi_{2,i}, p_i, \xi)$  by construction. Putting this all together, we get total variance

$$V_{1} + V_{2} + V_{3} = \operatorname{Var}(c(X_{i})) - E[\operatorname{Var}(c(X_{i})|\psi_{1,i}, q_{i}, \xi)|\xi]$$

$$+ E[q_{i}^{-1} \operatorname{Var}(c(X_{i})|\psi_{1,i}, q_{i}, \xi)|\xi] - E[q_{i}^{-1} \operatorname{Var}(c(X)|\psi_{2,i}, p_{i}, \xi)|\xi]$$

$$+ E[(q_{i}p_{i})^{-1} \operatorname{Var}(m_{1}(X_{i})|\psi_{2,i}, p_{i}, \xi)|\xi] + E[(q_{i}(1 - p_{i}))^{-1} \operatorname{Var}(m_{0}(X_{i})|\psi_{2,i}, p_{i}, \xi)|\xi]$$

$$+ E[(q_{i}p_{i})^{-1}\sigma_{1}^{2}(X_{i})|\xi] + E[(q_{i}(1 - p_{i}))^{-1}\sigma_{0}^{2}(X_{i})|\xi]$$

$$= T_{1} + T_{2} + T_{3} + T_{4} + T_{5} + T_{6} + T_{7} + T_{8}$$

Note that  $T_2 + T_3 = E[q_i^{-1}(1 - q_i) Var(c(X_i)|\psi_{1,i}, q_i, \xi)|\xi]$ . Also note that

$$-\operatorname{Var}(c(X_{i})|\psi_{2,i}, p_{i}, \xi) + p_{i}^{-1}\operatorname{Var}(m_{1}(X_{i})|\psi_{2,i}, p_{i}, \xi) + (1 - p_{i})^{-1}\operatorname{Var}(m_{0}(X_{i})|\psi_{2,i}, p_{i}, \xi)$$

$$= p_{i}^{-1}(1 - p_{i})\operatorname{Var}(m_{1}(X_{i})|\psi_{2,i}, p_{i}, \xi) + p_{i}(1 - p_{i})^{-1}\operatorname{Var}(m_{0}(X_{i})|\psi_{2,i}, p_{i}, \xi)$$

$$+ 2\operatorname{Cov}(m_{1}(X_{i}), m_{0}(X_{i})|\psi_{2,i}, p_{i}, \xi) = \operatorname{Var}(b(X_{i}; p_{i})|\psi_{2,i}, p_{i}, \xi)$$

Then we have  $T_4 + T_5 + T_6 = E[q_i^{-1} Var(b(X_i; p_i) | \psi_{2,i}, p_i, \xi) | \xi]$ . Then as claimed

$$V = \sum_{k=1}^{8} T_k = \operatorname{Var}(c(X)) + E[q_i^{-1}(1 - q_i) \operatorname{Var}(c(X_i)|\psi_{1,i}, q_i, \xi)|\xi]$$
  
+ 
$$E[q_i^{-1} \operatorname{Var}(b(X_i; p_i)|\psi_{2,i}, p_i, \xi)|\xi] + E\left[q_i^{-1} \left(\frac{\sigma_1^2(X_i)}{p_i} + \frac{\sigma_0^2(X_i)}{1 - p_i}\right) |\xi]\right].$$

Finally, note  $E_n[T_i] = E_n[T_i - q_i] + E_n[q_i] = o_p(n^{-1/2}) + E_n[q_i] = E[q_i|\xi] + O_p(n^{-1/2})$ . The second equality by Lemma A.3, and the third by conditional Chebyshev (Lemma C.2). Then  $\sqrt{n_T}(\widehat{\theta} - \text{ATE}) = \sqrt{n}(E_n[T_i])^{1/2}(\widehat{\theta} - \text{ATE}) = E[q_i|\xi]^{1/2}\sqrt{n}(\widehat{\theta} - \text{ATE}) + o_p(1) \Rightarrow N(0, E[q(X, \xi)] \cdot V)$  by continuous mapping theorem and Slutsky. This finishes the proof

#### A.4 Optimal Design

Proof of Proposition 4.1. Define  $V(q) = E[\bar{\sigma}^2(\psi)/q(\psi)]$ . Define the sets

$$\mathcal{Q}' = \{q \in \mathbb{R}^{\psi} : |q|_{\infty} < \infty, q > 0, E[C(\psi)q(\psi)] \le \bar{B}, V(q) < \infty\} \qquad \mathcal{Q} = \mathcal{Q}' \cap \{0 < q \le 1\}$$

and recall the candidate optimal solution  $q^*(\psi) = \bar{B} \cdot \bar{\sigma}(\psi)C(\psi)^{-1/2}/E[\bar{\sigma}(\psi)C(\psi)^{1/2}]$ . Let  $t \in [0,1]$  and  $q_1, q_2 \in \mathcal{Q}'$ . By convexity of  $y \to 1/y$  on  $(0,\infty)$ , for each  $\psi \in \psi$  we have

$$\frac{\bar{\sigma}^2(\psi)}{tq_1(\psi) + (1-t)q_2(\psi)} \le t\frac{\bar{\sigma}^2(\psi)}{q_1(\psi)} + (1-t)\frac{\bar{\sigma}^2(\psi)}{q_1(\psi)}$$

Taking expectations of both sides gives  $V(tq_1+(1-t)q_2) \leq tV(q_1)+(1-t)V(q_2)$ , so V is convex on  $\{q>0\}$  and  $\mathcal{Q}'$  is convex. We claim that  $q^*\in\mathcal{Q}'$ . First,  $q^*\in(0,1]$  by assumption. Since  $\sup_{\psi\in\psi}q^*\leq 1$  we have  $E[\bar{\sigma}(\psi)C(\psi)^{1/2}]>0$ . By Holder  $E[\bar{\sigma}(\psi)C(\psi)^{1/2}]\leq E[\bar{\sigma}^2(\psi)]^{1/2}E[C(\psi)]^{1/2}<\infty$ . Then we have  $V(q^*)=\bar{B}^{-1}E[\bar{\sigma}(\psi)C(\psi)^{1/2}]^2<\infty$ . Also clearly  $E[C(\psi)q^*(\psi)]=\bar{B}$ . This shows the claim. Next, suppose that  $q^*+t\Delta\in\mathcal{Q}'$  for some  $t\in[0,1]$  and  $|\Delta|_{\infty}< M$ . Since  $q^*\in\mathcal{Q}'$ , by convexity of  $\mathcal{Q}'$ ,  $q^*+t'\Delta\in\mathcal{Q}'$  for all  $0\leq t'\leq t$ . Then  $dV_{q^*}[\Delta]\equiv\limsup_{t\to 0^+}t^{-1}(V(q^*+t\Delta)-V(q^*))$  is well-defined. We claim that this limit exists. Under our assumptions  $q^*>q_l\geq 0$  for some  $q_l$ , so that for any  $\psi$  and all  $t\leq q_l^2/2M<\infty$ 

$$\left| t^{-1} \left( \frac{\bar{\sigma}^2(\psi)}{q^*(\psi) + t\Delta(\psi)} - \frac{\bar{\sigma}^2(\psi)}{q^*(\psi)} \right) \right| = \frac{|\bar{\sigma}^2(\psi)\Delta(\psi)|}{((q^*)^2 + q^*t\Delta)(\psi)} \le \frac{M|\bar{\sigma}^2(\psi)|}{q_l^2 - tM} \le \frac{M|\bar{\sigma}^2(\psi)|}{2q_l^2}$$

Since  $\|\bar{\sigma}^2\|_1 < \infty$ , dominated convergence implies

$$dV_{q^*}[\Delta] = \lim_{t \to 0^+} t^{-1}(V(q^* + t\Delta) - V(q^*)) = E\left[\lim_{t \to 0^+} \frac{-\bar{\sigma}^2(\psi)\Delta(\psi)}{((q^*)^2 + q^*t\Delta)(\psi)}\right]$$
$$= -E\left[\frac{\bar{\sigma}^2(\psi)\Delta(\psi)}{(q^*)^2(\psi)}\right] = (1/\bar{q})^2 E\left[C(\psi)\Delta(\psi)\right] E\left[\bar{\sigma}(\psi)C(\psi)^{1/2}\right]^2 = 0$$

The last line since  $q^* + t\Delta \in \mathcal{Q}'$  implies  $\bar{B} = E[q^*(\psi)C(\psi) + t\Delta(\psi)C(\psi)] = \bar{B} + tE[\Delta(\psi)C(\psi)]$ , so that  $E[\Delta(\psi)C(\psi)] = 0$ . Let  $q \in \mathcal{Q}'$ , so that  $\Delta = q - q^*$  has  $|\Delta|_{\infty} < \infty$ . Then by convexity  $V(q) - V(q^*) \ge dV_{q^*}[q - q^*] = 0$ , showing that  $q^* = \operatorname{argmin}_{q \in \mathcal{Q}'} V(q)$ . Since  $q^* \in \mathcal{Q}$  by assumption, it is optimal over  $\mathcal{Q} \subseteq \mathcal{Q}'$  as well.

Proof of Theorem 6.2. Suppose that  $T_{1:n} \sim \text{Loc}(\psi, \widehat{q}_n(\psi))$  and  $D_{1:n} \sim \text{Loc}(\psi, \widehat{p}_n(\psi))$ . Similar to the proof of Theorem 3.11, define  $\sigma$ -algebras  $\mathcal{F}_{1,n} = \sigma(\psi_{1:n}, \pi_n, \xi_n)$ ,  $\mathcal{F}_{2,n} = \sigma(\mathcal{F}_{1,n}, T_{1:n})$ , and  $\mathcal{F}_{3,n} = \sigma(\mathcal{F}_{2,n}, D_{1:n})$ . Next, expand the estimator

$$\widehat{\theta} - \theta = E_n[c(\psi_i) - \theta] + E_n\left[\frac{T_i - \widehat{q}_{i,n}}{\widehat{q}_{i,n}}c(\psi_i)\right] + E_n\left[\frac{T_i(D_i - \widehat{p}_{i,n})}{\widehat{q}_{i,n}\sqrt{\widehat{p}_{i,n}(1 - \widehat{p}_{i,n})}}b(\psi_i; \widehat{p}_n)\right] + E_n\left[\frac{D_i T_i \epsilon_i^1}{\widehat{p}_{i,n}\widehat{q}_{i,n}} + \frac{(1 - D_i) T_i \epsilon_i^0}{(1 - \widehat{p}_{i,n})\widehat{q}_{i,n}}\right] \equiv A_n + B_n + C_n + R_n$$

Our main task is to show that  $\sqrt{n}B_n$ ,  $\sqrt{n}C_n = o_p(1)$ . We do this by modifying the proof of Lemma A.3.

(1) Balancing Argument - Note that the term  $C_n$  has

$$C_n = E_n \left[ \frac{T_i(D_i - \widehat{p}_n(\psi_i))}{\widehat{q}_n(\psi_i)} \left( \frac{m_1(\psi_i)}{\widehat{p}_n(\psi_i)} + \frac{m_0(\psi_i)}{1 - \widehat{p}_n(\psi_i)} \right) \right] = C_{n1} + C_{n2}.$$

Recall  $q^*(\psi) = \bar{B}(\sigma_1(\psi) + \sigma_0(\psi))C(\psi)^{-1/2}/E[(\sigma_1(\psi) + \sigma_0(\psi))C(\psi)^{1/2}]$ . Under our assumptions, it's clear that  $\inf_{\psi} q^*(\psi) > 0$ . Consider the term above involving  $m_1(\psi)$ . We have  $E[m_1(\psi)^2/q^*(\psi)^2] \lesssim E[m_0(\psi)^2] < \infty$ . Then the construction in Lemma A.3 provides functions  $h_n \in L_2(\psi)$  with  $|h_n|_{lip} \vee |h_n|_{\infty} \leq c_n$  and  $|h_n - (m_1/q^*)|_{2,\psi} \to 0$ . Define  $\mathcal{F}_n = \sigma(\psi_{1:n}, \xi_n, \pi_n, \tau^t)$ . Note that  $\mathcal{G}_n, (q^*(\psi_i))_{1:n}, (\widehat{q}_n(\psi_i))_{1:n}, (\widehat{p}_n(\psi_i))_{1:n} \in \mathcal{F}_n$ . Then by Lemma A.2  $E[C_{n1}|\mathcal{F}_n] = 0$ . We can expand  $C_{n1}$  as

$$E_n \left[ \frac{T_i(D_i - \widehat{p}_n(\psi_i))}{\widehat{p}_n(\psi_i)} \left( \left( \frac{m_1(\psi_i)}{\widehat{q}_n(\psi_i)} - \frac{m_1(\psi_i)}{\widehat{q}(\psi_i)} \right) + \left( \frac{m_1(\psi_i)}{\widehat{q}(\psi_i)} - \frac{m_1(\psi_i)}{q^*(\psi_i)} \right) + \frac{m_1(\psi_i)}{q^*(\psi_i)} \right) \right]$$

and write  $C_{n1} = T_{n1} + T_{n2} + T_{n3}$ . Consider the first term. By construction,  $|\widehat{q}_n - \widehat{q}|_{\infty} \leq$ 

 $1/\overline{k}_n$ . Then by Lemma A.2 we have  $E[B_{n1}|\mathcal{F}_n]=0$  and

$$\operatorname{Var}(\sqrt{n}T_{n1}|\mathcal{F}_n) \lesssim E_n[m_1(\psi_i)^2(\widehat{q}_n - \widehat{q})^2(\psi_i)/\widehat{p}_n(\psi_i)^2] \lesssim o(1)E_n[m_1(\psi_i)^2] = o_p(1)$$

Again by Lemma A.2 we have

$$\operatorname{Var}(\sqrt{n}T_{n2}|\mathcal{F}_n) \lesssim E_n[m_1(\psi_i)^2(\widehat{q}-q^*)^2(\psi_i)/\widehat{p}_n(\psi_i)^2] \lesssim \max_{i=1}^n m_1(\psi_i)^2 E_n[(\widehat{q}-q^*)^2(\psi_i)]$$

The final expression is  $o_p(n^{2/\alpha_2-2r})+O(n^{2/\alpha_2}/\overline{k}_n^2)$ , using Lemma C.8 and the bound from Lemma C.1. This is  $o_p(1)$  under our assumptions. Consider the final term  $T_{n3}$ 

$$T_{n3} = E_n \left[ \frac{T_i(D_i - \widehat{p}_n(\psi_i))}{\widehat{p}_n(\psi_i)} \left( \left( \frac{m_1(\psi_i)}{q^*(\psi_i)} - h_n(\psi_i) \right) + h_n(\psi_i) \right) \right] = T_{n4} + T_{n5}$$

As above  $E[T_{n4}|\mathcal{F}_n] = 0$  and  $Var(\sqrt{n}T_{n4}|\mathcal{F}_n) \lesssim E_n[(m_1(\psi_i)/q^*(\psi_i) - h_n(\psi_i))^2] = o_p(1)$  by Markov inequality since  $|h_n - (m_1/q^*)|_{2,\mathcal{X}} \to 0$ . Finally, by the last part of Lemma A.2 we have  $E[T_{n5}|\mathcal{F}_n] = 0$  and

$$\operatorname{Var}(\sqrt{n}T_{n5}|\mathcal{F}_n) = n^{-1} \sum_{g \in \mathcal{G}_n} \frac{1}{|g|} \sum_{i,j \in g} (h_n(\psi_i) - h_n(\psi_i))^2 + n^{-1} \overline{k}_n |L_n| \max_{i=1}^n h_n(\psi_i)^2$$

$$\lesssim c_n^2 n^{-1} \sum_{g \in \mathcal{G}_n} \frac{1}{|g|} \sum_{i,j \in g} |\psi_i - \psi_j|_2^2 + n^{-1} \overline{k}_n |L_n| \max_{i=1}^n h_n(\psi_i)^2$$

$$\lesssim c_n^2 \max_{i=1}^n |\psi_i|_2^2 \cdot O((n/\overline{k}_n |L_n|)^{-2/(d+1)}) + n^{-1} \overline{k}_n |L_n| O_p(c_n^2)$$

$$= o_p(c_n^2 n^{2/\alpha_1 - 2/(d+1)} (\overline{k}_n |L_n|)^{2/(d+1)}) = o_p(1)$$

The first inequality by Lipschitz continuity, the second inequality by Theorem A.1. The final equality holds if  $\overline{k}_n|L_n| = o(n^{1-\frac{d+1}{\alpha_1}})$  and  $c_n = O(n^{2/\alpha_1 - 2/(d+1)}(\overline{k}_n|L_n|)^{2/(d+1)})$  with  $c_n \to \infty$ . This finishes the proof that  $\sqrt{n}B_n = o_p(1)$ . An identical proof shows that  $\sqrt{n}C_n = o_p(1)$ .

(2) CLT Argument - By the previous argument, we have  $\sqrt{n}(\widehat{\theta} - \theta) = \sqrt{n}A_n + \sqrt{n}R_n + o_p(1)$ .  $\sqrt{n}A_n \Rightarrow \mathcal{N}(0, V_1)$  with  $V_1 = \operatorname{Var}(c(\psi))$  by vanilla CLT. We want to apply Theorem A.5 to the term  $\sqrt{n}R_n$ . The moment bound is satisfied by assumption. For condition (a2), set  $\psi_{k,n}(\psi) = \psi$ ,  $p_i = p_i^*$ , and  $q_i = q_i^*$ . The propensity lower and upper bounds follow from our assumptions on  $\sigma_d(\psi)$ . Condition (c) is shown in Lemma C.1. Then by Theorem A.5  $\sqrt{n}R_n|\mathcal{F}_{3,n} \Rightarrow \mathcal{N}(0,V_2)$  with  $V_2 = E[(q_i^*p_i^*)^{-1}\sigma_1^2(\psi_i) + (q_i^*(1-p_i^*))^{-1}\sigma_0^2(\psi_i)]$  by Theorem A.5. Then by Lemma C.6,  $\sqrt{n}(A_n + R_n) \Rightarrow \mathcal{N}(0,V_1 + V_2)$ .

Applying Lemma A.2 with  $h_n = 1$  shows that  $\operatorname{Var}(E_n[(T_i - \widehat{q}_{i,n})]|\mathcal{F}_{1,n}) \leq n^{-1}\overline{k}_n|L_n|$ . Then  $E_n[T_i] = E_n[\widehat{q}_{i,n}] + O_p((\overline{k}_n|L_n|/n)^{1/2})$  and  $E_n[\widehat{q}_{i,n}] = E_n[\widehat{q}_i] + O(1/\overline{k}_n)$ , since  $|\widehat{q} - \widehat{q}_n|_{\infty} = O(1/\overline{k}_n)$  by discretization. Finally,  $E_n[\widehat{q}_i] = E_n[q_i^*] + o_p(1)$  by Lemma C.1. Putting this all together, we have  $E_n[T_i] = E_n[q_i^*] + o_p(1) = E[q_i^*] + o_p(1)$ , so that  $\sqrt{n_T}(\widehat{\theta} - ATE) = \sqrt{n}(E_n[T_i])^{1/2}(\widehat{\theta} - ATE) = E[q^*(\psi_i)]^{1/2}\sqrt{n}(\widehat{\theta} - ATE) + o_p(1) \Rightarrow N(0, E[q^*(\psi_i)] \cdot V)$  by continuous mapping theorem and Slutsky. This finishes the proof. The conclusion for Theorem 4.3 follows by setting  $\widehat{q} = q^*$  and  $\widehat{q}_n = q_n^*$ , so that the error  $T_{n2}$  above is identically zero.

Proof of Theorem 5.1. Fix  $P \in \mathcal{P}_{1/2}$ . By the fundamental expansion of the IPW estimator,  $\widehat{\theta} = E_n[c(X_i)] + 2E_n[(D_i - 1/2)b(X_i)] + 2E_n[D_i\epsilon_i^1 + (1 - D_i)\epsilon_i^0] \equiv A_n + B_n + C_n$ . Then by the law of total variance

$$\operatorname{Var}(\widehat{\theta}|X_{1:n}) = \operatorname{Var}(B_n + C_n|X_{1:n}) = E[\operatorname{Var}(B_n + C_n|X_{1:n}, D_{1:n})|X_{1:n}] + \operatorname{Var}(E[B_n + C_n|X_{1:n}, D_{1:n}]|X_{1:n}) = E[\operatorname{Var}(C_n|X_{1:n}, D_{1:n})|X_{1:n}] + \operatorname{Var}(B_n|X_{1:n})$$

The last line follows since  $E[C_n|X_{1:n}, D_{1:n}] = 0$ . One can show  $E[\operatorname{Var}(C_n|X_{1:n}, D_{1:n})|X_{1:n}] = (2/n)E_n[\sigma_1^2(X_i) + \sigma_0^2(X_i)]$ , which does not depend on P. Then  $\operatorname{argmin}_{P \in \mathcal{P}_{1/2}} \operatorname{Var}(\widehat{\theta}|X_{1:n}) = \operatorname{argmin}_{P \in \mathcal{P}_{1/2}} \operatorname{Var}(B_n|X_{1:n})$ . Denote  $Z_i = D_i - 1/2$ . Then  $n^2 \operatorname{Var}(B_n|X_{1:n})$  is equal to

$$E[(Z'_{1:n}b_{1:n})^2] = \sum_{d_{1:n} \in \{0,1\}^n} P(d_{1:n}|X_{1:n})(Z'_{1:n}b_{1:n})^2 \ge \min_{d_{1:n} \in \{0,1\}^n} ((D_i - 1/2)'_{1:n}b_{1:n})^2$$

Let  $d_{1:n}^* = d_{1:n}^*(X_{1:n})$  be a vector achieving the RHS minimum. Define  $P^* \in \mathcal{P}_{1/2}$  by  $P^*(d_{1:n}^*|X_{1:n}) = P^*(1 - d_{1:n}^*|X_{1:n}) = 1/2$ . Then

$$n^{2} \min_{P \in \mathcal{P}_{1/2}} \operatorname{Var}(B_{n}|X_{1:n}) \ge ((d_{1:n}^{*} - (1/2)\mathbb{1}_{n})'b_{1:n})^{2} = E_{P^{*}}[(D_{1:n} - (1/2)\mathbb{1}_{n})'b_{1:n})^{2}]$$
$$= n^{2} \operatorname{Var}_{P^{*}}(B_{n}|X_{1:n}) \ge n^{2} \min_{P \in \mathcal{P}_{1/2}} \operatorname{Var}(B_{n}|X_{1:n})$$

The final equality since  $P^* \in \mathcal{P}_{1/2}$  by construction. Then equality holds throughout, and  $P^* \in \operatorname{argmin}_{P \in \mathcal{P}_{1/2}} \operatorname{Var}(B_n|X_{1:n}) = \operatorname{argmin}_{P \in \mathcal{P}_{1/2}} \operatorname{Var}(\widehat{\theta}|X_{1:n})$ . Next, we characterize the optimal vector  $d_{1:n}^*$ . Observe that  $(d_i - 1/2)(d_j - 1/2) = (d_i - 1/2)(d_j - 1/2) - 1/4 + 1/4 = -(1/2)\mathbb{1}(d_i \neq d_j) + 1/4$ . Then  $\operatorname{argmin}_{d_{1:n} \in \{0.1\}^n}((d_{1:n} - (1/2)\mathbb{1}_n)'b_{1:n})^2$  is equal to

$$\underset{d_{1:n} \in \{0,1\}^n}{\operatorname{argmin}} \sum_{i,j=1}^n (d_i - 1/2)(d_j - 1/2)b_i b_j = \underset{d_{1:n} \in \{0,1\}^n}{\operatorname{argmax}} \sum_{i \neq j}^n \mathbb{1}(d_i \neq d_j)b_i b_j$$

The latter problem is equivalent to Max-Cut with edge weights  $w_{ij} = b_i b_j$ , as claimed.

A.5 Inference

Proof of Theorem 7.1. First, consider the sample variance. The second moment is

$$E_n \left[ \left( \frac{T_i(D_i - p(\psi_i))Y_i}{q(\psi_i)(p - p^2)(\psi_i)} \right)^2 \right] = E_n \left[ \frac{T_iD_iY_i(1)^2}{p_i^2 q_i^2} \right] + E_n \left[ \frac{T_i(1 - D_i)Y_i(0)^2}{(1 - p_i)^2 q_i^2} \right]$$

Consider the first term

$$E_n[T_iD_iY_i(1)^2/(p_i^2q_i^2)] = E_n[T_i(D_i - p_i)Y_i(1)^2/(p_i^2q_i^2)] + E_n[(T_i - q_i)Y_i(1)^2/(p_iq_i^2)] + E_n[Y_i(1)^2/(p_iq_i)] = E_n[Y_i(1)^2/(p_iq_i)] + o_p(1) = E[Y_i(1)^2/(p_iq_i)] + o_p(1)$$

The first equality is by Lemma A.2, and the second by WLLN. Then by symmetry  $E_n[T_i(1-D_i)Y_i(0)^2/(1-p_i)^2q_i^2] = E[Y_i(0)^2/(1-p_i)q_i] + o_p(1)$ . Then the sample variance in the theorem converges in probability to  $v = E[Y_i(1)^2/(p_iq_i)] + E[Y_i(0)^2/(1-p_i)q_i] - ATE^2$ . With V the limiting variance of Theorem 3.11, simple algebra shows that

$$v - V = E[m_{1i}^2(1 - p_i q_i)/p_i q_i] + E[m_{0i}^2(1 - q_i(1 - p_i))/(q_i(1 - p_i))] + 2E[m_{1i} m_{0i}].$$

Then the conclusion follows from the consistency results in Lemma A.6.  $\Box$ 

For variables  $A_i, B_i \in \sigma(W_i)$ , consider the matching corrections

$$\widehat{v}_{1} = n^{-1} \sum_{g \in \mathcal{G}_{n}^{\nu}} \frac{1}{a(g) - 1} \sum_{i \neq j \in g} A_{i} B_{j} D_{i} D_{j}$$

$$\widehat{v}_{0} = n^{-1} \sum_{g \in \mathcal{G}_{n}^{\nu}} \frac{1}{(k - a)(g) - 1} \sum_{i \neq j \in g} A_{i} B_{j} (1 - D_{i}) (1 - D_{j})$$

$$\widehat{v}_{10} = n^{-1} \sum_{g \in \mathcal{G}_{n}} \frac{k}{a(k - a)} (g) \sum_{i, j \in g} A_{i} B_{j} D_{i} (1 - D_{j})$$

**Lemma A.6** (Inference). Suppose  $E[A^2+B^2] < \infty$ . Then  $\widehat{v}_1 \stackrel{p}{\to} E[q_i p_i E[A_i | \psi_i] E[B_i | \psi_i]]$ ,  $\widehat{v}_0 \stackrel{p}{\to} E[q_i (1-p_i) E[A_i | \psi_i] E[B_i | \psi_i]]$ , and  $\widehat{v}_{10} \stackrel{p}{\to} E[q_i E[A_i | \psi_i] E[B_i | \psi_i]]$ .

*Proof.* First, we show the homogeneity condition  $n^{-1} \sum_{g \in \mathcal{G}_n^{\nu}} \sum_{i,j \in g} |\psi_i - \psi_j|_2^2 = o(1)$  also

holds for the matched groups  $\mathcal{G}_n^{\nu} = \{g \cup \nu(g) : g \in \mathcal{G}_n\}$ . Note that we may write

$$n^{-1} \sum_{g \in \mathcal{G}_n^{\nu}} \sum_{i,j \in g} |\psi_i - \psi_j|_2^2 = (2n)^{-1} \sum_{g \in \mathcal{G}_n} \sum_{i,j \in g \cup \nu(g)} |\psi_i - \psi_j|_2^2$$

$$= (2n)^{-1} \sum_{g \in \mathcal{G}_n} \sum_{i \in g, j \in \nu(g)} |\psi_i - \psi_j|_2^2 + (2n)^{-1} \sum_{g \in \mathcal{G}_n} \sum_{i \neq j} |\psi_i - \psi_j|_2^2 \mathbb{1}(ij \in g \text{ or } ij \in \nu(g))$$

The second term is o(1) by Theorem A.1. By Young's inequality, the first term is

$$\lesssim n^{-1} \sum_{g \in \mathcal{G}_n} \sum_{i \in g, j \in \nu(g)} |\psi_i - \bar{\psi}_g|_2^2 + |\bar{\psi}_g - \bar{\psi}_{\nu(g)}|_2^2 + |\bar{\psi}_{\nu(g)} - \psi_j|_2^2$$

$$\leq 2n^{-1} \sum_{g \in \mathcal{G}_n} k(g) \sum_{i \in g} |\psi_i - \bar{\psi}_g|_2^2 + \bar{k}^2 n^{-1} \sum_{g \in \mathcal{G}_n} |\bar{\psi}_g - \bar{\psi}_{\nu(g)}|_2^2$$

The second term is o(1) again by Theorem A.1. The first term is

$$2n^{-1} \sum_{g \in \mathcal{G}_n} k(g) \sum_{i \in g} |k(g)^{-1} \sum_{j \in g} (\psi_i - \psi_j)|_2^2 \le 2n^{-1} \sum_{g \in \mathcal{G}_n} \sum_{i,j \in g} |\psi_i - \psi_j|_2^2 = o(1)$$

again by triangle inequality, Jensen, and Theorem A.1. This finishes our proof of the claim.

Define  $A_i = v_a(\psi_i) + \epsilon_i^a$  with  $E[\epsilon_i^a|\psi_i] = 0$  and similarly for  $B_i$ . Denote  $v_{ia} = v_a(\psi_i)$  and  $v_{ib} = v_b(\psi_i)$ . Let  $c_n \to \infty$  be any sequence. By Lemma C.5, there exists sequences  $(z_n^a)_{n\geq 1}$  and  $(z_n^b)_{n\geq 1}$  of functions with  $|z_n^a|_{lip} \leq c_n$  and  $|z_n^a - v_a|_{2,\psi} = o(1)$  and similarly for b. Observe that  $|z_n^a|_{2,\psi} = O(1)$  since  $v_a \in L_2(\psi)$ . For matched groups  $g = g_1 \sqcup g_2$  with assignment propensities  $a_1/k_1$  and  $a_2/k_2$  in each group, define the group weight  $w_g = 1/(a_1 + a_2 - 1)$  and variance estimator

$$\widehat{v}_{1} = n^{-1} \sum_{g \in \mathcal{G}_{n}^{\nu}} w_{g} \sum_{i,j \in g} A_{i} B_{i} D_{i} D_{j} \mathbb{1}(i \neq j)$$

$$= n^{-1} \sum_{g \in \mathcal{G}_{n}^{\nu}} w_{g} \sum_{\substack{i,j \in g \\ i \neq j}} (m_{a}(\psi_{i}) + \epsilon_{i}^{a}) (m_{b}(\psi_{j}) + \epsilon_{j}^{b}) D_{i} D_{j} = A_{n} + B_{n} + C_{n} + R_{n}.$$

Consider  $A_n$ . Noting  $a_ib_j + b_ia_j = -(a_i - a_j)(b_i - b_j) + a_ib_i + a_jb_j$ , this is

$$n^{-1} \sum_{g \in \mathcal{G}_n^{\nu}} w_g \sum_{i < j \in g} (v_{ia}v_{jb} + v_{ja}v_{ib}) D_i D_j = n^{-1} \sum_{g \in \mathcal{G}_n^{\nu}} w_g \sum_{i < j \in g} (v_{ia}v_{ib} + v_{ja}v_{jb}) D_i D_j$$
$$- n^{-1} \sum_{g \in \mathcal{G}_n^{\nu}} w_g \sum_{i < j \in g} (v_{ia} - v_{ja}) (v_{ib} - v_{jb}) D_i D_j \equiv A_n^1 + A_n^2.$$

Denote  $z_{in}^a = z_n^a(\psi_i)$ ,  $z_{in}^b = z_n^b(\psi_i)$  and let  $\bar{k} = \max_{g \in \mathcal{G}} |g|$ . Expanding  $(v_{ia} - v_{ja})(v_{ib} - v_{jb})$  and by Young's inequality and Jensen inequality we have

$$|(v_{ia} - z_{in}^{a} + z_{in}^{a} - z_{jn}^{a} + z_{jn}^{a} - v_{ja})(v_{ib} - z_{in}^{b} + z_{in}^{b} - z_{jn}^{b} + z_{jn}^{b} - v_{jb})|$$

$$\lesssim |v_{ia} - z_{in}^{a} + z_{in}^{a} - z_{jn}^{a} + z_{jn}^{a} - v_{ja}|^{2} + |v_{ib} - z_{in}^{b} + z_{in}^{b} - z_{jn}^{b} + z_{jn}^{b} - v_{jb})|^{2}$$

$$\lesssim |v_{ia} - z_{in}^{a}|^{2} + |z_{in}^{a} - z_{jn}^{a}|^{2} + |z_{jn}^{a} - v_{ja}|^{2} + |v_{ib} - z_{in}^{b}|^{2} + |z_{in}^{b} - z_{jn}^{b}|^{2} + |z_{jn}^{b} - v_{jb}|^{2}.$$

Then by triangle inequality we have shown  $|A_{n2}| \leq |A_{n2}^a| + |A_{n2}^b|$  with

$$|A_{n2}^{a}| \lesssim n^{-1} \sum_{g \in \mathcal{G}_{n}^{\nu}} \sum_{i < j \in g} |v_{ia} - z_{in}^{a}|^{2} + |z_{in}^{a} - z_{jn}^{a}|^{2} + |z_{jn}^{a} - v_{ja}|^{2}$$

$$\lesssim 2\bar{k}n^{-1} \sum_{g \in \mathcal{G}_{n}^{\nu}} \sum_{i \in g} |v_{ia} - z_{in}^{a}|^{2} + c_{n}^{2}n^{-1} \sum_{g \in \mathcal{G}_{n}^{\nu}} \sum_{i,j \in g} |\psi_{i} - \psi_{j}|_{2}^{2}$$

$$= 2\bar{k}E_{n}[T_{i}|v_{ia} - z_{in}^{a}|^{2}] + o_{p}(1) \lesssim E_{n}[|v_{ia} - z_{in}^{a}|^{2}] + o_{p}(1) = o_{p}(1).$$

For the second to last inequality, set  $c_n = o(r_n^{-1/2})$  for  $n^{-1} \sum_{g \in \mathcal{G}_n^{\nu}} \sum_{i,j \in g} |\psi_i - \psi_j|_2^2 = O(r_n)$ , as guaranteed by Theorem A.1. The final equality is by Markov, since  $|z_n^a - v_a(\psi)|_{2,\psi} = o(1)$ . Then by symmetry  $A_{n2}^b = o_p(1)$  and  $A_{n2} = o_p(1)$ . Next consider  $A_{n1}$ 

$$n^{-1} \sum_{g \in \mathcal{G}_n^{\nu}} w_g \sum_{i < j \in g} (v_{ia}v_{ib} + v_{ja}v_{jb}) D_i D_j = n^{-1} \sum_{g \in \mathcal{G}_n^{\nu}} w_g \sum_{i \in g} D_i v_{ia} v_{ib} \left( \sum_{j \in g: j > i} D_j + \sum_{j \in g: j < i} D_j \right)$$

$$= n^{-1} \sum_{g \in \mathcal{G}_n^{\nu}} w_g \sum_{i \in g} D_i v_{ia} v_{ib} (a(g) - 1) = E_n [T_i D_i v_{ia} v_{ib}] = E_n [T_i (D_i - p_i) v_{ia} v_{ib}]$$

$$+ E_n [(T_i - q_i) p_i v_{ia} v_{ib}] + E_n [q_i p_i v_{ia} v_{ib}] = E[q_i p_i v_{ia} v_{ib}] + o_p (1).$$

The first equality by re-indexing, the third since  $w_g = (a(g) - 1)^{-1} = (a_1 + a_2 - 1)^{-1}$  and since  $\mathcal{G}_n^{\nu}$  partitions  $\{i: T_i = 1\}$ . The final equality follows by WLLN and Lemma A.2, since  $E[|q_i p_i v_{ia} v_{ib}|] \leq E[v_{ia}^2]^{1/2} E[v_{ib}^2]^{1/2} \lesssim E[A_i^2]^{1/2} E[B_i^2]^{1/2} < \infty$  by assumption.

Next claim that  $R_n = o_p(1)$ . It suffices to verify conditions of Lemma C.7 for

$$u_g = w_g \sum_{i,j \in g} \epsilon_i^a \epsilon_j^b D_i D_j \mathbb{1}(i \neq j) = w_g \sum_{i \neq j} \epsilon_i^a \epsilon_j^b D_i D_j \mathbb{1}(ij \in g)$$

Define  $\mathcal{F}_n = \sigma(\psi_{1:n}, \tau^t, \pi_n)$ , so that  $\mathcal{G}_n^{\nu} \in \mathcal{F}_n$ . Note that  $u_g \perp u_{g'}|\mathcal{F}_n$  for  $g \neq g'$  by Lemma C.9. We also need to show  $E[u_g|\mathcal{F}_n] = 0$  for each  $g \in \mathcal{G}_n^{\nu}$ . Note that  $E[u_g|\mathcal{F}_n] = E[E[u_g|\mathcal{F}_n']\mathcal{F}_n]$  with  $\mathcal{F}_n' = \sigma(\mathcal{F}_n, \tau^d)$  and  $D_{1:n} \in \mathcal{F}_n'$ . Repeatedly using the fact that  $(A, B) \perp C \Longrightarrow A \perp C|B$ , we have  $E[\epsilon_i^a \epsilon_j^b | \mathcal{F}_n'] = E[\epsilon_i^a \epsilon_j^b | \psi_i, \psi_j] = E[\epsilon_j^b E[\epsilon_i^a | \psi_i] | \psi_i, \psi_j] = 0$ . Then apparently  $E[u_g|\mathcal{F}_n] = 0$  for all  $g \in \mathcal{G}_n^{\nu}$ . Finally, Lemma C.7 requires the condition  $\frac{1}{n} \sum_{g \in \mathcal{G}_n^{\nu}} E[|u_g| \mathbb{1}(|u_g| > c_n) | \mathcal{F}_n] = o_p(1)$ . Observe that for any positive constants  $(a_k)_{k=1}^m$  we have  $\sum_k a_k \mathbb{1}(\sum_k a_k > c) \leq m \sum_k a_k \mathbb{1}(a_k > c/m)$  and  $ab\mathbb{1}(ab > c) \leq a^2\mathbb{1}(a^2 > c) + b^2\mathbb{1}(b^2 > c)$ . Let  $c_n \to \infty$  and let  $k = \max_{g \in \mathcal{G}_n^{\nu}} |g|$ . Using the indicator function facts above, for any group  $g \in \mathcal{G}_n^{\nu}$ ,  $E[|u_g|\mathbb{1}(|u_g| > c_n)|\mathcal{F}_n]$  is bounded above by

$$E\left[\sum_{\substack{i,j\in g}} |\epsilon_i^a| |\epsilon_j^b| \mathbb{1}(i \neq j) \mathbb{1}\left(\sum_{\substack{i,j\in g}} |\epsilon_i^a| |\epsilon_j^b| \mathbb{1}(i \neq j) > c_n\right) \middle| \mathcal{F}_n\right]$$

$$\leq \bar{k}^2 \sum_{\substack{i,j\in g\\i\neq j}} E\left[|\epsilon_i^a| |\epsilon_j^b| \mathbb{1}\left(|\epsilon_i^a| |\epsilon_j^b| > c_n/\bar{k}^2\right) \middle| \mathcal{F}_n\right]$$

The first line by triangle inequality and since  $w_g \leq 1$ . The inequality by the first indicator function fact. Using the second indicator fact, this is bounded above by

$$\leq \bar{k}^3 \sum_{i \in g} E\left[ (\epsilon_i^a)^2 \mathbb{1} \left( (\epsilon_i^a)^2 > c_n/\bar{k}^2 \right) \middle| \mathcal{F}_n \right] + \bar{k}^3 \sum_{i \in g} E\left[ (\epsilon_i^b)^2 \mathbb{1} \left( (\epsilon_i^b)^2 > c_n/\bar{k}^2 \right) \middle| \mathcal{F}_n \right] \\
= \bar{k}^3 \sum_{i \in g} E\left[ (\epsilon_i^1)^2 \mathbb{1} \left( (\epsilon_i^1)^2 > c_n/\bar{k}^2 \right) \middle| \psi_i \right] + \bar{k}^3 \sum_{i \in g} E\left[ (\epsilon_i^b)^2 \mathbb{1} \left( (\epsilon_i^b)^2 > c_n/\bar{k}^2 \right) \middle| \psi_i \right] \\$$

The last line again uses the fact that  $(A, B) \perp \!\!\! \perp C \implies A \perp \!\!\! \perp C | B$ , combined with iid sampling and independence of  $(\tau^t, \pi_n)$  from the data  $W_{1:n}$ . Then since  $\mathcal{G}_n^{\nu}$  is a partition of  $\{T_i = 1\} \subseteq [n]$ , we have

$$\frac{1}{n} \sum_{g \in \mathcal{G}_n^{\nu}} E[|u_g| \mathbb{1}(|u_g| > c_n) | \mathcal{F}_n] \lesssim \frac{\bar{k}^3}{n} \sum_{i=1}^n \sum_{c \in \{a,b\}} E\left[ (\epsilon_i^c)^2 \mathbb{1}\left( (\epsilon_i^c)^2 > c_n/\bar{k}^2 \right) \middle| \psi_i \right]$$

For c = a, taking an expectation of the RHS gives  $\bar{k}^3 E[(\epsilon_i^a)^2 \mathbb{1}((\epsilon_i^a)^2 > c_n/\bar{k}^2)] = o(1)$ 

as  $n \to \infty$  since  $E[(\epsilon_i^a)^2] \le E[\operatorname{Var}(A|\psi)] \lesssim \operatorname{Var}(A) < \infty$  and similarly for c = b. Then by Markov inequality  $\frac{1}{n} \sum_{g \in \mathcal{G}_n^{\vee}} E[|u_g|\mathbb{1}(|u_g| > c_n)|\mathcal{F}_n] = o_p(1)$ , so  $R_n = o_p(1)$  by Lemma C.7. An identical argument shows that  $B_n, C_n = o_p(1)$ . Then we have shown that  $\widehat{v}_1 = E[v_{ia}v_{ib}p_iq_i] + o_p(1)$ . By symmetry,  $\widehat{v}_0 = E[v_{ia}v_{ib}(1-p_i)q_i] + o_p(1)$ .

Next, consider the cross-term estimator.

$$\widehat{v}_{10} = n^{-1} \sum_{g \in \mathcal{G}_n} w_g \sum_{i,j \in g} A_i B_j D_i (1 - D_j)$$

$$= n^{-1} \sum_{g \in \mathcal{G}_n} w_g \sum_{i,j \in g} (m_{ai} + \epsilon_i^a) (m_{bj} + \epsilon_j^b) D_i (1 - D_j) = A_n + B_n + C_n + R_n$$

Let  $\mathcal{F}_n = \sigma(\psi_{1:n}, \tau^t, \pi_n)$  as before. Note the equality  $a_i b_j + b_i a_j = -(a_i - a_j)(b_i - b_j) + a_i b_i + a_j b_j$ . Then the conditional expectation  $E[A_n | \mathcal{F}_n]$  is equal to

$$n^{-1} \sum_{g \in \mathcal{G}_n} w_g \sum_{i,j \in g} E[v_i^a v_j^b D_i (1 - D_j) | \mathcal{F}_n] = n^{-1} \sum_{g \in \mathcal{G}_n} w_g \sum_{i,j \in g} v_i^a v_j^b \frac{a(k-a)}{k(k-1)} \mathbb{1}(i \neq j)$$

Expanding using the fact above gives

$$= n^{-1} \sum_{g \in \mathcal{G}_n} w_g \frac{a(k-a)}{k(k-1)} \sum_{i < j \in g} (v_i^a v_j^b + v_j^a v_i^b) = -n^{-1} \sum_{g \in \mathcal{G}_n} w_g \frac{a(k-a)}{k(k-1)} \sum_{i < j \in g} (v_i^a - v_j^a) (v_i^b - v_j^b)$$

$$+ n^{-1} \sum_{g \in \mathcal{G}_n} w_g \frac{a(k-a)}{k(k-1)} \sum_{i < j \in g} (v_i^a v_i^b + v_j^a v_j^b) \equiv T_{n1} + T_{n2}$$

First consider  $T_{n1}$ . By Young's inequality we have

$$|T_{n1}| \lesssim n^{-1} \sum_{g \in \mathcal{G}_n} \sum_{i < j \in g} |v_i^a - v_j^a| |v_i^b - v_j^b| \le (2n)^{-1} \sum_{g \in \mathcal{G}_n} \sum_{i,j \in g} |v_i^a - v_j^a|^2 + |v_i^b - v_j^b|^2$$

The form of each expression is identical to our analysis of  $A_n^1$  above. Then  $T_{n1} = o_p(1)$  by the same argument. Next consider  $T_{n2}$ . By counting, it's easy to see that  $\sum_{i < j \in g} (v_i^a v_i^b + v_j^a v_j^b) = (k-1) \sum_{i \in g} v_i^a v_i^b$ . Then setting  $w_g = k/(a(k-a))$  gives

$$T_{n2} = n^{-1} \sum_{g \in \mathcal{G}_n} w_g \frac{a(k-a)}{k(k-1)} (k-1) \sum_{i \in g} v_i^a v_i^b = n^{-1} \sum_{g \in \mathcal{G}_n} \sum_{i \in g} v_i^a v_i^b$$
$$= E_n[T_i v_i^a v_i^b] = E_n[q_i v_i^a v_i^b] + E_n[(T_i - q_i) v_i^a v_i^b] = E[q_i v_{ia} v_{ib}] + o_p(1)$$

The third equality since  $\mathcal{G}_n$  partitions the units  $\{T_i = 1\}$ . The final equality follows from

Lemma A.2. Next consider

$$A_n - E[A_n | \mathcal{F}_n] = n^{-1} \sum_{g \in \mathcal{G}_n} \sum_{i,j \in g} w_g v_i^a v_j^b \left( D_i (1 - D_j) - \frac{a(k-a)}{k(k-1)} \right) \mathbb{1}(i \neq j) \equiv n^{-1} \sum_{g \in \mathcal{G}_n} u_g$$

We have  $E[u_g|\mathcal{F}_n] = 0$  for all  $g \in \mathcal{G}_n$  by the calculation of  $E[A_n|\mathcal{F}_n]$  above. Also, note  $u_g \perp \!\!\!\perp u_{g'}|\mathcal{F}_n$  for all  $g \neq g'$  by Lemma C.9. Then by Lemma C.7, it suffices to show that  $\frac{1}{n} \sum_{g \in \mathcal{G}_n^v} E[|u_g|\mathbb{1}(|u_g| > c_n)|\mathcal{F}_n] = o_p(1)$  for some  $c_n \to \infty$  with  $c_n = o(n^{1/2})$ . It's easy to see that  $w_g \leq 2$ , so we have

$$|u_g| \le \sum_{i,j \in g} w_g |v_i^a| |v_j^b| \left| D_i (1 - D_j) - \frac{a(k-a)}{k(k-1)} \right| \mathbb{1}(i \ne j) \le \sum_{i,j \in g} |v_i^a| |v_j^b|$$

Then using the indicator function bounds in our analysis above,  $E[|u_g|\mathbb{1}(|u_g|>c_n)|\mathcal{F}_n]$  is bounded above by

$$E\left[\sum_{i,j\in g} |v_i^a| |v_j^b| \mathbb{1}\left(\sum_{i,j\in g} |v_i^a| |v_j^b| > c_n\right) |\mathcal{F}_n\right] \le \bar{k}^2 \sum_{i,j\in g} E\left[|v_i^a| |v_j^b| \mathbb{1}\left(|v_i^a| |v_j^b| > c_n/(\bar{k})^2\right) |\mathcal{F}_n\right]$$

$$\le \bar{k}^3 \sum_{i\in g} \left(E\left[|v_i^a|^2 \mathbb{1}\left(|v_i^a|^2 > c_n/(\bar{k})^2\right) |\mathcal{F}_n\right] + E\left[|v_i^b|^2 \mathbb{1}\left(|v_i^b|^2 > c_n/(\bar{k})^2\right) |\mathcal{F}_n\right]\right)$$

$$\le \bar{k}^3 \sum_{i\in g} \left(E\left[|v_i^a|^2 \mathbb{1}\left(|v_i^a|^2 > c_n/(\bar{k})^2\right) |\psi_i\right] + E\left[|v_i^b|^2 \mathbb{1}\left(|v_i^b|^2 > c_n/(\bar{k})^2\right) |\psi_i\right]\right)$$

Then  $\frac{1}{n} \sum_{g \in \mathcal{G}_n^v} E[|u_g|\mathbb{1}(|u_g| > c_n)|\mathcal{F}_n]$  is bounded above by

$$\begin{split} &\bar{k}^3 \frac{1}{n} \sum_{g \in \mathcal{G}_n^v} \sum_{i \in g} \left( E\left[ |v_i^a|^2 \mathbb{1} \left( |v_i^a|^2 > c_n/(\bar{k})^2 \right) |\psi_i \right] + E\left[ |v_i^b|^2 \mathbb{1} \left( |v_i^b|^2 > c_n/(\bar{k})^2 \right) |\psi_i \right] \right) \\ &= \bar{k}^3 E_n [T_i E[|v_i^a|^2 \mathbb{1} (|v_i^a|^2 > c_n/(\bar{k})^2) |\psi_i]] + E_n [T_i E[|v_i^b|^2 \mathbb{1} (|v_i^b|^2 > c_n/(\bar{k})^2) |\psi_i]] \\ &\leq \bar{k}^3 E_n [E[|v_i^a|^2 \mathbb{1} (|v_i^a|^2 > c_n/(\bar{k})^2) |\psi_i]] + E_n [E[|v_i^b|^2 \mathbb{1} (|v_i^b|^2 > c_n/(\bar{k})^2) |\psi_i]] \end{split}$$

Taking expectation of the final line gives  $\sum_{c=a,b} E[|v_i^c|^2 \mathbb{1}(|v_i^c|^2 > c_n/(\bar{k})^2)] \to 0$  as  $n \to \infty$  by dominated convergence. Then by Markov inequality, we have shown that  $\frac{1}{n} \sum_{g \in \mathcal{G}_n} E[|u_g| \mathbb{1}(|u_g| > c_n) | \mathcal{F}_n]$ , so  $A_n - E[A_n|\mathcal{F}_n] = o_p(1)$  by Lemma C.7. Next, note that  $B_n, C_n, R_n = o_p(1)$  by the exact argument used in our analysis of  $\widehat{v}_1$ . Then we have shown that  $\widehat{v}_{10} \stackrel{p}{\to} E[q_i v_{ia} v_{ib}]$  as claimed.

# Secondary Online Appendix to "Optimal Stratification of Survey Experiments"

#### Max Cytrynbaum

This secondary online appendix is not intended for publication. It contains our theoretical simulation results, as well as other non-essential supporting material.

#### **B** Simulations

This section presents simulations exhibiting the finite sample properties of our method. Our asymptotic results show separate variance reductions from each of the following: (a) finely treatment assignment, (b) finely stratified sampling and assignment, (c) using the optimal propensities  $q^*(\psi)$  and  $p^*(\psi)$  (generally infeasible), and (d) using pilot estimates  $\widehat{q}(\psi)$  and  $\widehat{p}(\psi)$  of the optimal propensities (feasible). In particular, designs (a)-(d) are weakly increasing in asymptotic efficiency. To quantify the marginal efficiency gain from each of our proposed methods in finite samples, we simulate unadjusted ATE estimation under the following designs:

**CR**: Complete randomization  $T_{1:n} \sim \operatorname{CR}(q_k^*)$  and  $D_{1:n} \sim \operatorname{CR}(p)$ , with  $q_k^*$  a discretization of the budget-exhausting sampling propensity  $q^* = \bar{B}/E[C(\psi)]$ .<sup>22</sup>

**CR**, **Loc**: As in CR but with stratified assignment  $D_{1:n} \sim \text{Loc}(\psi, p)$ .

**Loc**: Stratified sampling and assignment  $T_{1:n} \sim \text{Loc}(\psi, q_k^*)$  and  $D_{1:n} \sim \text{Loc}(\psi, p)$ .

**Hom**: As in **Loc** but with  $q_{hom,k}^*(\psi)$  a discretization of  $q_{hom}^*(\psi) = \bar{B} \cdot C(\psi)^{-1/2} / E[C(\psi)^{1/2}]$ , the optimal sampling propensity assuming homoskedasticity. This is feasible but may be misspecified.

**Opt**: As in **Loc** but with  $q_k^*(\psi)$  and  $p_k^{*23}$  discretizations of the optimal propensities from Section 4, using oracle knowledge of the heteroskedasticity functions  $\sigma_d^2(\psi)$  (infeasible).

**Pilot S/L**: As in **Opt**, replacing the unknown optimal propensities  $q_k^*(\psi)$  and  $p_k^*$  with  $\hat{q}_k(\psi)$  and  $\hat{p}_k$  estimated from a pilot of size (S)  $n_{pilot} = 100$  or (L)  $n_{pilot} = 400$ .

<sup>&</sup>lt;sup>22</sup>In particular, we let  $q_k^* = a/k$ , using the minimal k such that  $q_k^* \cdot E_n[C(\psi_i)] \in [.95\bar{B}, 1.05\bar{B}]$ .

<sup>&</sup>lt;sup>23</sup>For simplicity, we focus on the optimal constant assignment propensity under fine stratification (Equation 4.6).

Variance functions  $\sigma_d^2(\psi)$  are estimated using a modification of Fan and Yao (1998), see appendix section A.2 for details.

Discretization - In each of the designs with varying propensities we discretize by choosing  $q_k(\cdot)$  to minimize  $E_n[(q_k - q^*)^2(\psi_i)]$  over the set of discretizations  $\{q : q(\psi) \in a/10 : a = 1, ..., 10\}$  subject to number of propensity levels  $L = |\text{Image}(q)| \leq 3$ .

Theory Predictions. Our results predict that there will be large variance reduction from stratified assignment, design CR to CR, Loc in the notation above, if  $\psi$  predicts outcomes Y(d) well. Similarly, there will be large variance reductions from stratified sampling (CR, Loc to Loc) if  $\psi$  predicts treatment effects Y(1) - Y(0) well, from Loc to Hom if costs are heterogeneous and heteroskedasticity is mild, and from Hom to Opt if there is significant heteroskedasticity. Moreover, the confidence intervals from Section 7 should have close to nominal coverage. Let  $Y_i(d) = m_d(\psi_i) + \sigma_d^2(\psi_i)\epsilon_i^d$  with  $E[\epsilon_i^d|\psi_i] = 0$  and  $Var(\epsilon_i^d|\psi_i) = 1$  for d = 0, 1, and denote  $\nu = \dim(\psi)$ . To test the predictions of our theory, we simulate data from the following DGP's:

Model 1: Outcomes  $m_0(\psi) = \beta_0' \psi$  and  $m_1(\psi) = \beta_1' \psi + \psi' Q \psi$  with  $\beta_0 = 0$ ,  $\beta_1 = 3 \cdot \text{vec}(1/m : m \in [\nu])$ , and  $Q = (1/2)\mathbb{1}\mathbb{1}'$  with  $\psi \sim \text{Unif}([-1, 1]^{\nu})$ . Costs  $c(\psi) = \mathbb{1}(\psi_1 \leq 0) + 10 \cdot \mathbb{1}(\psi_1 > 0)$ , budget constraint  $\bar{B} = 4$ , and baseline treatment proportions p = 3/8. Residuals  $\epsilon^d \sim \mathcal{N}(0, I_{\nu})$  with  $\sigma_0^2 = 1$  and  $\sigma_1^2 = 9$ .

Model 2: As in Model 1, but  $c(\psi) = \mathbb{1}(\psi_1 \leq 0) + 4 \cdot \mathbb{1}(\psi_1 > 0)$ , budget constraint  $\bar{B} = 1$ , and p = 1/2. Heteroskedasticity functions  $\sigma_0^2(\psi) = 5$  and  $\sigma_1^2(\psi) = 5 + 30 \cdot \|\psi\|_2^2/\nu$  and  $\epsilon^d \sim \text{Unif}([-1,1])$ .

Model 3: As in Model 1, but  $c(\psi) = 1/2 + 10 \cdot ||\psi||_2^2/\nu$ ,  $\bar{B} = 2$ , and  $\sigma_d^2(\psi) = 2$ .

Model 4: As in Model 1, but with  $\beta_0 = 2 \cdot \text{vec}(1/k : k \in [\nu]) = (2/3)\beta_1$ , and Q = 211'. Costs as in Model 3 and heteroskedasticity as in Model 2.

Model 5: As in Model 1, but with  $m_d(\psi) = 5 \cdot g(\beta'_d \psi)$  for  $\beta_0 = \beta_1 = 10 \cdot \text{vec}(1/m : m \in [\nu])$  and g the Cauchy CDF, p = 1/2, and  $\sigma_d^2(\psi) = 2$ .

Model 6: As in Model 1, but outcomes  $m_1(\psi) = 4\sum_{m=1}^{\nu} \sin(\psi_m) + 2\mathbb{1}'\psi$  and  $m_0(\psi) = 2\sum_{m=1}^{\nu} \cos(\psi_m)$  and  $\psi \sim \text{Unif}([-\pi, \pi]^{\nu})$ , with p = 3/10 and  $\sigma_d^2(\psi) = 6$ .

Table 2 presents our main results, computed using 1000 Monte Carlo repetitions, discretizing propensities to level k=8 in all cases. "SD" denotes estimator standard

		$n = 800, \dim(\psi) = 2$						$n = 400, \dim(\psi) = 6$					
	Design, DGP	1	2	3	4	5	6	1	2	3	4	5	6
SD	CR	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
	CR, Loc	0.96	0.94	0.81	0.87	0.56	0.62	0.89	0.96	0.86	0.92	0.66	0.76
	Loc	0.90	0.93	0.74	0.84	0.54	0.58	0.89	0.94	0.81	0.86	0.67	0.73
	Hom.	0.93	0.91	0.74	0.89	0.55	0.58	0.88	0.93	0.81	0.88	0.66	0.74
	Opt.	0.80	0.87	0.72	0.79	0.56	0.55	0.81	0.90	0.68	0.76	0.64	0.59
	Pilot S	0.87	0.91	0.68	0.83	0.56	0.52	0.78	0.86	0.75	0.73	0.66	0.57
	Pilot L	0.82	0.87	0.70	0.77	0.56	0.52	0.78	0.90	0.74	0.70	0.65	0.56
$\%\Delta { m CI}$	CR	0	0	0	0	0	0	0	0	0	0	0	0
	CR, Loc	-7	-3	-18	-12	-42	-35	-7	-3	-9	-6	-30	-18
	Loc	-9	-6	-24	-13	-42	-40	-9	-5	-11	-7	-29	-20
	Hom.	-14	-9	-26	-14	-45	-41	-13	-8	-10	-5	-33	-23
	Opt.	-21	-12	-30	-24	-45	-47	-21	-9	-24	-21	-33	-43
	Pilot S	-21	-12	-29	-22	-43	-46	-20	-11	-21	-22	-30	-40
	Pilot L	-21	-13	-30	-24	-44	-46	-21	-11	-23	-25	-32	-40
Cover	CR	0.95	0.95	0.95	0.95	0.95	0.95	0.94	0.94	0.94	0.95	0.95	0.94
	CR, Loc	0.95	0.95	0.94	0.95	0.96	0.96	0.96	0.95	0.96	0.96	0.97	0.97
	Loc	0.95	0.95	0.95	0.96	0.95	0.96	0.95	0.95	0.97	0.96	0.97	0.97
	Hom.	0.92	0.95	0.96	0.95	0.95	0.90	0.94	0.94	0.97	0.97	0.95	0.96
	Opt.	0.92	0.96	0.95	0.96	0.95	0.87	0.94	0.95	0.97	0.96	0.96	0.94
	Pilot S	0.94	0.95	0.96	0.95	0.95	0.95	0.96	0.96	0.95	0.96	0.96	0.96
	Pilot L	0.94	0.96	0.94	0.95	0.95	0.96	0.95	0.95	0.95	0.96	0.96	0.96

Table 2: Simulation Results

deviation relative to design CR.<sup>24</sup> "% $\Delta$ CI" is percent change in confidence interval length relative to the length under CR, using the asymptotically exact confidence intervals from Section 7 for all designs.

Results. Our simulation results agree with the theory predictions above. For example, Models 5 and 6 show large variance reductions from stratified assignment, but not from stratified sampling since  $\psi$  is not predictive of treamtent effects Y(1) - Y(0) in these models. By contrast, stratified sampling significantly reduces variance in Models 1-3, where  $\psi$  is predictive of treatment effects. The simulation results also show efficiency gains from incorporating costs  $C(\psi)$  into the sampling propensity  $q_{hom}^*(\psi)$ , even without knowledge of the true heteroskedasticity function, as in design Hom. Models 2 and 4 have significant heteroskedasticity, and show further variance reduction from incorporating oracle knowledge of  $\sigma_d^2(\psi)$  into the globally optimal sampling propensity  $q^*(\psi)$  in Opt. Design Pilot S is less efficient than Opt due to noisy estimation of  $\sigma_d^2(\psi)$  using a small pilot, while Pilot L is almost optimal. The results also show approximately nominal coverage, and the confidence interval shrinkage in panel 2 reflects the efficiency gains in panel 1.

## C Supporting Theory

**Lemma C.1** (Propensity Convergence). Suppose that  $|\widehat{\sigma}_{d}^{2} - \sigma_{d}^{2}|_{2,\psi}^{2} = O_{p}(n^{-r})$  for d = 0, 1. Then  $|\widehat{p}_{i,n} - p_{i}^{*}|_{2,n}^{2} \vee |\widehat{q}_{i,n} - q_{i}^{*}|_{2,n}^{2} = O(1/\overline{k}_{n}^{2}) + O_{p}(n^{-r})$ .

*Proof.* We have  $|\widehat{p}_{i,n} - p_i^*|_{2,n}^2 \leq 2|\widehat{p}_{i,n} - \widehat{p}_i|_{2,n}^2 + 2|\widehat{p}_i - p_i^*|_{2,n}^2 \leq O(1/\overline{k}_n^2) + |\widehat{p}_i - p_i^*|_{2,n}^2$  by discretization, and similarly for  $|\widehat{q}_{i,n} - q_i^*|_{2,n}^2$ . Then it suffices to bound  $|\widehat{p}_i - p_i^*|_{2,n}^2$ . Note

$$|\widehat{\sigma}_d - \sigma_d|_{2,\psi}^2 = \int_{\psi} \frac{(\widehat{\sigma}_d^2 - \sigma_d^2)^2(\psi)}{(\widehat{\sigma}_d + \sigma_d)^2(\psi)} dP(\psi) \le c_l^{-1} |\widehat{\sigma}_d^2 - \sigma_d^2|_{2,\psi}^2 = O_p(n^{-r}).$$

Then  $|\widehat{p}_i - p_i^*|_{2,n}^2$  is equal to

$$E_{n}[(\widehat{\sigma}_{1i}/(\widehat{\sigma}_{1i}+\widehat{\sigma}_{0i})-\sigma_{1i}/(\sigma_{1i}+\sigma_{0i}))^{2}] \leq 4c_{l}^{-2}E_{n}[((\sigma_{1i}-\widehat{\sigma}_{1i})\widehat{\sigma}_{0i}+\widehat{\sigma}_{1i}(\widehat{\sigma}_{0i}-\sigma_{0i}))^{2}]$$

$$\lesssim E_{n}[(\sigma_{1i}-\widehat{\sigma}_{1i})^{2}\widehat{\sigma}_{0i}^{2}] + E_{n}[\widehat{\sigma}_{1i}^{2}(\widehat{\sigma}_{0i}-\sigma_{0i}))^{2}] \lesssim |\widehat{\sigma}_{0}-\sigma_{0i}|_{2,n}^{2} + |\widehat{\sigma}_{1}-\sigma_{1}|_{2,n}^{2}$$

The last expression is equal to  $\sum_{d=0,1} |\widehat{\sigma}_d - \sigma_d|_{2,\psi}^2 + O_p(n^{-1/2}) = O_p(n^{-r}) + O_p(n^{-1/2})$ 

Note that  $E[\widehat{\theta} - ATE] = 0$  for all designs and estimators, so we only report standard deviation.

by conditional Markov inequality. Next consider  $|\widehat{q} - q^*|_{2,n}^2$ . Denote  $C_i = C(\psi_i)$ . Define  $\mu_n = E_n[C_i^{1/2}(\widehat{\sigma}_{1i} + \widehat{\sigma}_{0i})]$  and  $\mu = E[C_i^{1/2}(\sigma_{1i} + \sigma_{0i})]$ . Using  $\xi_n \perp W_{1:n}$ , by conditional Chebyshev  $E_n[C_i^{1/2}\widehat{\sigma}_{di}] = E[C_i^{1/2}\widehat{\sigma}_{di}|\xi_n] + O_p(n^{-1/2})$ . Then we have

$$(\mu_n - \mu)^2 \lesssim \sum_{d=0,1} (E_n[C_i^{1/2}\widehat{\sigma}_{di}] - E[C_i^{1/2}\widehat{\sigma}_{di}|\xi_n] + E[C_i^{1/2}\widehat{\sigma}_{di}|\xi_n] - E[C_i^{1/2}\widehat{\sigma}_{di}])^2$$

$$\lesssim \sum_{d=0,1} (E_n[C_i^{1/2}\widehat{\sigma}_{di}] - E[C_i^{1/2}\widehat{\sigma}_{di}|\xi_n])^2 + |C|_{\infty} E_{\psi}[(\widehat{\sigma}_{di} - \sigma_{di})^2] = O_p(n^{-1}) + O_p(n^{-r})$$

The first inequality is Young's, the second by Young's and Jensen. Define  $\widehat{v}_i = C_i^{-1/2}(\widehat{\sigma}_{1i} + \widehat{\sigma}_{0i})$  and  $v_i = C_i^{-1/2}(\sigma_{1i} + \sigma_{0i})$ .

$$|\widehat{q} - q^*|_{2,n}^2 = \overline{q}^2 E_n[(\widehat{v}_i/\mu_n - v_i/\mu)^2] \lesssim (\mu_n \mu)^{-2} (E_n[\widehat{v}_i^2](\mu - \mu_n) + \mu_n E_n[(\widehat{v}_i - v_i)^2])$$

$$\lesssim (\mu - \mu_n)^2 + E_n[(\widehat{v}_i - v_i)^2] = O_p(n^{-r}) + O_p(n^{-1/2})$$

The first inequality is Young's, the second using our bounded variance assumption. The final equality follows from work above. This finishes the proof.  $\Box$ 

## C.1 Regression Equivalence Propositions

Proof of Proposition 3.6. First, consider the regression  $Y \sim 1 + D + \tilde{z} + D\tilde{z}$  defining  $\widehat{\tau}$  and  $\widehat{\beta}$ . Define the within-arm regression coefficients  $\widehat{\alpha}_d = \operatorname{Var}_n(\widetilde{z}_i|D_i = d, T_i = 1)^{-1} \operatorname{Cov}_n(\widetilde{z}_i, Y_i(d)|D_i = d, T_i = 1)$  for  $d \in \{0, 1\}$ . E.g. by the calculations in Lin (2013), we have  $\widehat{\beta} = \widehat{\alpha}_1 - \widehat{\alpha}_0$  and

$$\widehat{\tau} = \widehat{\theta} - (\widehat{\alpha}_1/p + \widehat{\alpha}_0/(1-p)) E_n [(D_i - p)\widetilde{z}_i | T_i = 1]$$

Consider  $\widehat{\alpha}_1$ , for instance.

$$Var_{n}(\tilde{z}_{i}|D_{i}=1, T_{i}=1) = \frac{E_{n}[\tilde{z}_{i}\tilde{z}'_{i}D_{i}T_{i}]}{E_{n}[D_{i}T_{i}]} - \frac{E_{n}[\tilde{z}_{i}D_{i}T_{i}]E_{n}[\tilde{z}'_{i}D_{i}T_{i}]}{E_{n}[D_{i}T_{i}]^{2}}$$

By Definition 2.1, we have  $E_n[D_iT_i] = E_n[(D_i-p)T_i] + pE_n[T_i-q] + pq = pq + O(1/n)$ . Similarly, we expand  $E_n[\tilde{z}_i\tilde{z}_i'D_iT_i] = E_n[\tilde{z}_i\tilde{z}_i'(D_i-p)T_i] + pE_n[\tilde{z}_i\tilde{z}_i'(T_i-q)] + pqE_n[\tilde{z}_i\tilde{z}_i']$  and  $E_n[\tilde{z}_i'D_iT_i] = E_n[\tilde{z}_i(D_i-p)T_i] + pE_n[\tilde{z}_i(T_i-q)] + pqE_n[\tilde{z}_i]$ . It's easy to check that the conditions of Lemma A.2 are satisfied, so that  $E_n[\tilde{z}_i\tilde{z}_i'D_iT_i] = pqE_n[\tilde{z}_i\tilde{z}_i'] + O_p(n^{-1/2})$  and  $E_n[\tilde{z}_iD_iT_i] = pqE_n[\tilde{z}_i] + O_p(n^{-1/2})$ . Putting these facts together gives  $Var_n(\tilde{z}_i|D_i=pqE_n[\tilde{z}_i]) = pqE_n[\tilde{z}_i] + O_p(n^{-1/2})$ .

 $1, T_i = 1$ ) =  $E_n[\tilde{z}_i \tilde{z}_i'] - E_n[\tilde{z}_i] E_n[\tilde{z}_i'] + O_p(n^{-1/2})$ . Similarly,  $E_n[z_i|T_i = 1] = E_n[z_i] + O_p(n^{-1/2})$  so

$$E_{n}[\tilde{z}_{i}\tilde{z}'_{i}] - E_{n}[\tilde{z}_{i}]E_{n}[\tilde{z}'_{i}] = E_{n}[z_{i}z'_{i}] - E_{n}[z_{i}]E_{n}[z'_{i}|T_{i} = 1] - E_{n}[z_{i}|T_{i} = 1]E_{n}[z'_{i}]$$

$$+ E_{n}[z_{i}|T_{i} = 1]E_{n}[z'_{i}|T_{i} = 1] = E_{n}[z_{i}z'_{i}] - E_{n}[z_{i}]E_{n}[z'_{i}] + O_{p}(n^{-1/2})$$

$$= \operatorname{Var}(z) + O_{p}(n^{-1/2})$$

Similar reasoning shows that  $\operatorname{Cov}_n(\tilde{z}_i,Y_i(d)|D_i=d,T_i=1)=\operatorname{Cov}(z,Y(d))+O_p(n^{-1/2})$  if  $E[Y(d)^2]<\infty$ . Note that  $\operatorname{Var}(z)\succ 0$  by the assumption that P(S=k)>0  $\forall k\in [m]$ . Then we have  $\widehat{\alpha}_d=\operatorname{Var}(z)^{-1}\operatorname{Cov}(z,Y(d))+O_p(n^{-1/2})$ . Recall  $z=(\mathbbm{1}(S=k))_{k=1}^{m-1}$ . For a function  $f(X)\in L_1(X)$  define  $\gamma(f)=\operatorname{Var}(z)^{-1}\operatorname{Cov}(z,f(X))$ . Then it's easy to see that  $\gamma(f)'z=E[f(X)|S]-E[f(X)|S=m]$ . Now by above work  $\widehat{\beta}=\widehat{\alpha}_1-\widehat{\alpha}_0=\operatorname{Var}(z)^{-1}\operatorname{Cov}(z,Y(1)-Y(0))+O_p(n^{-1/2})=\gamma(c)+O_p(n^{-1/2})$ . Similarly,  $\widehat{\alpha}_1/p+\widehat{\alpha}_0/(1-p)=\operatorname{Var}(z)^{-1}\operatorname{Cov}(z,Y(1)/p+Y(0)/(1-p))+O_p(n^{-1/2})=\gamma(b)(p-p)^{-1/2}+O_p(n^{-1/2})$ . Then by the fundamental expansion of the IPW estimator, we have

$$\check{\theta} = \widehat{\theta} - (\widehat{\alpha}_1/p + \widehat{\alpha}_0/(1-p)) E_n [(D_i - p)\tilde{z}_i|T_i = 1] - \widehat{\beta}' E_n \left[ \frac{z_i(T_i - q)}{q} \right] + O_p(n^{-1}) 
= \widehat{\theta} - \gamma(b)' E_n \left[ \frac{(D_i - p)z_i}{q\sqrt{p - p^2}} \right] - \gamma(c)' E_n \left[ \frac{z_i(T_i - q)}{q} \right] + O_p(n^{-1}) = E_n [c(X_i)] 
+ E_n \left[ \frac{T_i - q}{q} (c(X_i) - \gamma(c)'z_i) \right] + E_n \left[ \frac{T_i(D_i - p)}{q\sqrt{p - p^2}} (b(X_i) - \gamma(b)'z_i) \right] + R_n + O_p(n^{-1}) 
= E_n [c(X_i)] + E_n \left[ \frac{T_i - q}{q} (c(X_i) - E[c(X_i)|S_i]) \right] + E_n \left[ \frac{T_i(D_i - p)}{q\sqrt{p - p^2}} (b(X_i) - E[b|S_i]) \right] 
+ R_n + O_p(n^{-1})$$

The first line uses  $E_n[z_i|T_i=1]=E_n[z_i]/q+O(n^{-1})$  and  $E_n[(D_i-p)E_n[z_i|T_i=1]]=O(n^{-1})$  by stratification. The second line uses the probability limits established above and that  $E_n[(D_i-p)z_i]=O_p(n^{-1/2})$  and  $E_n[(T_i-q)z_i]=O_p(n^{-1/2})$ . The final equality follows from the characterization of  $\operatorname{Var}(z)^{-1}\operatorname{Cov}(z,f(X))$  above and since  $E_n[(D_i-p)E[b(X_i)|S_i=m]]=O(n^{-1})$  and  $E[(T_i-q)E[c(X_i)|S_i=m]]=O(n^{-1})$  by stratification. The final expansion is identical to that in the proof of Theorem 3.11. The conclusion then follows by the same argument.

Proof of Proposition 3.12. First we discuss cross-fitting. Denote  $Z_i = (W_i, D_i, T_i)$ . Let  $I_1 \sqcup I_2 = [n]$  be a random partition with  $|I_1| \asymp n$  and  $(I_1, I_2) \in \sigma(\pi_n)$  for randomness  $\pi_n \perp \!\!\! \perp Z_{1:n}$ . The estimator has form  $E_n[F(Z_i, \widehat{m}_{I(i)})]$ . Use the cross-fitting pattern  $I(i) = I_1$  if  $i \in I_2$  and similarly for  $i \in I_1$ . We may rearrange the summand of  $\widehat{\theta}_{adj}$  as

$$\begin{split} & \frac{T_i D_i Y_i}{q_i p_i} - \frac{Y_i (1 - D_i) T_i}{q_i (1 - p_i)} + \widehat{m}_1(\psi_i) - \widehat{m}_0(\psi_i) - \frac{T_i}{q_i} \left( \frac{D_i \widehat{m}_1(\psi_i)}{p_i} - \frac{(1 - D_i) \widehat{m}_0(\psi_i)}{(1 - p_i)} \right) \\ & = \frac{T_i D_i Y_i}{q_i p_i} - \frac{Y_i (1 - D_i) T_i}{q_i (1 - p_i)} + \widehat{m}_1(\psi_i) - \widehat{m}_0(\psi_i) - \frac{T_i}{q_i} \left( \widehat{m}_1(\psi_i) \right) - \widehat{m}_0(\psi_i))) \\ & - \frac{T_i (D_i - p_i)}{q_i} \left( \frac{\widehat{m}_1(\psi_i)}{p_i} - \frac{\widehat{m}_0(\psi_i)}{(1 - p_i)} \right) \end{split}$$

Continuing the calculation, this is

$$\begin{split} &= \frac{T_i D_i Y_i}{q_i p_i} - \frac{Y_i (1 - D_i) T_i}{q_i (1 - p_i)} - \frac{(T_i - q_i)}{q_i} \widehat{c}(\psi_i) - \frac{T_i (D_i - p_i)}{q_i (p_i - p_i^2)^{1/2}} \widehat{b}(\psi_i) \\ &= c(\psi_i) + \frac{(T_i - q_i)}{q_i} (c - \widehat{c})(\psi_i) - \frac{T_i (D_i - p_i)}{q_i (p_i - p_i^2)^{1/2}} (b - \widehat{b})(\psi_i) + \frac{D_i T_i \epsilon_i^1}{p_i q_i} + \frac{(1 - D_i) T_i \epsilon_i^0}{(1 - p_i) q_i} \end{split}$$

Consider the term  $T_{1,n}=n^{-1}\sum_{i\in I_1}q_i^{-1}(T_i-q_i)(c-\widehat{c})(\psi_i,Z_{I_2})$ . By Lemma C.9 with  $m=2,\ g=I$  and  $h,\tau_s=1$  we have  $Z_{I_1}\perp\!\!\!\perp Z_{I_2}|\pi_n$ . Then applying Lemma C.9

$$E[nT_{1,n}^{2}|\pi_{n}, Z_{I_{2}}] = n^{-1} \sum_{i \in I_{1}} E[q_{i}^{-2}(T_{i} - q_{i})^{2}(c - \widehat{c})(\psi_{i}, Z_{I_{2}})^{2}|\pi_{n}, Z_{I_{2}}]$$

$$= n^{-1} \sum_{i \in I_{1}} E[q_{i}^{-1}(1 - q_{i})(c - \widehat{c})(\psi_{i}, Z_{I_{2}})^{2}|\pi_{n}, Z_{I_{2}}]$$

$$= n^{-1}|I_{1}| \int (1 - q)(\psi)/q(\psi)(c - \widehat{c})(\psi, Z_{I_{2}})^{2}dP(\psi) \lesssim |c - \widehat{c}(Z_{I_{2}})|_{2,\psi} = o_{p}(1)$$

Then  $\sqrt{n}T_{1,n} = o_p(1)$ . Then by symmetry  $\sqrt{n}E_n[q_i^{-1}(T_i - q_i)(c - \hat{c})(\psi_i)] = o_p(1)$ . Similarly,  $\sqrt{n}E_n[\frac{T_i(D_i - p_i)}{q_i(p_i - p_i^2)^{1/2}}(b - \hat{b})(\psi_i)] = o_p(1)$ . The claim now follows from vanilla CLT, noting that  $n_T/n \stackrel{p}{\to} E[q_i]$ .

## C.2 Lemmas

**Lemma C.2** (Conditional Convergence). Let  $(\mathcal{G}_n)_{n\geq 1}$  and  $(A_n)_{n\geq 1}$  a sequence of  $\sigma$ -algebras and RV's. Define conditional convergence

$$A_n = o_{p,\mathcal{G}_n}(1) \iff P(|A_n| > \epsilon | \mathcal{G}_n) = o_p(1) \quad \forall \epsilon > 0$$
  
 $A_n = O_{p,\mathcal{G}_n}(1) \iff P(|A_n| > s_n | \mathcal{G}_n) = o_p(1) \quad \forall s_n \to \infty$ 

Then the following results hold

(i) 
$$A_n = o_p(1) \iff A_n = o_{p,\mathcal{G}_n}(1)$$
 and  $A_n = O_p(1) \iff A_n = O_{p,\mathcal{G}_n}(1)$ 

(ii) 
$$E[|A_n||\mathcal{G}_n] = o_p(1)/O_p(1) \implies A_n = o_p(1)/O_p(1)$$

(iii) 
$$\operatorname{Var}(A_n|\mathcal{G}_n) = o_p(c_n^2)/O_p(c_n^2) \implies A_n - E[A_n|\mathcal{G}_n] = o_p(c_n)/O_p(c_n).$$

(iv) If 
$$(A_n)_{n\geq 1}$$
 has  $A_n \leq \bar{A} < \infty$   $\mathcal{G}_n$ -a.s.  $\forall n$  and  $A_n = o_p(1) \implies E[|A_n||\mathcal{G}_n] = o_p(1)$ 

*Proof.* (i) Consider that for any  $\epsilon > 0$ 

$$P(|A_n| > \epsilon) = E[\mathbb{1}(|A_n| > \epsilon)] = E[E[\mathbb{1}(|A_n| > \epsilon)|\mathcal{G}_n]] = E[P(|A_n| > \epsilon|\mathcal{G}_n)]$$

If  $A_n = o_p(1)$ , then  $E[P(|A_n| > \epsilon | \mathcal{G}_n)] = o(1)$ , so  $P(|A_n| > \epsilon | \mathcal{G}_n) = o_p(1)$  by Markov inequality. Conversely, if  $P(|A_n| > \epsilon | \mathcal{G}_n) = o_p(1)$ , then  $E[P(|A_n| > \epsilon | \mathcal{G}_n)] = o(1)$  since  $(P(|A_n| > \epsilon | \mathcal{G}_n))_{n \geq 1}$  is uniformly bounded, hence UI. Then  $P(|A_n| > \epsilon) = o(1)$ . The second equivalence follows directly from the first. (ii) follows from (i) and conditional Markov inequality. (iii) is an application of (ii). For (iv), note that for any  $\epsilon > 0$ 

$$E[|A_n||\mathcal{G}_n] \le \epsilon + E[|A_n|\mathbb{1}(|A_n| > \epsilon)|\mathcal{G}_n] \le \epsilon + \bar{A}P(|A_n| > \epsilon|\mathcal{G}_n) = \epsilon + o_p(1)$$

The equality is by (i) and our assumption. Since  $\epsilon > 0$  was arbitrary  $E[|A_n||\mathcal{G}_n] = o_p(1)$ .

**Definition C.3** (Conditional Weak Convergence). For random variables  $A_n, A \in \mathbb{R}^d$  and  $\sigma$ -algebras  $(\mathcal{F}_n)_n$ ,  $\mathcal{G}$  define conditional weak convergence

$$A_n|\mathcal{F}_n \Rightarrow A|\mathcal{G} \iff E[e^{it'A_n}|\mathcal{F}_n] = E[e^{it'A}|\mathcal{G}] + o_p(1) \quad \forall t \in \mathbb{R}^d$$

We require a slight modification of the martingale difference CLT in Billingsley (1995), allowing the weak limit to be a mixture of normals.

**Proposition C.4** (MDS-CLT). Consider probability spaces  $(\Omega_n, \mathcal{G}_n, P_n)$  each equipped with filtration  $(\mathcal{F}_{k,n})_{k\geq 0}$ . Suppose  $(Y_{k,n})_{k=1}^n$  is adapted to  $(\mathcal{F}_{k,n})_{k\geq 0}$  and has  $E[Y_{k,n}|\mathcal{F}_{k-1,n}] = 0$  for all  $k \geq 1$  with  $n \to \infty$ . Make the following definitions

$$S_{k,n} = \sum_{j=1}^{k} Y_{k,n}$$
  $\sigma_{k,n}^2 = E[Y_{k,n}^2 | \mathcal{F}_{k-1,n}]$   $\Sigma_{k,n} = \sum_{j=1}^{k} \sigma_{k,n}^2$ 

Denote  $S_n \equiv S_{n,n}$  and  $\Sigma_n \equiv \Sigma_{n,n}$ . Suppose that  $\sigma_{k,n}^2 \in \mathcal{F}_{0,n}$  for all k, n and  $\Sigma_n = \sigma^2 + o_p(1)$  with  $\sigma^2 \in \mathcal{F}_{0,n}$ . Also, suppose for each  $\epsilon > 0$ 

$$L_n^{\epsilon} = \sum_{k=1}^n E[Y_{k,n}^2 \mathbb{1}(|Y_{k,n}| \ge \epsilon) | \mathcal{F}_{0,n}] = o_p(1)$$
 (C.1)

Then  $E[e^{itS_n}|\mathcal{F}_{0,n}] = e^{-\frac{1}{2}t^2\sigma^2} + o_p(1).$ 

*Proof.* We modify the argument in Theorem 35.12 of Billingsley (1995).

$$E\left[e^{itS_n} - e^{-\frac{1}{2}t^2\sigma^2}|\mathcal{F}_{0,n}\right] = E\left[e^{itS_n}(1 - e^{\frac{1}{2}t^2\Sigma_n}e^{-\frac{1}{2}t^2\sigma^2})|\mathcal{F}_{0,n}\right] + E\left[e^{-\frac{1}{2}t^2\sigma^2}(e^{\frac{1}{2}t^2\Sigma_n}e^{itS_n} - 1)|\mathcal{F}_{0,n}\right]$$

For the first term, by conditional Jensen inequality

$$|E[e^{itS_n}(1 - e^{\frac{1}{2}t^2\Sigma_n}e^{-\frac{1}{2}t^2\sigma^2})|\mathcal{F}_{0,n}]| \le E[|(1 - e^{\frac{1}{2}t^2\Sigma_n}e^{-\frac{1}{2}t^2\sigma^2})||\mathcal{F}_{0,n}]|$$

$$= |(1 - e^{\frac{1}{2}t^2\Sigma_n}e^{-\frac{1}{2}t^2\sigma^2})| = o_n(1)$$

The first equality since  $\Sigma_n$ ,  $\sigma^2 \in \mathcal{F}_{0,n}$ . Since  $\Sigma_n = \sigma^2 + o_p(1)$ , the second equality follows by continuous mapping. The second term has

$$|E[e^{-\frac{1}{2}t^{2}\sigma^{2}}(e^{\frac{1}{2}t^{2}\Sigma_{n}}e^{itS_{n}}-1)|\mathcal{F}_{0,n}]| = e^{-\frac{1}{2}t^{2}\sigma^{2}}|E[(e^{\frac{1}{2}t^{2}\Sigma_{n}}e^{itS_{n}}-1)|\mathcal{F}_{0,n}]|$$

$$= e^{-\frac{1}{2}t^{2}\sigma^{2}}\left|\sum_{k=1}^{n} E[e^{itS_{k-1,n}}e^{\frac{1}{2}t^{2}\Sigma_{k,n}}(e^{itY_{k,n}}-e^{-\frac{1}{2}t^{2}\sigma_{k,n}^{2}})|\mathcal{F}_{0,n}]\right|$$

$$\leq e^{-\frac{1}{2}t^{2}\sigma^{2}}e^{\frac{1}{2}t^{2}\Sigma_{n}}\sum_{k=1}^{n} E[|e^{itS_{k-1,n}}E[e^{itY_{k,n}}-e^{-\frac{1}{2}t^{2}\sigma_{k,n}^{2}}|\mathcal{F}_{k-1,n}]||\mathcal{F}_{0,n}]$$

$$= e^{-\frac{1}{2}t^{2}\sigma^{2}}e^{\frac{1}{2}t^{2}\Sigma_{n}}\sum_{k=1}^{n} E[|E[e^{itY_{k,n}}-e^{-\frac{1}{2}t^{2}\sigma_{k,n}^{2}}|\mathcal{F}_{k-1,n}]||\mathcal{F}_{0,n}] \equiv o_{p}(1)Z_{n}$$

The first equality since  $\sigma^2 \in \mathcal{F}_{0,n}$ . The second equality by telescoping. The first inequality by triangle inequality and since  $\Sigma_{k,n} \in \mathcal{F}_{0,n}$ ,  $\Sigma_{k,n} \leq \Sigma_n$ , and  $S_{k-1,n} \in \mathcal{F}_{k-1,n}$  for  $1 \leq k \leq n$ . The final equality by continuous mapping since  $\Sigma_n \stackrel{p}{\to} \sigma^2$ . We want to show that  $Z_n = O_p(1)$ . Fix  $\epsilon > 0$  and let  $I_{k,n} = \mathbb{1}(|Y_{k,n}| > \epsilon)$ . Note the facts  $|e^{ix} - (1+ix-(1/2)x^2)| \leq (1/6)|x|^3 \wedge |x|^2$  and  $|e^z - (1+z)| \leq |z|^2 e^{|z|}$  for real x, complex z. By the MDS property and  $E[Y_{k,n}^2|\mathcal{F}_{k-1,n}] = \sigma_{k,n}^2$ , combined with these facts

$$|E[e^{itY_{k,n}} - e^{-\frac{1}{2}t^2\sigma_{k,n}^2}|\mathcal{F}_{k-1,n}]| \leq E[|tY_{k,n}|^3 \wedge |tY_{k,n}|^2 + (1/4)t^4\sigma_{k,n}^4 e^{\frac{1}{2}t^2\sigma_{k,n}^2}|\mathcal{F}_{k-1,n}]$$

$$\leq (t^2 + t^4 + |t|^3 + e^{\frac{1}{2}t^2\Sigma_n})E[(\epsilon|Y_{k,n}|^2 + |Y_{k,n}|^2I_{k,n} + \sigma_{k,n}^4)|\mathcal{F}_{k-1,n}]$$

$$\equiv A_{n,t}(\epsilon\sigma_{k,n}^2 + E[|Y_{k,n}|^2I_{k,n}|\mathcal{F}_{k-1,n}] + E[\sigma_{k,n}^4|\mathcal{F}_{k-1,n}])$$

Then we have

$$Z_{n} \leq A_{n,t} \sum_{k=1}^{n} E[\epsilon \sigma_{k,n}^{2} + E[|Y_{k,n}|^{2} I_{k,n}|\mathcal{F}_{k-1,n}] + E[\sigma_{k,n}^{4}|\mathcal{F}_{k-1,n}]|\mathcal{F}_{0,n}]$$

$$= A_{n,t}(\epsilon \Sigma_{n} + L_{n}^{\epsilon}) + A_{n,t} \sum_{k=1}^{n} E[\sigma_{k,n}^{4}|\mathcal{F}_{0,n}] \leq A_{n,t}(\epsilon \Sigma_{n} + L_{n}^{\epsilon} + \Sigma_{n}(\epsilon^{2} + L_{n}^{\epsilon}))$$

To see the final inequality, note that  $\sigma_{k,n}^4 \leq \sigma_{k,n}^2 \max_{k=1}^n \sigma_{k,n}^2$  and We have  $\sigma_{k,n}^2 = E[Y_{k,n}^2 | \mathcal{F}_{k-1,n}] \leq \epsilon^2 + E[Y_{k,n}^2 I_{k,n} | \mathcal{F}_{k-1,n}] \leq \epsilon^2 + \sum_{j=1}^n E[Y_{j,n}^2 I_{j,n} | \mathcal{F}_{j-1,n}]$ . Taking  $\max_{k=1}^n$  on both sides gives  $\max_{k=1}^n \sigma_{k,n}^2 \leq \epsilon^2 + \sum_{j=1}^n E[Y_{j,n}^2 I_{j,n} | \mathcal{F}_{j-1,n}]$ . Then  $\sum_{k=1}^n E[\sigma_{k,n}^4 | \mathcal{F}_{0,n}] \leq \sum_{k=1}^n E[\sigma_{k,n}^2 (\epsilon^2 + \sum_{j=1}^n E[Y_{j,n}^2 I_{j,n} | \mathcal{F}_{j-1,n}]) | \mathcal{F}_{0,n}] = \sum_n (\epsilon^2 + L_n^{\epsilon})$ . Note that since  $\sum_n \stackrel{p}{\to} \sigma^2$ , we have  $A_{n,t}, \sum_n = O_p(1)$  and  $L_n^{\epsilon} = o_p(1)$  by assumption. Since  $\epsilon$  was arbitrary, this shows  $Z_n = o_p(1)$ .

**Lemma C.5** (Lipschitz Approximation). Let  $Z \in \mathbb{R}^d$  be a random variable. Define  $\mathcal{L} = \{g(Z) \in L_2(Z) : |g|_{lip} \lor |g|_{\infty} < \infty\}$ . Then  $\mathcal{L}$  is dense in  $L_2(Z)$ .

Proof. Let  $\mathbb{1}(Z \in A)$  P-measurable for non-empty A. Define  $f_n(z) = (1 + nd(z, A))^{-1}$  with  $d(z, A) = \inf_{y \in A} |z - y|_2$ . The function  $z \to d(z, A)$  is 1-Lipschitz (e.g. reverse triangle inequality). Then  $|f_n(z) - f_n(y)| \le n|z - y|_2$  for any  $z, y \in \mathbb{R}^d$  and  $|f_n|_\infty \le 1$  so  $f_n(Z) \in \mathcal{L}$ . Observe that  $f_n(z) \to \mathbb{1}(z \in A)$  pointwise as  $n \to \infty$ . Then by dominated convergence  $\int (f_n(z) - \mathbb{1}(z \in A))^2 dP(z) \to 0$ , since the integrand converges pointwise and is dominated by  $2 \in L_1(Z)$ . Then bounded Lipschitz functions are dense in the set of indicator functions of measurable sets. Next, consider a simple function  $\sum_k a_k \mathbb{1}(Z \in A_k)$  with  $|a_k| < \infty$  for all k. If  $g_{nk}(z) = (1 + nd(z, A_k))^{-1}$  the same argument shows that  $\sum_k a_k g_{nk}(Z) - \sum_k a_k \mathbb{1}(Z \in A_k) \to 0$  in  $L_2(Z)$ . The left hand sum is bounded Lipschitz,

showing that the Lipschitz functions are dense in the set of simple functions in  $L_2(Z)$ . The bounded simple functions are dense in  $L_2(Z)$  (e.g. Folland (1999)), so bounded Lipschitz functions are dense in  $L_2(Z)$  by transitivity.

**Lemma C.6** (Asymptotic Independence). Consider a probability space  $(\Omega, \mathcal{G}, P)$  with  $\sigma$ -algebras  $\mathcal{F} = \mathcal{F}_{n,0}$  and  $\mathcal{F}_{n,k} \subseteq \mathcal{F}_{n,k+1} \subseteq \mathcal{G}$  for all  $n \geq 1$  and  $0 \leq k \leq m-1$ . Let  $X_{n,k}$  be  $\mathcal{F}_{n,k}$ -measurable random variables for all n and  $1 \leq k \leq m$ . Suppose that  $X_{n,k}|\mathcal{F}_{n,k-1} \Rightarrow L_k|\mathcal{F}$ , as in Definition C.3. Then  $(X_{n,1},\ldots,X_{n,m})|\mathcal{F} \Rightarrow (L_1,\ldots,L_m)|\mathcal{F}$ , with jointly independent limit.

Proof. By Levy continuity, it suffices to show  $E[e^{it'(X_{1,n},...X_{m,n})}|\mathcal{F}] \to \prod_{k=1}^m E[e^{it_kL_k}|\mathcal{F}]$  for all  $t \in \mathbb{R}^m$ . We work by induction on k. By assumption,  $E[e^{itX_{n,1}}|\mathcal{F}] \xrightarrow{p} E[e^{itL_1}|\mathcal{F}]$  for all  $t \in \mathbb{R}$ . Assume by induction that the conclusion holds for  $1 \le k \le k' \le m$ . Then

$$E[e^{i\sum_{k=1}^{k'+1}t_kX_{n,k}}|\mathcal{F}] = E[e^{i\sum_{k=1}^{k'}t_kX_{n,k}}E[e^{it_{k'+1}X_{n,k'+1}}|\mathcal{F}_{n,k'}]|\mathcal{F}]$$

$$= E[e^{i\sum_{k=1}^{k'}t_kX_{n,k}}(E[e^{it_{k'+1}X_{n,k'+1}}|\mathcal{F}_{n,k'}] - E[e^{it_{k'+1}L_{k'+1}}|\mathcal{F}])|\mathcal{F}]$$

$$+ E[e^{it_{k'+1}L_{k'+1}}|\mathcal{F}]E[e^{i\sum_{k=1}^{k'}t_kX_{n,k}}|\mathcal{F}] = \prod_{k=1}^{k'+1}E[e^{it_{k'+1}L_{k'+1}}|\mathcal{F}] + o_p(1)$$

The first equality is by tower law and our measurability and increasing  $\sigma$ -algebra assumption. For the final equality, note that  $|e^{i\sum_{k=1}^{k'}t_kX_{n,k}}(E[e^{it_{k'+1}X_{n,k'+1}}|\mathcal{F}_{n,k'}]-E[e^{it_{k'+1}L_{k'+1}}|\mathcal{F}])| \leq |E[e^{it_{k'+1}X_{n,k'+1}}|\mathcal{F}_{n,k'}]-E[e^{it_{k'+1}L_{k'+1}}|\mathcal{F}]| \stackrel{p}{\to} 0$ . Then the first term in the sum above is  $o_p(1)$  since the integrand converges in probability and is bounded, hence UI. The final equality also uses our inductive hypothesis. This finishes the proof.

**Lemma C.7** (LLN). Consider  $A_n = n^{-1} \sum_{g \in \mathcal{G}_n} u_g$ , with  $\mathcal{G}_n$  a collection of disjoint subsets of [n]. Let  $(\mathcal{F}_n)_{n\geq 1}$  be  $\sigma$ -algebras such that  $\mathcal{G}_n$  is  $\mathcal{F}_n$ -measurable,  $E[u_g|\mathcal{F}_n] = 0$ , and for all  $g \neq g' \in \mathcal{G}_n$   $u_g \perp \!\!\!\perp u_{g'}|\mathcal{F}_n$ . If  $n^{-1} \sum_{g \in \mathcal{G}_n} E[|u_g|\mathbb{1}(|u_g| > c_n)|\mathcal{F}_n] \stackrel{p}{\to} 0$  for  $c_n = \omega(1)$ ,  $c_n = o(n^{1/2})$ , then  $A_n \stackrel{p}{\to} 0$ .

*Proof.* By disjointness  $|\mathcal{G}_n| \leq n$ . Fix an indexing  $\mathcal{G}_n = \{g_s : 1 \leq s \leq n\}$ , possibly with  $g_s = \emptyset$  for some s. Define  $\bar{u}_{sn} = u_s \mathbb{1}(|u_s| \leq c_n)$  and  $\bar{\mu}_{sn} = E[u_s \mathbb{1}(|u_s| \leq c_n)|\mathcal{F}_n]$ . Expand

$$\frac{1}{n} \sum_{g \in \mathcal{G}_n} u_g = \frac{1}{n} \sum_{s=1}^n u_s = \frac{1}{n} \sum_{s=1}^n \left[ (u_s - \bar{u}_{sn}) + (\bar{u}_{sn} - \bar{\mu}_{sn}) + \bar{\mu}_{sn} \right] = T_{n1} + T_{n2} + T_{n3}$$

Observe that  $E[|T_{n1}||\mathcal{F}_n] \leq (1/n) \sum_{s=1}^n E[|u_s|\mathbb{1}(|u_s| > c_n)|\mathcal{F}_n] = o_p(1)$  by assumption. Then  $T_{n1} = o_p(1)$  by conditional Markov (Lemma C.2). Next consider  $T_{n2}$ .

Note that by definition  $E[\bar{u}_{sn} - \bar{\mu}_{sn}|\mathcal{F}_n] = 0$  for each  $1 \leq s \leq n$ . Note that for  $s \neq s'$  Cov $(\bar{u}_{sn}, \bar{u}_{s'n}|\mathcal{F}_n) = 0$  by the conditional independence assumption. Then  $\operatorname{Var}(T_{n2}|\mathcal{F}_n) = n^{-2} \sum_{s=1}^n \operatorname{Var}(\bar{u}_{sn}|\mathcal{F}_n) \leq n^{-2} \sum_{s=1}^n E[\bar{u}_{sn}^2|\mathcal{F}_n] \leq n^{-1}c_n^2 = o(1)$ , so that  $T_{n2} = o_p(1)$  by conditional Chebyshev. Finally, since  $E[u_s|\mathcal{F}_n] = 0$ , we have  $\bar{\mu}_{sn} = -E[u_s\mathbb{1}(|u_s| > c_n)|\mathcal{F}_n]$ . Then  $E[|T_{n3}||\mathcal{F}_n] \leq (1/n) \sum_{s=1}^n E[|u_s|\mathbb{1}(|u_s| > c_n)|\mathcal{F}_n] = o_p(1)$ , so that  $T_{n3} = o_p(1)$  by conditional Markov as before. This finishes the proof.

**Lemma C.8.** Suppose  $E[|X|^p] < \infty$  for p > 0. Then  $\max_{i=1}^n |X_i| = o_p(n^{1/p})$ .

Proof. For  $\epsilon > 0$  we have  $P(\max_{i=1}^n |X_i| > \epsilon n^{1/p}) \leq nP(|X_i| > \epsilon n^{1/p}) = nP(|X_i|^p > \epsilon^p n) \leq n(\epsilon^p n)^{-1}E[|X_i|^p\mathbb{1}(|X_i|^p > \epsilon^p n)] \lesssim E[|X_i|^p\mathbb{1}(|X_i|^p > \epsilon^p n)] \to 0$ . The first inequality by union bound, the equality by monotonicity of  $x \to x^p$ . The second inequality is Markov's, and the final statement by dominated convergence, since  $E[|X_i|^p] < \infty$ .

**Lemma C.9** (Random Partitions). Let  $\mathcal{G}_n = \{g_s\}_{s=1}^m$  a random collection of disjoint subsets of [n]. Let variables  $((\tau_s)_s, W_{1:n}, \pi)$  jointly independent for some random elements  $\pi$  and  $(\tau_s)_{s=1}^m$ . Let  $h_i = h(W_i)$  for a fixed measurable function h and suppose that the partition  $\mathcal{G}_n$  is  $\mathcal{F}_n$ -measurable for  $\mathcal{F}_n = \sigma(h_{1:n}, \pi)$ . Then for  $s \neq r$  and measurable  $F_s, F_r$ , we have  $F_s((W_i)_{i \in q_s}, \tau_s) \perp \!\!\! \perp F_r((W_i)_{i \in q_r}, \tau_r) | \mathcal{F}_n$ .

*Proof.* Since  $F_s$ ,  $F_r$  are arbitrary, it suffices to show  $E[F_sF_r|\mathcal{F}_n] = E[F_s|\mathcal{F}_n]E[F_s|\mathcal{F}_n]$ . Denote  $W_I = (W_i)_{i \in I}$  and similarly for  $h_I$ . Then  $F_s = \sum_{I \in 2^{[n]}} \mathbb{1}(g_s = I)F_s(W_I, \tau_s)$ . We claim that it suffices to show

$$E[F_s(W_I, \tau_s)F_r(W_J, \tau_r)|\mathcal{F}_n] = E[F_s(W_I, \tau_s)|\mathcal{F}_n]E[F_r(W_J, \tau_r)|\mathcal{F}_n]$$

for all disjoint  $I \cap J = \emptyset$ . To see this, note that in this case by measurability of  $\mathcal{G}_n$  with respect to  $\mathcal{F}_n$  and disjointness of the groups we would have

$$E[F_{s}F_{r}|\mathcal{F}_{n}] = E\left[\sum_{I \in 2^{[n]}} \sum_{J \in 2^{[n]}} \mathbb{1}(g_{s} = I)\mathbb{1}(g_{r} = J)F_{s}(W_{I}, \tau_{s})F_{r}(W_{J}, \tau_{r})|\mathcal{F}_{n}\right]$$

$$= \sum_{\substack{I,J \in 2^{[n]}\\I \cap J = \emptyset}} \mathbb{1}(g_{s} = I)\mathbb{1}(g_{r} = J)E[F_{s}(W_{I}, \tau_{s})|\mathcal{F}_{n}]E[F_{r}(W_{J}, \tau_{r})|\mathcal{F}_{n}] = E[F_{s}|\mathcal{F}_{n}]E[F_{r}|\mathcal{F}_{n}]$$

Then consider such  $I \cap J = \emptyset$ . Note the fact (1) if  $(A, B) \perp L$  then  $A \perp L \cap L$ . By applying (1) with  $A = (W_I, \tau_s, W_J, \tau_r)$ ,  $B = h_{1:n}$  and  $C = \pi$ , we have  $E[F_s(W_I, \tau_s)F_r(W_J, \tau_r)|\mathcal{F}_n] = E[F_s(W_I, \tau_s)F_r(W_J, \tau_r)|h_{1:n}]$ . Then it suffices to show that (a)  $(W_I, \tau_s) \perp L \cap L$  then  $L \cap L$  then L then

By fact (1) to show (a) it suffices to prove (b)  $(W_I, \tau_s, h_I) \perp \!\!\! \perp (W_J, \tau_r) | h_{I^c}$ . By fact (1) again, it suffices to show (c)  $(W_I, \tau_s, h_I) \perp \!\!\! \perp (W_J, \tau_r, h_{I^c})$ . This is true by disjointness and joint independence of the  $(\tau_s)_s$ , which finishes the proof.

**Lemma C.10** (Design Properties). Let  $D_{1:n} \sim \operatorname{Loc}(\psi_n, p_n)$ . Denote group randomization variables  $\tau^d = (\tau_{a,s}^d)_{a,s}$ , jointly independent with  $(\tau_{a,s,\ell}^d)_{\ell=1}^{k_a} \sim \operatorname{CR}(q_a/k_a)$  for  $1 \leq s \leq n-1$  and remainder group  $(\tau_{a,n,\ell}^d)_{\ell=1}^{k_a} \sim \operatorname{SRS}(q_a/k_a)$ . Let  $(\mathcal{F}_n)_{n\geq 0}$  a sequence of  $\sigma$ -algebras with  $\mathcal{G}_n \subseteq \mathcal{F}_n$  and  $\mathcal{F}_n \perp \!\!\! \perp \tau^d$ . Then the following hold

- (i) For each  $i \in [n]$  we have  $E[D_i | \mathcal{F}_n] = \sum_{a=1}^{|L_n|} \sum_{s=1}^n \mathbb{1}(i \in g_{a,s}) \cdot p_a$ . In particular,  $E[D_i \mathbb{1}(i \in g_{a,s}) | \mathcal{F}_n] = \mathbb{1}(i \in g_{a,s}) \cdot p_a$ .
- (ii) For  $1 \le i \le n$  and  $1 \le s \le n$  we have  $Var(D_i|\mathcal{F}_n)\mathbb{1}(i \in g_{a,s}) = p_a(1-p_a)\mathbb{1}(i \in g_{a,s})$ . For  $1 \le i, j \le n$  distinct indices and  $1 \le s \le n-1$

$$Cov(D_i, D_j | \mathcal{F}_n) \mathbb{1}(i, j \in g_{a,s}) = -\frac{q_a(k_a - q_a)}{k_a^2(k_a - 1)} \mathbb{1}(i, j \in g_{a,s})$$

In particular,  $|\operatorname{Cov}(D_i, D_j | \mathcal{F}_n) \mathbb{1}(i, j \in g_{a,s})| \leq k_a^{-1} \mathbb{1}(i, j \in g_{a,s}) \mathbb{1}(s \neq n)$ . Moreover,  $\operatorname{Cov}(D_i, D_j | \mathcal{F}_n) \mathbb{1}(g(i) \neq g(j)) = 0$ .

*Proof.* For the first statement, note that

$$D_i = \sum_{a=1}^{|L_n|} \sum_{s=1}^n \sum_{\ell=1}^{k_a} D_i \mathbb{1}(i = g_{a,s,l}) = \sum_{a=1}^{|L_n|} \sum_{s=1}^n \sum_{\ell=1}^{k_a} \tau_{a,s,\ell}^d \mathbb{1}(i = g_{a,s,l})$$

Then since  $\mathcal{G}_n \in \mathcal{F}_n$  and  $\tau_{a,s,\ell}^d \perp \!\!\! \perp \mathcal{F}_n$  we have

$$E[D_{i}|\mathcal{F}_{n}] = \sum_{a=1}^{|L_{n}|} \sum_{s=1}^{n} \sum_{\ell=1}^{k_{a}} E[\mathbb{1}(i = g_{a,s,\ell})\tau_{a,s,\ell}^{d}|\mathcal{F}_{n}] = \sum_{a=1}^{|L_{n}|} \sum_{s=1}^{n} \sum_{\ell=1}^{k_{a}} \mathbb{1}(i = g_{a,s,\ell})E[\tau_{a,s,\ell}^{d}|\mathcal{F}_{n}]$$

$$= \sum_{a=1}^{|L_{n}|} \sum_{s=1}^{n} \sum_{\ell=1}^{k_{a}} \mathbb{1}(i = g_{a,s,\ell})E[\tau_{a,s,\ell}^{d}] = \sum_{a=1}^{|L_{n}|} \sum_{s=1}^{n} \sum_{\ell=1}^{k_{a}} \mathbb{1}(i = g_{a,s,\ell})p_{a}$$

To finish, note that  $\sum_{\ell=1}^{k_a} \mathbb{1}(i = g_{a,s,\ell}) = \mathbb{1}(i \in g_{a,s})$  by definition. For (ii), by the decomposition above and measurability assumption, for  $1 \leq j \neq i \leq n$ 

$$Cov(D_i, D_j | \mathcal{F}_n) = \sum_{a, a'=1}^{|L_n|} \sum_{s, s'=1}^n \sum_{\ell=1}^{k_a} \sum_{\ell'=1}^{k_{a'}} \mathbb{1}(i = g_{a, s, \ell}) \mathbb{1}(j = g_{a', s', \ell'}) Cov(\tau_{a, s, \ell}^d, \tau_{a', s', \ell'}^d | \mathcal{F}_n)$$

By  $\sigma$ -algebra independence and joint independence of groupwise randomizations

$$Cov(\tau_{a,s,\ell}^d, \tau_{a',s',\ell'}^d | \mathcal{F}_n) = Cov(\tau_{a,s,\ell}^d, \tau_{a',s',\ell'}^d)$$

$$= \begin{cases} 0 & (a,s) \neq (a',s') \\ p_a - p_a^2 & (a,s,\ell) = (a',s',\ell') \\ -\frac{q_a(k_a - q_a)}{k_a^2(k_a - 1)} & (a,s) = (a',s'); \quad \ell \neq \ell' \quad 1 \leq s < n \\ 0 & (a,s) = (a',s'); \quad \ell \neq \ell' \quad s = n \end{cases}$$

The third line follows since by definition of  $CR(q_a/k_a)$ , for (a, s) = (a', s') we have

$$\operatorname{Cov}(\tau_{a,s,\ell}^d, \tau_{a',s',\ell'}^d) = P(\tau_{a,s,\ell}^d = \tau_{a,s,\ell'}^d = 1) - (q_a/k_a)^2 = \binom{k_a}{q_a}^{-1} \binom{k_a - 2}{q_a - 2} - (q_a/k_a)^2$$
$$= \frac{q_a(q_a - 1)}{k_a(k_a - 1)} - (q_a/k_a)^2 = -\frac{q_a(k_a - q_a)}{k_a^2(k_a - 1)}$$

The bounds follow by inspection.