Design-based theory for cluster rerandomization

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Abstract

Complete randomization balances covariates on average, but covariate imbalance often exists in finite samples. Rerandomization can ensure covariate balance in the realized experiment by discarding the undesired treatment assignments. Many field experiments in public health and social sciences assign the treatment at the cluster level due to logistical constraints or policy considerations. Moreover, they are frequently combined with rerandomization in the design stage. We refer to cluster rerandomization as a cluster-randomized experiment compounded with rerandomization to balance covariates at the individual or cluster level. Existing asymptotic theory can only deal with rerandomization with treatments assigned at the individual level, leaving that for cluster rerandomization an open problem. To fill the gap, we provide a design-based theory for cluster rerandomization. Moreover, we compare two cluster rerandomization schemes that use prior information on the importance of the covariates: one based on the weighted Euclidean distance and the other based on the Mahalanobis distance with tiers of covariates. We demonstrate that the former dominates the latter with optimal weights and orthogonalized covariates. Last but not least, we discuss the role of covariate adjustment in the analysis stage and recommend covariate-adjusted procedures that can be conveniently implemented by least squares with the associated robust standard errors.

Key words: cluster randomization; cluster-robust standard error; constrained randomization; covariate balance
1. Introduction

Cluster randomization has been widely used in public health (Donner and Klar, 2000; Turner et al., 2017a,b; Hayes and Moulton, 2017) and social sciences (Raudenbush, 1997; Schochet, 2013; Athey and Imbens, 2017; Schochet, 2020). It assigns the treatments at the cluster level, with units within a cluster receiving the same treatment or control condition, which helps to avoid interference within clusters and is applicable when individual-level assignments are logistically infeasible.

Before experiments, researchers often collect covariates at the individual or cluster level. For instance, in clinical trials, individual-level covariates may include gender, race, age, and education of patients while cluster-level covariates may include the capacity of the clinics and whether they are in a metropolitan area (Li et al., 2016). The probability of having imbalance in covariates after treatment assignments is non-negligible and would complicate the interpretation of the experimental results, especially if some particular covariates are predictive to the outcome.

A common approach to tackle covariate imbalance is to perform regression adjustment in the analysis stage of an experiment (Lin, 2013; Su and Ding, 2021). In contrast, rerandomization actively reduces the imbalance in the design stage. Rerandomization, also known as constrained randomization (Moulton, 2004; Morgan and Rubin, 2012; Li et al., 2016, 2017, 2018), is a procedure where one discards the undesired assignments that result in highly unbalanced covariates and repeats randomization until a proper assignment appears. The existing design-based theory for rerandomization assumes that the treatments are assigned at the individual level (Morgan and Rubin, 2012; Li et al., 2018), leaving it unclear how rerandomization would theoretically work in cluster experiments. The overarching goal of this paper is to fill this gap.

We study cluster rerandomization with both individual- and cluster-level covariates, and derive an asymptotic theory for estimators either with or without regression adjustment. Our theory precisely quantifies the asymptotic efficiency gain of performing cluster rerandomization at both levels. We further show that under cluster rerandomization, the adjusted estimators based on linear regressions recommended by Su and Ding (2021) still have desired theoretical guarantees. All these inferential procedures can be conveniently realized by standard statistical packages. Moreover, previous asymptotic theory mainly focuses on the rerandomization scheme based on the Mahalanobis distance (Morgan and Rubin, 2012; Li et al., 2018, 2020) while we also discuss a distinct but widely-adopted practical scheme based on the weighted Euclidean distance where one could utilize prior knowledge of the covariate importance (Raab and Butcher, 2001; Wight et al., 2002; Althabe et al., 2008; de Hoop et al., 2012; Li et al., 2016, 2017; Hayes and Moulton, 2017; Dempsey et al., 2018). We show that for orthogonalized covariates with optimal weights, it dominates the cluster rerandomization with tiers of covariates, another scheme accounting for the covariate importance, the non-cluster version of which is proposed in Morgan and Rubin (2015).

To facilitate the discussion, we introduce the following notation. Let $\text{det}(\cdot)$ denote the determinant of a matrix. For a real-valued matrix $A$, we write $A > 0$ if $A$ is strictly positive definite. For a finite population $\{a_1, \ldots, a_M\}$, let $\text{var}_f(a) = (M - 1)^{-1} \sum_{i=1}^{M} (a_i - \bar{a})^2$ denote its finite-population variance, where $\bar{a} = M^{-1} \sum_{i=1}^{M} a_i$. Analogously, let $\text{cov}_f$ denote the finite-population covariance. For two
random sequences $A$ and $B$, let $A \sim B$ indicate that they have the same asymptotic distribution. Let $\text{pr}_a$, $\text{var}_a$, and $\text{cov}_a$ denote the asymptotic probability, variance, and covariance, respectively. Besides, our asymptotic theory requires mild moment conditions, but we relegate them to the appendix to avoid clutter in the main text.

2. Notation and review for cluster-randomized experiments

Consider a cluster-randomized experiment with a finite population of $N$ units grouped into $M$ clusters. The experimenter randomly assigns $M_1$ clusters to the treatment arm and $M_0 = M - M_1$ clusters to the control arm, with units in the same cluster receiving the same treatment or control. For cluster $i$, let $Z_i$ be the treatment indicator with $Z_i = 1$ when it is assigned to the treatment arm and $Z_i = 0$ when it is assigned to the control arm. Let $n_i$ be the size of cluster $i$, with $\sum_{i=1}^M n_i = N$. Let $(i, j)$ or simply $ij$ to index unit $j$ in cluster $i$. Let $Z_{ij}$ be the treatment indicator for unit $(i, j)$ and by design, $Z_{ij} = Z_i$ for $j = 1, \ldots, n_i$. Let $N_1 = \sum_{i=1}^M Z_i n_i$ and $N_0 = N - N_1$ denote the numbers of units assigned to the treatment and control arms, respectively. Importantly, $N_1$ and $N_0$ are random if the $n_i$’s vary. Let $Y_{ij}(1)$ and $Y_{ij}(0)$ denote the potential outcomes of unit $(i, j)$ under the treatment and control, respectively. We adopt the design-based framework by conditioning on the potential outcomes with the $Z_i$’s being the only source of randomness. The observed outcome $Y_{ij} = Z_i Y_{ij}(1) + (1 - Z_i) Y_{ij}(0)$ is random in general due to the random $Z_i$’s. We are interested in estimating the average treatment effect

$$\tau = N^{-1} \sum_{i=1}^M \sum_{j=1}^{n_i} \{Y_{ij}(1) - Y_{ij}(0)\}$$

based on the observed data.

The difference-in-means estimator of $\tau$ is given by

$$\hat{\tau}_{\text{haj}} = N_1^{-1} \sum_{i=1}^M \sum_{j=1}^{n_i} Z_{ij} Y_{ij} - N_0^{-1} \sum_{i=1}^M \sum_{j=1}^{n_i} (1 - Z_{ij}) Y_{ij},$$

with the subscript “haj” signifying that it is the Hajek estimator based on the inverse of the treatment probabilities (Su and Ding, 2021). As pointed out by Middleton and Aronow (2015), the random denominators in $\hat{\tau}_{\text{haj}}$ can result in bias when the $n_i$’s vary. The unbiased Horvitz–Thompson estimator replaces the random denominators $N_1$ and $N_0$ with their expectations:

$$\hat{\tau}_{\text{ht}} = (NM_1/M)^{-1} \sum_{i=1}^M Z_i \sum_{j=1}^{n_i} Y_{ij} - (NM_0/M)^{-1} \sum_{i=1}^M (1 - Z_i) \sum_{j=1}^{n_i} Y_{ij}.$$

Define the scaled cluster total potential outcome as $\tilde{Y}_i(z) = \sum_{j=1}^{n_i} Y_{ij}(z) M/N$ so that $\tau = \sum_{i=1}^M \sum_{j=1}^{n_i} \{Y_{ij}(1) - Y_{ij}(0)\}$.
\[ M^{-1} \sum_{i=1}^{M} \{ \hat{Y}_i(1) - \hat{Y}_i(0) \}. \] Based on the observed analog \( \hat{Y}_i = Z_i \tilde{Y}_i(1) + (1 - Z_i) \tilde{Y}_i(0) \), the Horvitz–Thompson estimator simplifies to

\[ \hat{\tau}_{ht} = M^{-1} \sum_{i=1}^{M} Z_i \tilde{Y}_i - M^{-1} \sum_{i=1}^{M} (1 - Z_i) \tilde{Y}_i. \]

This is unbiased for \( \tau \) because it is the scaled difference in means of the potential outcomes if each cluster is treated as a whole.

Both \( \hat{\tau}_{ht} \) and \( \hat{\tau}_{haj} \) are asymptotically normal under some mild regularity conditions (Su and Ding, 2021). Let \( e_\tau = M_2/M \) be the proportion of clusters assigned to the treatment arm \( z \) \((z = 0, 1)\). Denote the normalized cluster size vector by \( \tilde{\omega} = (\tilde{\omega}_1, \ldots, \tilde{\omega}_M)^t \), with \( \tilde{\omega}_i = n_i M/N \). Let \( \hat{Y}(z) = N^{-1} \sum_{i=1}^{M} \sum_{j=1}^{n_i} Y_{ij}(z) \). Define \( \tilde{\varepsilon}(z) = (\tilde{\varepsilon}_1(z), \ldots, \tilde{\varepsilon}_M(z))^t \) and \( \bar{Y}(z) = (\bar{Y}_1(z), \ldots, \bar{Y}_M(z))^t \), where

\[ \tilde{\varepsilon}_i(z) = \hat{Y}_i(z) - \bar{\omega}_i \bar{Y}(z) = \sum_{j=1}^{n_i} \varepsilon_{ij}(z) M/N, \quad \varepsilon_{ij}(z) = Y_{ij}(z) - \bar{Y}(z). \]

Su and Ding (2021) showed that \( M^{1/2}(\hat{\tau}_{ht} - \tau) \sim \mathcal{N}(0, V_{ht, \tau \tau}) \) for \( \star = ht, haj \), where

\begin{align*}
V_{ht, \tau \tau} & = e^{-1} \text{var} \{ \tilde{Y}(1) \} + e^{-1} \text{var} \{ \tilde{Y}(0) \} - \text{var} \{ \tilde{Y}(1) - \tilde{Y}(0) \}, \\
V_{haj, \tau \tau} & = e^{-1} \text{var} \{ \tilde{\varepsilon}(1) \} + e^{-1} \text{var} \{ \tilde{\varepsilon}(0) \} - \text{var} \{ \tilde{\varepsilon}(1) - \tilde{\varepsilon}(0) \}.
\end{align*}

Therefore, \( \hat{\tau}_{ht} \) is unbiased in finite samples and \( \hat{\tau}_{haj} \) is unbiased asymptotically. By Middleton and Aronow (2015) and Su and Ding (2021), \( \hat{\tau}_{haj} \) often practically outperforms \( \hat{\tau}_{ht} \) in terms of the mean squared error.

3. Cluster rerandomization using the Mahalanobis distance

3.1. Design

In a cluster-randomized experiment, suppose we observe baseline covariates at the individual or cluster level. Let \( x_{ij} = (x_{ij1}, \ldots, x_{ijK})^t \) denote the individual-level covariates for unit \((i, j)\), and \( c_i = (c_{i1}, \ldots, c_{iK})^t \) be the cluster-level covariates for cluster \(i\). To simplify the presentation, we center them to ensure that \( \bar{x} = N^{-1} \sum_{i=1}^{M} \sum_{j=1}^{n_i} x_{ij} = 0 \) and \( M^{-1} \sum_{i=1}^{M} c_i = 0 \), and use the same \( K \) to denote their dimensions, although they may differ. Let \( \bar{x}_i = \sum_{j=1}^{n_i} x_{ij} M/N \) be the scaled cluster totals, concatenated as \( \bar{X} = (\bar{x}_1, \ldots, \bar{x}_M)^t \). Similarly, let \( C = (c_1, \ldots, c_M)^t \).

Two types of covariates suggest two schemes of cluster rerandomization. The first one is based on the Mahalanobis distance of covariates at the cluster level. Define

\[ \hat{\tau}_{ht,c} = M^{-1} \sum_{i=1}^{M} Z_i c_i - M^{-1} \sum_{i=1}^{M} (1 - Z_i) c_i \]
as the Horvitz–Thompson estimator applied to the cluster-level covariates. For a pre-determined threshold \( a > 0 \), cluster rerandomization based on cluster-level covariates accepts the treatment assignment if and only if the following event happens:

\[
\mathcal{M}_c = \{ \hat{\tau}^T_{ht,c} \text{cov}(\hat{\tau}_{ht,c})^{-1} \hat{\tau}_{ht,c} \leq a \} = \{ e_1 e_0 M \hat{\tau}^T_{ht,c} \text{cov}_f(C)^{-1} \hat{\tau}_{ht,c} \leq a \}.
\]

The second one is based on the Mahalanobis distance of covariates at the individual level. Define

\[
\hat{\tau}_{haj,x} = N_i^{-1} \sum_{i=1}^{M} Z_i \sum_{j=1}^{n_i} x_{ij} - N_0^{-1} \sum_{i=1}^{M} (1 - Z_i) \sum_{j=1}^{n_i} x_{ij}
\]

as the difference in means of the individual-level covariates. For a pre-determined threshold \( a > 0 \), cluster rerandomization based on individual-level covariates accepts the treatment assignment if and only if the following event happens:

\[
\mathcal{M}_x = \{ \hat{\tau}^T_{haj,x} \text{cov}_{A}(\hat{\tau}_{haj,x})^{-1} \hat{\tau}_{haj,x} \leq a \} = \{ e_1 e_0 M \hat{\tau}^T_{haj,x} \text{cov}_f(\tilde{X})^{-1} \hat{\tau}_{haj,x} \leq a \}. \tag{3}
\]

We use the same threshold \( a \) for two types of cluster rerandomization to simplify the notation. Due to the complicated form of the exact covariance of \( \hat{\tau}_{haj,x} \), we have used its asymptotic analog in (3), with more details given in Proposition 1 in the next section.

The definition of cluster-level or individual-level covariates can be subtle, and different levels of covariates could be used interchangeably. On the one hand, we could take some statistics of aggregated individual-level covariates within a cluster to construct cluster-level covariates. For instance, we could define \( c_i = \tilde{x}_{i} \). On the other hand, it is common that only cluster-level covariates \( c_i \) are observed prior to rerandomization, in which case we can define individual-level covariates as \( x_{ij} = c_i \) for all \( j \) in cluster \( i \). Hence, both cluster rerandomization schemes are applicable.

### 3.2. Asymptotic distributions

We have introduced two estimators \( \hat{\tau}_{ht} \) and \( \hat{\tau}_{haj} \) for \( \tau \), and two cluster rerandomization schemes \( \mathcal{M}_c \) and \( \mathcal{M}_x \). Theoretically, they generate four combinations. Nevertheless, it is more natural to consider the design and analysis with the same type. Therefore, we will focus on the asymptotic distributions of \( \hat{\tau}_{ht} \) given \( \mathcal{M}_c \) and \( \hat{\tau}_{haj} \) given \( \mathcal{M}_x \). We start with unconditional joint asymptotic distributions of \( (\hat{\tau}_{haj}, \hat{\tau}_{haj,x}) \) and \( (\hat{\tau}_{ht}, \hat{\tau}_{ht,c}) \) as shown in Proposition 1 below.

**Proposition 1.** Under regularity conditions,

\[
M^{1/2} \left( \begin{array}{c} \hat{\tau}_{haj} - \tau \\ \hat{\tau}_{haj,x} \end{array} \right) \sim \mathcal{N} \left( 0, \begin{bmatrix} V_{haj,\tau} & V_{haj,\tau x} \\ V_{haj,x\tau} & V_{haj,xx} \end{bmatrix} \right),
\]

\[
M^{1/2} \left( \begin{array}{c} \hat{\tau}_{ht} - \tau \\ \hat{\tau}_{ht,c} \end{array} \right) \sim \mathcal{N} \left( 0, \begin{bmatrix} V_{ht,\tau} & V_{ht,\tau c} \\ V_{ht,c\tau} & V_{ht,cc} \end{bmatrix} \right),
\]

4
where $V_{ht,\tau}$ and $V_{haj,\tau}$ are defined in (1) and (2), respectively, and

$$V_{haj,xt} = (V_{haj,xx})^T = e_1^{-1} \text{cov}_t \{ \tilde{X}, \tilde{\epsilon}(1) \} + e_0^{-1} \text{cov}_t \{ \tilde{X}, \tilde{\epsilon}(0) \}, \quad V_{haj,xx} = (e_1 e_0)^{-1} \text{cov}_t (\tilde{X}),$$

$$V_{ht,ct} = (V_{ht,cc})^T = e_1^{-1} \text{cov}_t \{ C, \tilde{\epsilon}(1) \} + e_0^{-1} \text{cov}_t (C, \tilde{\epsilon}(0) \}, \quad V_{ht,cc} = (e_1 e_0)^{-1} \text{cov}_t (C).$$

By Proposition 1, the Mahalanobis distances based on $\hat{\tau}_{haj}$ and $\hat{\tau}_{ht}$ converge in distribution to $X^2_K$. This provides a guidance for choosing $a$. For example, we can choose $a$ as the $a$th quantile of $\chi^2_K$ to ensure an asymptotic acceptance rate of $\alpha$. Morgan and Rubin (2012) suggested $\alpha = 0.001$ when the cluster numbers are moderate or large. However, practitioners need to be aware that with small $M$ and $a$, we do not have enough randomizations and asymptotic approximation can be poor. We suggest the Fisher randomization tests in such situations, where the threshold $a$ is chosen to ensure non-trivial powers (Johansson et al., 2021).

Proposition 1 provides the basis for deriving the conditional asymptotic distributions, $\hat{\tau}_{ht}$ given $\mathcal{M}_c$ and $\hat{\tau}_{haj}$ given $\mathcal{M}_x$, which are the asymptotic distributions of $\hat{\tau}_{haj}$ and $\hat{\tau}_{ht}$ under cluster rerandomization. Extending Li et al. (2018), we introduce two squared multiple correlations:

$$R^2_c = \text{cov}_a (\hat{\tau}_{ht}, \hat{\tau}_{haj}) \text{cov}_a (\hat{\tau}_{haj}, \hat{\tau}_{ht})^{-1} \text{cov}_a (\hat{\tau}_{haj}, \hat{\tau}_{ht}) / \text{var}_a (\hat{\tau}_{ht}),$$

$$R^2_x = \text{cov}_a (\hat{\tau}_{haj}, \hat{\tau}_{ht}) \text{cov}_a (\hat{\tau}_{ht}, \hat{\tau}_{haj})^{-1} \text{cov}_a (\hat{\tau}_{ht}, \hat{\tau}_{ht}) / \text{var}_a (\hat{\tau}_{haj}).$$

Moreover, let $L_{K,a} \sim D_1 | D^T D \leq a$ where $D = (D_1, \ldots, D_K)^T$ is a $K$-dimensional standard normal random vector, and let $\epsilon$ be a standard normal random variable independent of $L_{K,a}$. These quantities play important roles in Theorem 1 below.

**Theorem 1.** Under regularity conditions,

$$M^{1/2} (\hat{\tau}_{haj} - \tau) | \mathcal{M}_x \sim (V_{haj,\tau\tau})^{1/2} \{ (1 - R^2_x)^{1/2} \epsilon + R_x L_{K,a} \},$$

$$M^{1/2} (\hat{\tau}_{ht} - \tau) | \mathcal{M}_c \sim (V_{ht,\tau\tau})^{1/2} \{ (1 - R^2_c)^{1/2} \epsilon + R_c L_{K,a} \}.$$
Corollary 1. Under regularity conditions, if \( c_i = (n_i, \tilde{x}_i^T)^T \), then \( V_{\text{haj}, \tau \tau} (1 - R^2_x) \geq V_{\text{ht}, \tau \tau} (1 - R^2_c) \).

With a small threshold \( a > 0 \), the variance of \( L_{K,a} \) is small, and therefore, \( V_{\text{haj}, \tau \tau} (1 - R^2_x) \) and \( V_{\text{ht}, \tau \tau} (1 - R^2_c) \) are the leading terms of the asymptotic variances of \( \hat{\tau}_{\text{haj}} \) and \( \hat{\tau}_{\text{ht}} \), respectively. Corollary 1 demonstrates that based on the asymptotic variances, \( M_c \) with cluster-level covariates dominates \( M_x \) with individual-level covariates if the cluster-level covariates include the cluster size and scaled cluster totals of the individual-level covariates. A key requirement of Corollary 1 is that the cluster size must be used as a cluster-level covariate. This parallels the theory for regression adjustment in the analysis of cluster-randomized experiments that the regression-adjusted estimator based on scaled cluster totals dominates the regression-adjusted estimator based on individual-level data with properly defined covariates (Su and Ding, 2021).

4. Cluster rerandomization with prior knowledge on covariate importance

4.1. Weighted Euclidean distance criterion

The cluster rerandomization schemes in Section 3 view all covariates as equally important. Although they have the advantage of being invariant to non-degenerate linear transformation of the covariates, they are not ideal in experiments with prior knowledge about the relative importance of the covariates. In those cases, a better choice is cluster rerandomization with the weighted Euclidean distance, which has been frequently used in practice (Wight et al., 2002; Althabe et al., 2008; Li et al., 2016, 2017; Hayes and Moulton, 2017; Dempsey et al., 2018). We will study its design-based properties in this subsection.

Consider cluster rerandomization schemes defined by general quadratic forms of the measures of covariate imbalance:

\[
D_x(A_x) = \{ M \tilde{\tau}_{\text{haj}, x}^T A_x \tilde{\tau}_{\text{haj}, x} \leq a \}, \quad D_c(A_c) = \{ M \tilde{\tau}_{\text{ht}, c}^T A_c \tilde{\tau}_{\text{ht}, c} \leq a \},
\]

where \( A_x > 0 \) and \( A_c > 0 \). They reduce to cluster rerandomization schemes in Section 3 if \( A_x = M^{-1} \text{cov}_a(\tilde{\tau}_{\text{haj}, x})^{-1} \) and \( A_c = M^{-1} \text{cov}(\tilde{\tau}_{\text{ht}, c})^{-1} \), respectively. The weighted Euclidean distances correspond to diagonal \( A_x \) and \( A_c \). Theorem 2 below provides the basis for inference under \( D_x(A_x) \) and \( D_c(A_c) \).

Theorem 2. Under regularity conditions,

\[
M^{1/2}(\tilde{\tau}_{\text{haj}} - \tau) \mid D_x(A_x) \sim V_{\text{haj}, \tau \tau}^{1/2} \{ (1 - R^2_x)^{1/2} \epsilon + R_x \mu_x^T \eta \mid \eta^T V_{\text{haj}, xx} V_{\text{haj}, xx}^{1/2} \eta \leq a \},
\]

\[
M^{1/2}(\tilde{\tau}_{\text{ht}} - \tau) \mid D_c(A_c) \sim V_{\text{ht}, \tau \tau}^{1/2} \{ (1 - R^2_c)^{1/2} \epsilon + R_c \mu_c^T \eta \mid \eta^T V_{\text{ht}, cc} V_{\text{ht}, cc}^{1/2} \eta \leq a \},
\]
where η = (η₁, ..., ηₖ)ᵗ, ε, η₁, ..., ηₖ are independent standard normal random variables, and

\[ \mu_x^T = (V_{haj,xx}^{-1}V_{haj,xt}V_{haj,xx})^{-1/2}V_{haj,xx}^{-1/2}, \quad \mu_c^T = (V_{ht,cc}^{-1}V_{ht,cr})^{-1/2}V_{ht,cc}^{-1/2}. \]

Theorem 2 is similar to Theorem 1 in that the asymptotic distributions have two components: one is normal, and the other is truncated normal. It allows us to derive properties of \( \hat{\tau}_{haj} \) and \( \hat{\tau}_ht \) under cluster rerandomization.

**Proposition 2.** Under regularity conditions, (i) the asymptotic distributions in Theorem 2 are symmetric around zero and unimodal, and (ii) \( \text{pr}_a\{M^{1/2} | \hat{\tau}_{haj} - \tau| < \delta | \mathcal{D}_x(A_x)\} \) is a non-decreasing function of \( R_x^2 \) and \( \text{pr}_a\{M^{1/2} | \hat{\tau}_ht - \tau| < \delta | \mathcal{D}_c(A_c)\} \) is a non-decreasing function of \( R_c^2 \) for any fixed \( \delta > 0 \).

Proposition 2 (i) ensures that the asymptotic distributions in Theorem 2 are both bell-shaped, although they differ from normal distributions. Proposition 2 (ii) ensures that the asymptotic distributions in Theorem 2 are more concentrated at zero than those under standard cluster rerandomization.

To compare the asymptotic efficiency of the two cluster rerandomization schemes, we can compare their variance reductions given the same acceptance rate. Let \( \alpha \) denote the common asymptotic acceptance rate:

\[ \alpha = \text{pr}_a\{\mathcal{D}_x(A_x)\} = \text{pr}_a\{M^{1/2}_{haj,x} A_x \hat{\tau}_{haj,x} \leq a\}, \quad \alpha = \text{pr}_a\{\mathcal{D}_c(A_c)\} = \text{pr}_a\{M^{1/2}_{ht,c} A_c \hat{\tau}_{ht,c} \leq a\}. \]

Let \( \Gamma(\cdot) \) be the Gamma function and

\[ p_K = \frac{2\pi}{K + 2} \left\{ \frac{2\pi^{K/2}}{K \Gamma(K/2)} \right\}^{-2/K}. \]

The expansions in Theorem 3 below provide the basis for comparing asymptotic efficiency.

**Theorem 3.** Under regularity conditions,

\[
\begin{align*}
\var_x\{M^{1/2} (\hat{\tau}_{haj} - \tau) \mid \mathcal{D}_x(A_x)\} &= V_{haj,xx}^{-1}V_{haj,xt}V_{haj,xx}\det(A_x)^{1/K}\det(V_{haj,xx})^{1/K}, \\
\var_c\{M^{1/2} (\hat{\tau}_ht - \tau) \mid \mathcal{D}_c(A_c)\} &= V_{ht,cc}^{-1}V_{ht,cr}V_{ht,cc}\det(A_c)^{1/K}\det(V_{ht,cc})^{1/K},
\end{align*}
\]

for a small \( \alpha \), where

\[
\begin{align*}
\nu_x(A_x) &= \frac{V_{haj,xx}^{-1}V_{haj,xt}V_{haj,xx}\det(A_x)^{1/K}\det(V_{haj,xx})^{1/K}}{V_{haj,xx}V_{haj,xt}}, \\
\nu_c(A_c) &= \frac{V_{ht,cc}^{-1}V_{ht,cr}V_{ht,cc}\det(A_c)^{1/K}\det(V_{ht,cc})^{1/K}}{V_{ht,cc}V_{ht,cr}},
\end{align*}
\]

As a sanity check, the cluster rerandomization schemes using the Mahalanobis distances lead to \( \nu_x(A_x) = \nu_x(V_{haj,xx}^{-1}) = 1 \) and \( \nu_c(A_c) = \nu_c(V_{ht,cc}^{-1}) = 1 \). Given the same \( R_x^2 \) or \( R_c^2 \) in Theorem 3,
the asymptotic efficiency of using $D_x(A_x)$ or $D_c(A_c)$ depends only on $\nu_x(A_x)$ or $\nu_c(A_c)$, respectively. Cluster rerandomization schemes using the weighted Euclidean distances have diagonal $A_x$ and $A_c$, which allows us to derive the optimal weighting matrices as shown in Theorem 4 below. Let $\xi_k$ denote a $K$-dimensional vector with 1 at the $k$th dimension and 0 at other dimensions.

**Theorem 4.** Under regularity conditions, if $V_{\text{haj},tx}V_{\text{haj},xx}^{-1}\xi_k$ and $V_{\text{ht},tc}V_{\text{ht},cc}^{-1}\xi_k$ are nonzero for all $k = 1, \ldots, K$, then $\nu_x\{\text{diag}(w_1, \ldots, w_K)\}$ reaches minimum if $w_k \propto (V_{\text{haj},tx}V_{\text{haj},xx}^{-1}\xi_k)^2$ for $k = 1, \ldots, K$, and $\nu_c\{\text{diag}(w_1, \ldots, w_K)\}$ reaches minimum if $w_k \propto (V_{\text{ht},tc}V_{\text{ht},cc}^{-1}\xi_k)^2$ for $k = 1, \ldots, K$.

Based on Theorem 4, let $A_x^{\text{opt}}$ and $A_c^{\text{opt}}$ denote the optimal weighting matrices at the individual level and cluster level, respectively. Recall Proposition 1 to obtain that

$$V_{\text{haj},tx}V_{\text{haj},xx}^{-1} = \text{cov}_i\{e_1\tilde{\varepsilon}(0) + e_0\tilde{\varepsilon}(1), \tilde{X}\}\{\text{cov}_i(\tilde{X})\}^{-1},$$
$$V_{\text{ht},tc}V_{\text{ht},cc}^{-1} = \text{cov}_i\{e_1\tilde{Y}(0) + e_0\tilde{Y}(1), C\}\{\text{cov}_i(C)\}^{-1}.$$

Therefore, the optimal weights in $A_x^{\text{opt}}$ and $A_c^{\text{opt}}$ correspond to the squared coefficients obtained from regressing $e_1\tilde{\varepsilon}(0) + e_0\tilde{\varepsilon}(1)$ on $\tilde{X}$ and regressing $e_1\tilde{Y}(0) + e_0\tilde{Y}(1)$ on $C$, respectively.

**Remark 1.** Orthogonalizing the covariates ensures that $V_{\text{haj},xx}^{-1}$ and $V_{\text{ht},cc}^{-1}$ are both diagonal. Then the optimality of $A_x^{\text{opt}}$ or $A_c^{\text{opt}}$ implies $\nu_x(A_x^{\text{opt}}) \leq \nu_x(V_{\text{haj},xx}^{-1}) = 1$ or $\nu_c(A_c^{\text{opt}}) \leq \nu_c(V_{\text{ht},cc}^{-1}) = 1$, respectively. Therefore, with orthogonalized covariates, the cluster rerandomization schemes based on the optimal weighted Euclidean distances are superior to those based on the Mahalanobis distances. However, this conclusion does not hold without orthogonalizing the covariates. We give a counterexample in the appendix.

### 4.2. Comparison with cluster rerandomization with tiers of covariates

With prior knowledge on the importance of the covariates, Morgan and Rubin (2015) proposed rerandomization with tiers of covariates as an alternative to rerandomization with the weighted Euclidean distance. Morgan and Rubin (2015) and Li et al. (2018) derived its properties under the assumption that treatments are assigned at the individual level. The theory for the cluster analog is still missing. Moreover, no comparison has been made between these two rerandomization schemes. We fill these gaps in this subsection.

Similar to Remark 1, the comparison does not yield definite answers with general covariates. However, we can demonstrate that rerandomization with the optimal weighted Euclidean distance is superior to rerandomization with tiers of covariates when the covariates are orthogonalized. In this subsection, we focus on cluster rerandomization with individual-level covariates; in the appendix, we give the corresponding results for cluster rerandomization with cluster-level covariates.

Orthogonalization is applied on the scaled cluster totals. The procedure proceeds as follows: first, find the upper triangular matrix $U$ by applying Gram–Schmidt orthogonalization to $\tilde{x}_i$ such that $U\tilde{x}_i$ has orthogonal components, and then transform the individual-level covariates to $Ux_{ij}$. To
simplify the presentation, we assume that $x_{ij} = (x_{ij1}, \ldots, x_{ijK})^T$ are already orthogonalized by the aforementioned procedure and are ordered in decreasing importance.

We first re-stated the results for cluster rerandomization with orthogonalized covariates. Let

$$V_{haj,xx} = \text{diag}(V_{haj,x_1x_1}, \ldots, V_{haj,x_Kx_K}), \quad V_{haj,\tau x} = (V_{haj,\tau x_1}, \ldots, V_{haj,\tau x_K}).$$

Define the squared multiple correlation for the $k$th covariate as

$$R^2_{xk} = V^2_{haj,\tau x_k} / (V_{haj,\tau x} V_{haj,x_kx_k}), \quad k = 1, \ldots, K.$$ 

Then by Theorem 4, the cluster rerandomization scheme based on the optimal weighted Euclidean distance is

$$D_x(A_x^{\text{opt}}) = \{ M\hat{\tau}^T_{haj,x} A^{\text{opt}}_x \hat{\tau}_{haj,x} \leq a \}$$

with the optimal diagonal matrix

$$A^{\text{opt}}_x = \text{diag}\{(V_{haj,\tau x_1} V^{-1}_{haj,x_1x_1})^2, \ldots, (V_{haj,\tau x_K} V^{-1}_{haj,x_Kx_K})^2\}.$$ 

Corollary 2 below is a special case of Theorem 3.

**Corollary 2.** Under regularity conditions with orthogonalized covariates and optimal weighted Euclidean distance, if $V_{haj,\tau x_k} V^{-1}_{haj,x_kx_k}$ are nonzero for all $k = 1, \ldots, K$, then

$$\text{var}_a\{M^{1/2}(\hat{\tau}_{haj} - \tau) \mid D_x(A_x^{\text{opt}})\} = V_{haj,\tau \tau} \left\{ (1 - R_x^2) + K \left( \prod_{k=1}^K R^2_{x_k} \right)^{1/K} p_K a^{2/K} + o(a^{2/K}) \right\},$$

for a small $\alpha$.

By Theorem 3, we can obtain that

$$\text{var}_a\{M^{1/2}(\hat{\tau}_{haj} - \tau) \mid M_x\} = V_{haj,\tau \tau} \left\{ (1 - R_x^2) + R_x^2 p_K a^{2/K} + o(a^{2/K}) \right\}.$$ 

Comparing it with Corollary 2 above, we can see that cluster rerandomization with the optimal weighted Euclidean distance is indeed superior to cluster rerandomization with the Mahalanobis distance due to $K \left( \prod_{k=1}^K R^2_{x_k} \right)^{1/K} \leq R_x^2$ by the inequality of arithmetic and geometric means, which echoes Remark 1.

In rerandomization with tiers of covariates, Morgan and Rubin (2015) partitioned the covariates into $L$ tiers by their importance with $K_l$ covariates in tier $l$, for $l = 1, \ldots, L$ and $\sum_{l=1}^L K_l = K$. Let $x^{[l]}$ be the covariates in the $l$th tier. Then $x = (x^{[1]}, \ldots, x^{[L]})$. Morgan and Rubin (2015) originally used the block-wise Gram–Schmidt orthogonalization, but we use the above element-wise orthogonalization because it is notionally simpler and leads to the same asymptotic distribution.

Within tier $l$, define $\hat{\tau}_{haj,x^{[l]}}$ as the difference in means of covariates, $V_{haj,x^{[l]}x^{[l]}}$ as its covariance, $M^{[l]}_x$ as the event that the corresponding Mahalanobis distance is smaller than or equal to the threshold $a^{[l]}$, $R^2_{x^{[l]}}$ as the corresponding $R^2$, and $\alpha^{[l]}$ as the asymptotic acceptance rate. The overall asymptotic acceptance rate satisfies $\alpha = \prod_{l=1}^L \alpha^{[l]}$ due to the orthogonalization of the covariates.
Corollary 3. Under regularity conditions,

\[ \text{var}_a \{ M^{1/2}(\hat{\tau}_{\text{haj}} - \tau) \mid M_{[1]}, \ldots, M_{[L]} \} = V_{\text{haj}, \tau} \left\{ (1 - R_x^2) + \sum_{l=1}^{L} R_{x[l]}^2 p_{K_l} \alpha^{2/K_l} + o(\alpha^{2/K_l}) \right\}, \]

for small \( \alpha[l] \), \( l = 1, \ldots, L \).

Given \( \alpha = \prod_{l=1}^{L} \alpha[l] > 0 \), to minimize the second term in the asymptotic variance in Corollary 3, we must choose

\[ \alpha[l] = \left( c_0 R_{x[l]}^2 / K_l \right)^{-K_l/2} \quad (l = 1, \ldots, L), \]

for some positive constant \( c_0 \). Theorem 5 below compares the second terms in the asymptotic variances in Corollaries 2 and 3.

Theorem 5. Under regularity conditions with orthogonalized covariates, the following inequality holds for any \( \alpha[1], \ldots, \alpha[L] \) satisfying \( \alpha = \prod_{l=1}^{L} \alpha[l] \):

\[ \sum_{l=1}^{L} R_{x[l]}^2 p_{K_l} \alpha^{2/K_l} \geq K \left( \prod_{k=1}^{K} R_{x[k]}^2 \right)^{1/K} p_K \alpha^{2/K}. \]

Based on the comparison of the asymptotic variances, Theorem 5 quantifies the superiority of cluster rerandomization with the optimal weighted Euclidean distance when the covariates are orthogonalized.

5. Rerandomization and regression adjustment

Rerandomization uses covariates in the design stage (Morgan and Rubin, 2012), and regression adjustment uses covariates in the analysis stage (Lin, 2013). Li et al. (2018) pointed out that they are dual in the design and analysis of randomized experiments with treatments assigned at the individual level. Moreover, Li and Ding (2020) showed that they could be used simultaneously. In this section, we will show that analogous results hold under cluster rerandomization and point out some subtle differences.

Under \( D_x(A_x) \), we can use the coefficient of \( Z_{ij} \) in the least squares fit of \( Y_{ij} \) on \( (1, Z_{ij}, x_{ij}, Z_{ij}x_{ij}) \) to estimate \( \tau \), and use the cluster-robust standard error to approximate the true asymptotic standard error (Liang and Zeger, 1986); under \( D_c(A_c) \), we can use the coefficient of \( Z_i \) in the least squares fit of \( \tilde{Y}_i \) on \( (1, Z_i, c_i, Z_i c_i) \) to estimate \( \tau \), and use the heteroskedasticity-robust standard error to approximate the true asymptotic standard error (Huber, 1967; White, 1980). Denote the two sets of regression coefficient and variance estimator by \( (\hat{\tau}_{\text{haj}}, \hat{V}_{\text{haj}}) \) and \( (\hat{\tau}_{\text{adj}}, \hat{V}_{\text{adj}}) \), respectively. Let \( z_\varsigma (0 < \varsigma < 1) \) be the \( \varsigma \)th quantile of a standard normal distribution. Theorem 6 below summarizes the important results about cluster rerandomization combined with regression adjustment.
Theorem 6. Assume regularity conditions hold.

(i) Under $\mathcal{D}_c(A_c)$, the estimator $\hat{\tau}_{\text{adj}}^{c}$ is consistent for $\tau$ and asymptotically normal, the probability limit of $M_V^{\hat{\tau}_{\text{adj}}^{c}}$ is larger than or equal to the true asymptotic variance of $M^{1/2}\hat{\tau}_{\text{adj}}^{c}$, and the $1-\varsigma$ confidence interval
\[
\left[\hat{\tau}_{\text{adj}}^{c} + (V_{\text{adj}}^{c})^{1/2}z_{\varsigma/2}, \hat{\tau}_{\text{adj}}^{c} + (V_{\text{adj}}^{c})^{1/2}z_{1-\varsigma/2}\right]
\]
has asymptotic coverage rate $\geq 1-\varsigma$;

(ii) Under $\mathcal{D}_x(A_x)$, the estimator $\hat{\tau}_{\text{adj}}^{x}$ is consistent for $\tau$ and its asymptotic distribution is a convolution of normal and truncated normal, the probability limit of $M_V^{\hat{\tau}_{\text{adj}}^{x}}$ is larger than or equal to the true asymptotic variance of $M^{1/2}\hat{\tau}_{\text{adj}}^{x}$, and the $1-\varsigma$ confidence interval
\[
\left[\hat{\tau}_{\text{adj}}^{x} + (V_{\text{adj}}^{LZ})^{1/2}z_{\varsigma/2}, \hat{\tau}_{\text{adj}}^{x} + (V_{\text{adj}}^{LZ})^{1/2}z_{1-\varsigma/2}\right]
\]
has asymptotic coverage rate $\geq 1-\varsigma$;

(iii) If $c_i = (n_i, \bar{x}_i^T)^T$, the asymptotic distribution of $\hat{\tau}_{\text{adj}}^{c}$ | $\mathcal{D}_c(A_c)$ is more concentrated at $\tau$ than $\hat{\tau}_{\text{adj}}^{x}$ | $\mathcal{D}_x(A_x)$, in the sense that for any $\delta > 0$, we have
\[
\Pr_{\text{a}}\{M^{1/2}|\hat{\tau}_{\text{adj}}^{c} - \tau| < \delta | \mathcal{D}_c(A_c)\} \leq \Pr_{\text{a}}\{M^{1/2}|\hat{\tau}_{\text{adj}}^{x} - \tau| < \delta | \mathcal{D}_x(A_x)\}.
\]

To avoid notation complexity, we relegate the details of the asymptotic distributions of $\hat{\tau}_{\text{adj}}^{c}$ given $\mathcal{D}_c(A_c)$ and $\hat{\tau}_{\text{adj}}^{x}$ given $\mathcal{D}_x(A_x)$ to Theorem 7 in the appendix. Theorem 6 parallels the key results in Su and Ding (2021) without rerandomization. It justifies the standard Wald-type inference based on appropriate regressions and standard errors, which can be conveniently obtained by standard statistical software packages. It also extends the results in Li and Ding (2020) from classic rerandomization to cluster rerandomization. However, some asymptotic results differ from those under rerandomization with treatments assigned at the individual level. In particular, with cluster rerandomization and regression adjustment using individual-level covariates, the asymptotic distribution is not normal anymore; see Theorem 7 in the appendix for more details. Moreover, Theorem 6 (iii) extends the theory in Su and Ding (2021) that regression adjustment using cluster size and scaled cluster totals outperforms regression adjustment using individual-level covariates.

Remark 2. Li and Ding (2020) also discussed the scenarios that the designer and analyzer do not communicate well, allowing the covariates used in the analysis stage be different from those used in the design stage. One important special case is that the set of covariates used in the analysis stage is empty. To be specific, under $\mathcal{D}_x(A_x)$, we can use the coefficient of $Z_{ij}$ in the least squares fit of $Y_{ij}$ on $(1, Z_{ij})$ to estimate $\tau$, and use the cluster-robust standard error to approximate the true asymptotic standard error; under $\mathcal{D}_c(A_c)$, we can use the coefficient of $Z_i$ in the least squares fit of $\hat{Y}_i$ on $(1, Z_i)$ to estimate $\tau$, and use the heteroskedasticity-robust standard error to approximate the true asymptotic standard error. These point estimators correspond to the Hajek and Horvitz–Thompson estimators.
discussed in Section 2, with standard errors \((\hat{V}_{LZ}^{\text{adj}})^{1/2}\) and \((\hat{V}_{HW}^{\text{adj}})^{1/2}\), respectively. Analogous to Theorem 6, these point estimators are still consistent for \(\tau\) and converge in distribution to convolutions of normal and truncated normal under cluster rerandomization. Moreover, the normal-based confidence intervals are still asymptotically conservative. However, different from the results in Su and Ding (2021), the standard errors \((\hat{V}_{LZ}^{\text{adj}})^{1/2}\) and \((\hat{V}_{HW}^{\text{adj}})^{1/2}\) are overly conservative because they ignore the truncated normal components in the asymptotic distributions. Due to the technical complexities, we relegate the theory and improved inference methods to the appendix.

**Remark 3.** Our asymptotic theory requires a large number of clusters, which may be unrealistic in many cluster randomized experiments. When \(M\) is small, one alternative approach is to use a mixed-effects model by imposing modelling assumptions on the data generating process. Another alternative approach is to use Fisher randomization tests that deliver finite-sample exact \(p\)-values under the sharp null hypothesis. See Zhao and Ding (2021, Section 4) for more details. Importantly, the Fisher randomization tests must follow the same treatment assignment rule of cluster rerandomization.

### 6. Numeric Examples

#### 6.1. Simulation

In this section, we conduct simulation to assess the finite-sample performances of all eight combinations with binary choices for three orthogonal axes, individual-level (X) versus cluster-level (C), the Mahalanobis distance (M) versus the optimal weighted Euclidean distance without orthogonalization (W), and using regression adjustment (.adj) or not. We also consider two baseline methods: Hajek (Haj) and Horvitz–Thompson (HT) estimators without using cluster rerandomization for better comparison. The names of the methods are written as ReMC, ReWC, ReMI, ReWI, ReMC.adj, ReWC.adj, ReMI.adj, and ReWI.adj, where the first two letters refer to cluster rerandomization and the rest correspond to the aforementioned three axes.

We generate potential outcomes from the following model:

\[
Y_{ij}(z) = g(n_i) + x_{ij}^T \beta_{iz} + \varepsilon_{ij}(z) \quad (i = 1, \ldots, M, \ j = 1, \ldots, n_i, \ z = 0,1).
\]

Here \(g(n_i)\) captures the cluster effects on individuals and \(\varepsilon_{ij}(z)\)'s are independent \(\mathcal{N}(0,16)\). Pre-treatment covariates \(x_{ij}\) are generated from a \(K\)-dimensional normal distribution with mean 0 and covariance matrix \(\Sigma\), where \(\Sigma_{ij} = (1 - \rho)\delta_{ij} + \rho\), with \(\delta_{ij} = 1\) if \(i = j\) and 0 otherwise. We fix \(M = 100\), with 50 assigned to the treatment arm and 50 to the control arm. We also conduct simulations with relatively small \(M\), and assess the validity of such asymptotic inference. The results are shown in the appendix. The size of each cluster is sampled uniformly from \(\{m \in \mathbb{N} \mid 4 \leq m \leq 10\}\). The coefficients are generated from \(\beta_{iz} = \beta_z + U(-0.1,0.1)\), where \(U(\cdot,\cdot)\) denotes uniform distribution. Here each component of \(\beta_1\) is sampled from \(\{0.5\gamma, \gamma, 1.5\gamma\}\) with equal probabilities, and \(\beta_0 = 2\gamma 1_K - \beta_1\), where \(1_K\) is a \(K\)-dimensional all-one vector, and \(\gamma\) is chosen to ensure the proportion of variance contributed by the covariates to be 0.5. These \(K\) covariates are used to generate the potential
outcomes, conduct cluster rerandomization, and perform regression adjustment. We use the scaled cluster totals of individual-level covariates together with cluster size as cluster-level covariates. Each cluster rerandomization is conducted with an acceptance rate $\alpha = 0.1\%$. We consider four scenarios with parameters given in Table 1.

Once generated, the potential outcomes and covariates are fixed throughout the simulation. We repeat the simulation for each scenario, draw treatment assignments 1000 times, and report the biases, standard deviations (SD), root mean squared errors (RMSE), and empirical coverage probabilities (CP) of 95% confidence intervals, and mean lengths of such intervals (CI Length). In particular, coverage probability is the percentage of confidence intervals that cover the true value of the average treatment effect from the 1000 replications. We consider two methods for constructing confidence intervals: the normal-based method given in Theorem 6 and Remark 2 and improved method provided in the appendix.

As shown in Table 2 and Figure 1, the combination of cluster rerandomization and regression adjustment results in better performance for all four scenarios. However, in some occasions, the combination has small improvement over cluster rerandomization only. This is because using cluster rerandomization only already has significant improvement, as the standard deviations are 30%–50% smaller than the two baseline methods. Moreover, the biases are negligible for all methods.

In Scenarios 1 and 3, cluster rerandomization schemes based on the optimal weighted Euclidean distances outperform cluster rerandomization schemes based on the Mahalanobis distances. This is due to the positively correlated covariates. On the contrary, in Scenarios 2 and 4, cluster rerandomization schemes based on the Mahalanobis distances are better because the covariates are negatively correlated. We conclude that the correlation structure between covariates can severely influence the efficiency of the balancing criterion.

Moreover, cluster rerandomization with cluster-level covariates outperforms cluster rerandomization with individual-level covariates in Scenarios 1 and 2, whereas cluster rerandomization with individual-level covariates is slightly better in Scenarios 3 and 4. To illustrate this, if the potential outcomes are not influenced by cluster size like in Scenarios 3 and 4, especially if the potential outcomes have a small variation across units, cluster rerandomization with individual-level covariates could be better. This is because they are based on the Hajek estimator, which partially eliminates the effect of cluster size by using $\tilde{\varepsilon}$ instead of $Y$ and fits a more precise model for this particular situation.

On the other hand, we recommend cluster rerandomization with cluster-level covariates, especially when the potential outcomes depend heavily on cluster size, because in such settings, the effect

| Scenario | $K$ | $\rho$ | $\gamma$ | $g(n_i)$ |
|----------|-----|-------|---------|---------|
| 1        | 7   | 0.8   | 1       | $(n_i - 7)/2$ |
| 2        | 7   | -0.15 | 5       | $(n_i - 7)/2$ |
| 3        | 12  | 0.4   | 0.5     | 6       |
| 4        | 12  | -0.09 | 12      | 6       |
Figure 1: Comparison results in simulation.
Table 2: Comparison results in simulation

| Method     | Bias  | SD    | RMSE | Normal-based | Improved |
|------------|-------|-------|------|--------------|----------|
|            | CP    | SD    | RMSE | CP           | CI Length | CP    | CI Length |
| Scenario 1 |       |       |      |              |          |       |          |
| ReMC       | -0.01 | 0.29  | 0.29 | 1.00         | 2.53     | 0.97  | 1.24     |
| ReWC       | 0.00  | 0.23  | 0.23 | 1.00         | 2.53     | 0.98  | 1.07     |
| ReMX       | -0.01 | 0.30  | 0.30 | 1.00         | 2.53     | 0.97  | 1.28     |
| ReWX       | 0.01  | 0.27  | 0.27 | 1.00         | 2.54     | 0.96  | 1.20     |
| Haj        | -0.02 | 0.62  | 0.62 | 0.96         | 2.53     | -     | -        |
| HT         | -0.03 | 0.62  | 0.62 | 0.95         | 2.53     | -     | -        |
| ReMC.adj   | 0.00  | 0.22  | 0.22 | 0.98         | 1.04     | -     | -        |
| ReWC.adj   | 0.00  | 0.22  | 0.22 | 0.97         | 1.05     | -     | -        |
| ReMX.adj   | 0.00  | 0.27  | 0.27 | 0.98         | 1.29     | 0.96  | 1.19     |
| ReWX.adj   | 0.00  | 0.28  | 0.28 | 0.98         | 1.29     | 0.97  | 1.22     |
| Scenario 2 |       |       |      |              |          |       |          |
| ReMC       | 0.00  | 0.24  | 0.24 | 1.00         | 2.18     | 0.98  | 1.14     |
| ReWC       | 0.01  | 0.30  | 0.30 | 1.00         | 2.17     | 0.96  | 1.23     |
| ReMX       | -0.01 | 0.27  | 0.27 | 1.00         | 2.17     | 0.97  | 1.21     |
| ReWX       | 0.00  | 0.32  | 0.32 | 1.00         | 2.18     | 0.95  | 1.31     |
| Haj        | -0.01 | 0.38  | 0.38 | 1.00         | 2.17     | -     | -        |
| HT         | -0.01 | 0.41  | 0.41 | 0.99         | 2.16     | -     | -        |
| ReMC.adj   | 0.00  | 0.22  | 0.22 | 0.98         | 1.04     | -     | -        |
| ReWC.adj   | 0.02  | 0.23  | 0.23 | 0.97         | 1.05     | -     | -        |
| ReMX.adj   | -0.01 | 0.28  | 0.28 | 0.98         | 1.29     | 0.96  | 1.20     |
| ReWX.adj   | 0.00  | 0.27  | 0.27 | 0.99         | 1.30     | 0.97  | 1.20     |
| Scenario 3 |       |       |      |              |          |       |          |
| ReMC       | 0.00  | 0.27  | 0.27 | 1.00         | 2.12     | 0.97  | 1.19     |
| ReWC       | 0.00  | 0.20  | 0.20 | 1.00         | 2.12     | 0.99  | 1.03     |
| ReMX       | -0.01 | 0.24  | 0.24 | 1.00         | 1.58     | 0.97  | 1.07     |
| ReWX       | 0.01  | 0.20  | 0.20 | 1.00         | 1.58     | 0.99  | 1.02     |
| Haj        | -0.01 | 0.35  | 0.35 | 0.97         | 1.58     | -     | -        |
| HT         | 0.01  | 0.50  | 0.50 | 0.95         | 2.10     | -     | -        |
| ReMC.adj   | 0.00  | 0.21  | 0.21 | 0.98         | 0.99     | -     | -        |
| ReWC.adj   | -0.01 | 0.21  | 0.21 | 0.98         | 1.01     | -     | -        |
| ReMX.adj   | 0.00  | 0.20  | 0.20 | 1.00         | 1.16     | 0.99  | 1.00     |
| ReWX.adj   | -0.01 | 0.21  | 0.21 | 1.00         | 1.16     | 0.98  | 1.01     |
| Scenario 4 |       |       |      |              |          |       |          |
| ReMC       | -0.01 | 0.27  | 0.27 | 1.00         | 4.50     | 0.98  | 1.34     |
| ReWC       | 0.01  | 0.41  | 0.41 | 1.00         | 4.49     | 0.97  | 1.76     |
| ReMX       | 0.01  | 0.23  | 0.23 | 1.00         | 4.29     | 0.99  | 1.20     |
| ReWX       | 0.01  | 0.31  | 0.31 | 1.00         | 4.30     | 0.97  | 1.49     |
| Haj        | -0.01 | 0.32  | 0.32 | 1.00         | 4.27     | -     | -        |
| HT         | 0.01  | 0.49  | 0.49 | 1.00         | 4.48     | -     | -        |
| ReMC.adj   | 0.00  | 0.20  | 0.20 | 0.98         | 0.99     | -     | -        |
| ReWC.adj   | 0.00  | 0.21  | 0.21 | 0.98         | 0.99     | -     | -        |
| ReMX.adj   | 0.00  | 0.20  | 0.20 | 1.00         | 1.16     | 0.99  | 1.01     |
| ReWX.adj   | 0.01  | 0.21  | 0.21 | 1.00         | 1.16     | 0.98  | 1.00     |
of cluster size is not directly accounted for if we use cluster rerandomization with individual-level covariates. Finally, by Corollary 1, with a sufficient small threshold, cluster rerandomization with cluster-level covariates is more efficient than cluster rerandomization with individual-level covariates in terms of variance reduction.

6.2. Child growth monitoring data

Tembo et al. (2017) conducted a cluster-randomized experiment in developing countries to study the effect of community-based monitoring on child growth faltering. We use part of this dataset to illustrate our theoretical results. We use two arms of the study, community-based monitoring as treatment and no monitoring as control. In the experiment, 41 communities were randomly assigned to the treatment arm while 41 to the control arm. The mean, median, and maximum of cluster size are 3.085, 3, and 8, respectively. We choose 6 individual-level covariates, including the child age, family background information, and some baseline growth data. We use cluster size and scaled cluster totals of individual-level covariates as cluster-level covariates. The height of a child is used as the outcome. As the potential outcomes are not completely available, we fit two simple linear regression models to impute the missing potential outcomes, and perform simulation based on the imputed dataset. The overall acceptance rate of all cluster rerandomization schemes are approximately 0.1%, computed from the quantile of the empirical distances. We use 4 covariates at the design stage for cluster rerandomization and 6 covariates at the analysis stage for regression adjustment.

Table 3 and Figure 2 show that cluster rerandomization always improves the performance, and cluster rerandomization schemes based on the weighted Euclidean distances are better than cluster rerandomization schemes based on the Mahalanobis distances. In the case when cluster-level covariates are used, the standard deviations under cluster rerandomization schemes using the weighted Euclidean distances are about half of those using the Mahalanobis distances. The combinations of cluster rerandomization and regression adjustment perform the best, and they have almost the same standard deviations and mean squared errors.

For this particular dataset, the covariates and outcomes are all positive. All cluster-level covariates and outcomes are strongly correlated with cluster size and there exists strong collinearity between covariates, which helps to explain why cluster rerandomization with the weighted Euclidean distance is much better than cluster rerandomization with the Mahalanobis distance. For cluster rerandomization with cluster-level covariates, the existence of collinearity and the fact that the weighted Euclidean distance puts more weights on more important covariates give rise to a dramatic increase of efficiency. The outcomes in this dataset, children’s heights, have a small variation across units, which helps to explain why the Hajek estimator performs much better than the Horvitz–Thompson estimator.

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Figure 2: Comparison results on the child monitoring data.

Table 3: Comparison results on the child monitoring data

| Method       | Bias | SD  | RMSE | Normal-based | Improved |
|--------------|------|-----|------|--------------|----------|
|              |      |     |      | CP           | CP       |
|              |      |     |      | CI Length    | CI Length|
| ReMC         | -0.01| 0.25| 0.25 | 1.00         | 0.94     |
|              |      |     |      | 4.63         | 0.95     |
| ReWC         | -0.01| 0.14| 0.14 | 1.00         | 0.93     |
|              |      |     |      | 4.63         | 0.54     |
| ReMX         | -0.01| 0.13| 0.13 | 0.99         | 0.94     |
|              |      |     |      | 0.72         | 0.51     |
| ReWX         | 0.00 | 0.13| 0.13 | 0.99         | 0.95     |
|              |      |     |      | 0.72         | 0.52     |
| Haj          | 0.00 | 0.17| 0.17 | 0.96         | –        |
|              |      |     |      | 0.72         | –        |
| HT           | -0.05| 1.20| 1.20 | 0.94         | –        |
|              |      |     |      | 4.60         | –        |
| ReMC.adj     | 0.00 | 0.07| 0.07 | 0.97         | –        |
|              |      |     |      | 0.31         | –        |
| ReWC.adj     | 0.00 | 0.07| 0.07 | 0.97         | –        |
|              |      |     |      | 0.31         | –        |
| ReMX.adj     | 0.00 | 0.06| 0.06 | 0.99         | 0.99     |
|              |      |     |      | 0.34         | 0.31     |
| ReWX.adj     | 0.00 | 0.06| 0.06 | 0.99         | 0.98     |
|              |      |     |      | 0.34         | 0.32     |
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A. Additional Simulation

Let $I_K$ denote a $K \times K$ identity matrix. We generate potential outcomes from the following model:

$$Y_{ij}(z) = f(2 + \epsilon_{iz} + x_{ij}^T \beta_{iz}) + \varepsilon_{ij}(z) \quad (i = 1, \ldots, M, \ j = 1, \ldots, n_i, \ z = 0, 1),$$

where $\beta_{iz} = \beta_z + \varsigma_{iz}$ with the components of $\beta_z$ ($z = 0, 1$) being independently generated from the $t$-distribution with three degrees of freedom and $\varsigma_{iz}$ ($i = 1, \ldots, M, z = 0, 1$) being independently generated from $N(0, I_K)$. We independently generate $x_{ij}$ ($i = 1, \ldots, M, j = 1, \ldots, n_i$) from $N(0, I_K)$ and $\epsilon_{iz}$ ($i = 1, \ldots, M, z = 0, 1$) from $N(0, 1)$. The error terms $\varepsilon_{ij}(z)$ ($i = 1, \ldots, M, j = 1, \ldots, n_i, z = 0, 1$) are independently generated from $N(0, \sigma_z^2)$, where $\sigma_z^2$ ($z = 0, 1$) are chosen so that the $f(2 + \epsilon_{iz} + x_{ij}^T \beta_{iz})$ ($i = 1, \ldots, M, j = 1, \ldots, n_i$) constitute half of the variation of $Y_{ij}(z)$. We use $(\tilde{x}_i, n_i) \in \mathbb{R}^{K+1}$ in cluster rerandomization using Mahalanobis distance and regression adjustment. We view simulation as a full factorial experiment and generate data under all combinations of the following five factors:

- Number of clusters $M = \{20 + 4k \mid k \in \mathbb{N}, \ 0 \leq k \leq 15\}$;
• Variance of cluster sizes $v_n = \{H, L\}$. If $v_n = H$, $n_i$’s are generated uniformly from $\{m \in \mathbb{N} \mid 2 \leq m \leq 16\}$; if $v_n = L$, $n_i$’s are generated uniformly from $\{m \in \mathbb{N} \mid 4 \leq m \leq 10\}$;

• Type of outcome-generating functions $f_n = \{\text{linear}, \text{nonlinear}\}$. $f(t) = t$ for $f_n = \text{linear}$; $f(t) = t^3$ for $f_n = \text{nonlinear}$;

• Dimension of covariates $K = \{1, 5\}$;

• Acceptance rate $\alpha = \{0.001, 0.1\}$.

Each of the $16 \times 2 \times 2 \times 2 \times 2 = 256$ scenarios is replicated under 100 random seeds. In each scenario under each random seed, we draw assignments for 1000 times with half of the clusters being assigned to the treatment arm. We construct 95% normal-based confidence intervals by the method provided in Section C based on the regression residuals. We compute the empirical coverage probabilities (CP) and percentages of reduction in root mean squared errors (RMSE) of the combination of cluster rerandomization and regression adjustment relative to two benchmark estimators without using cluster rerandomization, i.e., the Horvitz–Thompson estimator $\hat{\tau}_{ht}$ and Hajek estimator $\hat{\tau}_{haj}$ under classic cluster randomization.

As shown in Figure 3, the asymptotic inference does not vary much between $v_n=H$ and $v_n=L$ and between $f_n=\text{linear}$ and $f_n=\text{nonlinear}$. The dimension of covariates plays an important role in the validity of asymptotic inference. When $K = 1$, $M = 20$ is enough for the validity of the confidence interval under half of the random seeds and $M = 24$ is enough for the validity of the confidence interval under most of the random seeds. When $K = 5$, $M$ must be greater than 44 to ensure the validity of asymptotic inference.

Figures 4–5 show the percentages of reduction in RMSE. We can see that the combination of cluster rerandomization and regression adjustment is beneficial in reducing RMSE relative to the two benchmark estimators under most of the random seeds for all values of $M$. The benefit is more evident relative to the Horvitz–Thompson estimator than to the Hajek estimator.

The asymptotic inference is more likely to be valid and the regression adjustment provides more efficiency gains under more balanced assignments with $\alpha = 0.001$ than with $\alpha = 0.1$. This demonstrates the benefit of cluster rerandomization.

B. More detailed results on cluster rerandomization and regression adjustment

B.1. Asymptotic properties of regression-adjusted estimators under cluster rerandomization

In general, the covariates used in the analysis stage can be different from those used in the design stage. In the analysis stage, we use $w_{ij}$ for individual-level covariates and $v_i$ for cluster-level covariates.
Figure 3: Coverage probabilities for different values of $M$, $K$, and variance of cluster sizes.
Figure 4: Percentages of reduction in RMSE relative to the Horvitz–Thompson estimator without using cluster rerandomization for different values of $M$, $K$, and variance of cluster sizes.

(a) $fn = \text{linear}$

(b) $fn = \text{nonlinear}$
Figure 5: Percentages of reduction in RMSE relative to the Hajek estimator without using cluster rerandomization for different values of $M$, $K$, and variance of cluster sizes.

(a) $fn = \text{linear}$

(b) $fn = \text{nonlinear}$
Suppose that all these covariates are centered such that $\sum_{i=1}^{M} \sum_{j=1}^{n_i} w_{ij} = 0$ and $\sum_{i=1}^{M} v_i = 0$. Define $\bar{v}_i = \sum_{j=1}^{n_i} w_{ij} M/N$. Let $V$ and $\bar{W}$ be the concatenations of $v_i$ and $\bar{v}_i$ respectively.

With a slight abuse of notation, let $\bar{z}_{\text{ht}}$ denote the coefficient of $Z_{\text{ht}}$ obtained from the ordinary least squares fit of $Y_{ij}$ on $(1, Z_{ij}, w_{ij}, Z_{ij} w_{ij})$ in the individual-level regression adjustment, and $\bar{z}_{\text{ht}}$ denote the coefficient of $Z_{\text{ht}}$ obtained from the ordinary least squares fit of $\bar{Y}_i$ on $(1, Z_i, v_i, Z_i v_i)$ in the cluster-level regression adjustment.

Li and Ding (2020) derived the asymptotic distributions of the regression-adjusted estimators under rerandomization with treatments assigned at the individual level. We extend their results to cluster rerandomization. Define, for $z = 0, 1$,

$$\beta_w(z) = \arg \min_{\beta} \sum_{i=1}^{M} \sum_{j=1}^{n_i} \{Y_{ij}(z) - \bar{Y}(z) - w_{ij}^T \beta \}^2,$$

$$\beta_v(z) = \arg \min_{\beta} \sum_{i=1}^{M} \{\bar{Y}_i(z) - \bar{Y}(z) - v_i^T \beta \}^2.$$

Let $V_{\text{ht,}\tau,\nu}', V_{\text{ht,}\tau,\nu}', V_{\text{ht,}\tau,\nu}', V_{\text{ht,}\tau,\nu}'$, and $(R_x^\nu)^2$ be the quantities defined similarly to those in Proposition 1 except that we replace $Y_{ij}(z)$ by $Y_{ij}(z) - w_{ij}^T \beta_w(z)$, $z = 0, 1$. Let $V_{\text{ht,}\tau,\nu}', V_{\text{ht,}\tau,\nu}', V_{\text{ht,}\tau,\nu}'$, $V_{\text{ht,}\tau,\nu}'$ and $(R_c^\nu)^2$ be the quantities defined similarly to those in Proposition 1 except that we replace $\bar{Y}_i(z)$ by $\bar{Y}_i(z) - v_i^T \beta_v(z)$, $z = 0, 1$. Their limits exist under regularity conditions given in Section F.1, and we use the same notation to denote their limits if no confusion arises. We have the following result.

**Theorem 7.** Under regularity conditions, cluster rerandomization with individual-level covariates satisfies

$$M^{1/2}(\bar{z}_{\text{ht,}\nu} - \tau) \mid \mathcal{M}_x \sim (V_{\text{ht,}\tau,\nu}')^{1/2} \left[ \{1 - (R_x^\nu)^2\}^{1/2} \epsilon + R_x^{\nu} L_{K,a} \right],$$

$$M^{1/2}(\bar{z}_{\text{ht,}\nu} - \tau) \mid \mathcal{D}_x(A_x) \sim (V_{\text{ht,}\tau,\nu}')^{1/2} \left[ \{1 - (R_x^\nu)^2\}^{1/2} \epsilon + R_x^{\nu} \mu_a^T \eta \right],$$

and cluster rerandomization with cluster-level covariates satisfies

$$M^{1/2}(\bar{z}_{\text{ht,}\nu} - \tau) \mid \mathcal{M}_c \sim (V_{\text{ht,}\tau,\nu}')^{1/2} \left[ \{1 - (R_c^\nu)^2\}^{1/2} \epsilon + R_c^{\nu} L_{K,a} \right],$$

$$M^{1/2}(\bar{z}_{\text{ht,}\nu} - \tau) \mid \mathcal{D}_c(A_c) \sim (V_{\text{ht,}\tau,\nu}')^{1/2} \left[ \{1 - (R_c^\nu)^2\}^{1/2} \epsilon + R_c^{\nu} \mu_a^T \eta \right] V_{\text{ht,cc}} V_{\text{ht,cc}}^T \eta \leq a,$$

where $\eta = (\eta_1, \ldots, \eta_K)^T$, $\epsilon, \eta_1, \ldots, \eta_K$ are independent standard normal random variables, and

$$\mu_a^T = V_{\text{ht,}\tau,\nu}^{-1/2} / \{V_{\text{ht,}\tau,\nu} V_{\text{ht,}\tau,\nu}^T \}^{1/2}, \quad \mu_c^T = V_{\text{ht,}\tau,\nu}^{-1/2} / \{V_{\text{ht,}\tau,\nu} V_{\text{ht,}\tau,\nu}^T \}^{1/2}.$$
B.2. The gains from cluster rerandomization and regression adjustment

To compare the efficiency, Li and Ding (2020) introduced the notion of S-optimality to refer to the coefficient vector $\beta$ that could lead to the shortest asymptotic quantile range among all adjusted estimators. For cluster rerandomization with cluster-level covariates, the coefficient vector with respect to S-optimal regression-adjusted average treatment effect estimator coincides with $\beta_v(z)$ when $v_i = Bc_i$ or $c_i = Bv_i$ for certain matrix $B$. For cluster rerandomization with individual-level covariates, it may not be $\beta_w(z)$, which is the coefficient vector of $w_{ij}$ from the ordinary least squares fit of $Y_{ij}(z)$ on $(1, w_{ij})$. Instead, it equals the coefficient vector of $\tilde{w}_i$ from the ordinary least squares fit of $\tilde{Y}_i(z)$ on $(1, \tilde{w}_i)$. Su and Ding (2021) concluded that the individual-level regression adjustment is suboptimal, so we will not discuss the efficiency gains from the individual-level regression adjustment.

Li et al. (2020) proved the efficiency gain for the combination of rerandomization and regression adjustment with treatments assigned at the individual level if we use more or less information in the regression adjustment. We reexamine their results under cluster rerandomization using cluster-level covariates. We consider two special cases of cluster-level regression adjustment: $v_i = Bc_i$ or $c_i = Bv_i$. The former indicates that there is less information at the analysis stage, whereas the latter indicates that there is more information at the analysis stage. For the latter case, Corollary 4 below shows that regression adjustment can further improve the efficiency.

Corollary 4. Under regularity conditions, if $c_i = Bv_i$,

$$M^{1/2}(\hat{\tau}_{ht}^{adj} - \tau) \mid D(c) \sim (V_{ht,\tau})^{1/2} (1 - R^2) \epsilon,$$

where $\epsilon$ is a standard normal random variable, and $R^2$ is the squared multiple correlation defined similarly to $R^2_c$ with $c$ being replaced by $v$.

Corollary 4 can be interpreted as follows. If we use cluster-level covariates and have more information in the analysis stage, then using the combination of cluster rerandomization and regression adjustment is asymptotically equivalent to using regression adjustment only, which is no worse than using cluster rerandomization only.

For the case we have less information in the analysis stage, we have the following corollaries.

Corollary 5. Under regularity conditions, if $v_i = Bc_i$,

$$M^{1/2}(\hat{\tau}_{ht}^{adj} - \tau) \mid D(c) \sim (V_{ht,\tau})^{1/2} \{(1 - R^2)^{1/2} \epsilon + R_c \mu^T \eta \mid \eta^T V_{ht,cc}^{-1/2} \leq a\},$$

where $\eta = (\eta_1, \ldots, \eta_K)^T$, $\epsilon$, $\eta_1$, $\ldots$, $\eta_K$ are independent standard normal random variables,

$$\mu^T = (\mu_1, \ldots, \mu_K) = \{V_{ht,\tau} V_{ht,cc}^{-1} V_{ht,cr}\}^{-1/2} V_{ht,cc}^{-1/2} H = \mu_c^T H,$$

and

$$H = I_K - V_{ht,cc}^{1/2} B (BV_{ht,cc} B^T)^{-1} BV_{ht,cc}^{1/2}.$$
Corollary 6. Suppose that the covariates are orthogonalized. If we use the first $J < K$ covariates in the regression adjustment, then under regularity conditions,

$$\text{var}_a\{M^{1/2}(\hat{\tau}_{\text{adj}} - \tau) \mid \mathcal{D}_c(A_c)\} \leq \text{var}_a\{M^{1/2}(\hat{\tau}_{\text{int}} - \tau) \mid \mathcal{D}_c(A_c)\}.$$ 

By Corollary 5, the asymptotic distribution of $M^{1/2}(\hat{\tau}_{\text{adj}} - \tau)$ under $\mathcal{D}_c(A_c)$ is determined by the direction and length of the vector $\mu$. For an ellipsoidal acceptance region of the cluster rerandomization criterion, some directions lead to variance reduction while others do not. Regression adjustment is equivalent to a projection of $\mu_c$ onto a direction determined by $H$. However, such projection might not be in a favorable direction and there is no guarantee of efficiency gain in general. For some special cases as stated in Corollary 6, the asymptotic variance can be reduced. Moreover, if we use cluster rerandomization based on the Mahalanobis distance, the acceptance region is a ball and regression adjustment as a projection decreases the length of the vector $\mu_c$, leading to variance reduction. This echoes the result in Li et al. (2020) that regression adjustment improves the precision when we have less information in the analysis stage.

The gain from cluster rerandomization can be seen directly from Theorem 7 and Proposition 2 where $R_{c\text{adj}}$ and $R_{x\text{adj}}$ are equal to 0 without cluster rerandomization and greater than or equal to 0 with cluster rerandomization.

B.3. Estimating the sampling distributions of regression-adjusted estimators

In the main text, we discuss the validity of $\hat{V}_{LZ\text{adj}}$ and $\hat{V}_{HW\text{adj}}$ when $c_i = v_i$ and $x_{ij} = w_{ij}$. Theorem 8 below states general results without assuming $c_i = v_i$ and $x_{ij} = w_{ij}$.

Theorem 8. Under regularity conditions,

$$MV_{LZ\text{adj}}^{\tau} - V_{\text{adj}}^{\tau} \mid \mathcal{D}_x(A_x) \geq_p 0, \quad MV_{HW\text{adj}}^{\tau} - V_{\text{adj}}^{\tau} \mid \mathcal{D}_c(A_c) \geq_p 0,$$

where a random variable $\geq_p 0$ means that its probability limit is greater than or equal to 0.

By Theorem 8, the two types of robust standard errors are asymptotically conservative under cluster rerandomization.

C. Improvement for variance estimation and confidence intervals

Although $\hat{V}_{HW\text{adj}}^{\tau}$ and $\hat{V}_{LZ\text{adj}}^{\tau}$ are valid under cluster rerandomization, they can be overly conservative partly because they ignore that the asymptotic distributions have truncated normal components due to cluster rerandomization. We can derive better variance and confidence interval estimators by better estimating the sampling distributions.
In Theorem 7, we have derived the asymptotic distributions of \(M^{1/2}(\mathbf{v}_{\text{ht}} - \tau)\) and \(M^{1/2}(\mathbf{v}_{\text{haj}} - \tau)\) under cluster rerandomization. First, we derive better estimators of \(V_{\text{haj},\tau\tau}\) and \(V_{\text{ht},\tau\tau}\). Define the adjusted potential outcomes as \(\hat{Y}_{i}^{\text{adj}}(z) = \hat{Y}_{i}(z) - \mathbf{v}_{i}^{T}\beta_{v}(z)\) and \(\varepsilon_{ij}^{\text{adj}}(z) = \varepsilon_{ij}(z) - w_{ij}^{T}\beta_{w}(z)\), for \(z = 0, 1\). Let \(\hat{\varepsilon}_{i}^{\text{adj}}(z)\) be the scaled cluster total of \(\varepsilon_{ij}(z)\). Denote \(\hat{Y}_{i}^{\text{adj}}(z)\) and \(\hat{\varepsilon}_{i}^{\text{adj}}(z)\) as the vectors of \(\hat{Y}_{i}^{\text{adj}}(z)\) and \(\hat{\varepsilon}_{i}^{\text{adj}}(z)\), respectively. Recall that \(V_{\text{haj},\tau\tau}\) and \(V_{\text{ht},\tau\tau}\) are defined similarly as \(V_{\text{haj},\tau\tau}\) and \(V_{\text{ht},\tau\tau}\) except that we replace \(\varepsilon_{ij}(z)\) by \(\hat{\varepsilon}_{ij}(z)\) and \(\hat{Y}_{i}(z)\) by \(\hat{Y}_{i}^{\text{adj}}(z)\), for \(z = 0, 1\).

Define the variance of the linear projection of \(\hat{Y}_{i}^{\text{adj}}(z)\) on \(C\) as

\[
\text{var}_f\{\hat{Y}_{i}^{\text{adj}}(z) \mid C\} = \text{cov}_f\{\hat{Y}_{i}^{\text{adj}}(z), C\}\{\text{cov}_f(C)\}^{-1} \text{cov}_f\{C, \hat{Y}_{i}^{\text{adj}}(z)\}, \quad z = 0, 1.
\]

Similarly, define

\[
\text{var}_f\{\hat{\varepsilon}_{i}^{\text{adj}}(z) \mid \tilde{X}\} = \text{cov}_f\{\hat{\varepsilon}_{i}^{\text{adj}}(z), \tilde{X}\}\{\text{cov}_f(\tilde{X})\}^{-1} \text{cov}_f\{\tilde{X}, \hat{\varepsilon}_{i}^{\text{adj}}(z)\}, \quad z = 0, 1.
\]

Let \(\tilde{D}\) be the vector of residuals of the cluster-level regression adjustment. Let \(u_{ij}\) be the residual of the individual-level regression adjustment, \(\tilde{u}_{i}\), be its scaled cluster total, and \(\tilde{U}\) be the vector of \(\tilde{u}_{i}\). Denote by \(\text{var}_f(\cdot)\) and \(\text{cov}_f(\cdot)\) the sample variance and covariance under treatment arm \(z\). Let \(\tilde{G}\) be the union of \(\tilde{X}\) and \(\tilde{W}\). To simplify the presentation, we assume that \(\text{cov}_f(\tilde{G})\) is invertible.

Following the results of Li et al. (2018), less conservative estimators of \(V_{\text{haj},\tau\tau}\) and \(V_{\text{ht},\tau\tau}\) are

\[
\hat{V}_{\text{haj},\tau\tau}^{\text{adj}} = e_1^{-1} \text{var}_f\{\hat{\varepsilon}_{i}^{\text{adj}}(1)\} + e_0^{-1} \text{var}_f\{\hat{\varepsilon}_{i}^{\text{adj}}(0)\} - \text{var}_f\{\hat{\varepsilon}_{i}^{\text{adj}}(1) - \hat{\varepsilon}_{i}^{\text{adj}}(0) \mid \tilde{G}\},
\]

\[
\hat{V}_{\text{ht},\tau\tau}^{\text{adj}} = e_1^{-1} \text{var}_f\{\hat{Y}_{i}^{\text{adj}}(1)\} + e_0^{-1} \text{var}_f\{\hat{Y}_{i}^{\text{adj}}(0)\} - \text{var}_f\{\hat{Y}_{i}^{\text{adj}}(1) - \hat{Y}_{i}^{\text{adj}}(0) \mid C\},
\]

where \(\text{var}_f\{\hat{\varepsilon}_{i}^{\text{adj}}(z)\} = \text{var}_f(\tilde{U}), \text{var}_f\{\hat{Y}_{i}^{\text{adj}}(z)\} = \text{var}_f(\tilde{D})\), for \(z = 0, 1\), and

\[
\text{var}_f\{\hat{Y}_{i}^{\text{adj}}(1) - \hat{Y}_{i}^{\text{adj}}(0) \mid C\} = \left(\text{cov}_f(1)(D, C) - \text{cov}_f(0)(D, C)\right)\{\text{cov}_f(C)\}^{-1}\left(\text{cov}_f(1)(C, D) - \text{cov}_f(0)(C, D)\right),
\]

\[
\text{var}_f\{\hat{\varepsilon}_{i}^{\text{adj}}(1) - \hat{\varepsilon}_{i}^{\text{adj}}(0) \mid \tilde{G}\} = \left(\text{cov}_f(1)(\tilde{U}, \tilde{G}) - \text{cov}_f(0)(\tilde{U}, \tilde{G})\right)\{\text{cov}_f(\tilde{G})\}^{-1}\left(\text{cov}_f(1)(\tilde{G}, \tilde{U}) - \text{cov}_f(0)(\tilde{G}, \tilde{U})\right).
\]

Second, we estimate \(R_{x}^{\text{adj}}\) and \(R_{c}^{\text{adj}}\). Recall that \(R_{x}^{\text{adj}}\) and \(R_{c}^{\text{adj}}\) are defined similarly as \(R_{x}\) and \(R_{c}\) except that we replace \(Y_{ij}(z)\) by \(Y_{ij}(z) - w_{ij}^{T}\beta_{w}(z)\) and \(\hat{Y}_{i}(z)\) by \(\hat{Y}_{i}^{\text{adj}}(z) = \hat{Y}_{i}(z) - v_{i}^{T}\beta_{v}(z)\), for \(z = 0, 1\). Applying Proposition 1 of Li et al. (2018), we obtain the following results for \(R_{x}^{\text{adj}}\) and \(R_{c}^{\text{adj}}\).

**Proposition 3.** Under regularity conditions, \((R_{x}^{\text{adj}})^{2}\) or \((R_{c}^{\text{adj}})^{2}\) can be expressed in terms of the variances of the adjusted potential outcomes and of their projections on \(\tilde{X}\) or \(C\):

\[
(R_{x}^{\text{adj}})^{2} = \frac{e_1^{-1} \text{var}_f\{\hat{\varepsilon}_{i}^{\text{adj}}(1) \mid \tilde{X}\} + e_0^{-1} \text{var}_f\{\hat{\varepsilon}_{i}^{\text{adj}}(0) \mid \tilde{X}\} - \text{var}_f\{\hat{\varepsilon}_{i}^{\text{adj}}(1) - \hat{\varepsilon}_{i}^{\text{adj}}(0) \mid \tilde{X}\}}{e_1^{-1} \text{var}_f\{\hat{\varepsilon}_{i}^{\text{adj}}(1)\} + e_0^{-1} \text{var}_f\{\hat{\varepsilon}_{i}^{\text{adj}}(0)\} - \text{var}_f\{\hat{\varepsilon}_{i}^{\text{adj}}(1) - \hat{\varepsilon}_{i}^{\text{adj}}(0)\}},
\]

\[
(R_{c}^{\text{adj}})^{2} = \frac{e_1^{-1} \text{var}_f\{\hat{Y}_{i}^{\text{adj}}(1) \mid C\} + e_0^{-1} \text{var}_f\{\hat{Y}_{i}^{\text{adj}}(0) \mid C\} - \text{var}_f\{\hat{Y}_{i}^{\text{adj}}(1) - \hat{Y}_{i}^{\text{adj}}(0) \mid C\}}{e_1^{-1} \text{var}_f\{\hat{Y}_{i}^{\text{adj}}(1)\} + e_0^{-1} \text{var}_f\{\hat{Y}_{i}^{\text{adj}}(0)\} - \text{var}_f\{\hat{Y}_{i}^{\text{adj}}(1) - \hat{Y}_{i}^{\text{adj}}(0)\}}.
\]
The denominator of (4) is equal to $V_{\text{haj},\tau r}^{\text{adj}}$ and the denominator of (5) is equal to $V_{\text{ht},\tau r}^{\text{adj}}$. Following the results of Li et al. (2018), we can estimate $\text{var}_f\{\bar{Y}^{\text{adj}}(z) \mid C\}$ by

$$\text{var}_f\{\bar{Y}^{\text{adj}}(z) \mid C\} = \text{cov}_{f,z}(D,C)\{\text{cov}_{f,z}(C)\}^{-1}\text{cov}_{f,z}(C,D).$$

Similarly, $\text{var}_f\{\bar{Y}^{\text{adj}}(1) - \bar{Y}^{\text{adj}}(0) \mid C\}$ can be estimated by $\text{var}_f\{\bar{Y}^{\text{adj}}(1) - \bar{Y}^{\text{adj}}(0) \mid C\}$. Then we get an estimator for the numerator of (5). Thus, we estimate $\langle \hat{\mu} \rangle$.

Again we derive a consistent estimator for the numerator of (4). Thus, we estimate $\langle \hat{\mu} \rangle$.

Finally, we estimate $\hat{\mu}_x$ and $\hat{\mu}_c$ defined in Theorem 7. Recall that

$$\hat{\mu}_x^T = V_{\text{haj},\tau r}^{\text{adj}}V_{\text{haj},\tau r}^{-1/2}/\{V_{\text{haj},\tau r}^{\text{adj}}V_{\text{haj},\tau r}^{-1}\}^{1/2},$$

$$\hat{\mu}_c^T = V_{\text{ht},\tau c}^{\text{adj}}V_{\text{ht},\tau c}^{-1/2}/\{V_{\text{ht},\tau c}^{\text{adj}}V_{\text{ht},\tau c}^{-1}\}^{1/2}. \quad (6)$$

The denominators of (6) and (7) equal the square roots of the numerators of (4) and (5), respectively. We have derived their consistent estimators. Recall that

$$V_{\text{haj},\tau r}^{\text{adj}} = (V_{\text{haj},\tau r}^{\text{adj}})^T = e_1^{-1}\text{cov}_f\{\bar{X},\bar{z}^{\text{adj}}(1)\} + e_0^{-1}\text{cov}_f\{\bar{X},\bar{z}^{\text{adj}}(0)\},$$

$$V_{\text{ht},\tau c}^{\text{adj}} = (V_{\text{ht},\tau c}^{\text{adj}})^T = e_1^{-1}\text{cov}_f\{C,\bar{Y}^{\text{adj}}(1)\} + e_0^{-1}\text{cov}_f\{C,\bar{Y}^{\text{adj}}(0)\}. $$

We estimate $\text{cov}_f\{\bar{X},\bar{z}^{\text{adj}}(z)\}$ by $\text{cov}_{f,z}(\bar{X},\bar{U})$ and $\text{cov}_f\{C,\bar{Y}^{\text{adj}}(z)\}$ by $\text{cov}_{f,z}(C,\bar{D})$. Plugging in these terms, we derive consistent estimators of $\mu_x$ and $\mu_c$, denoted as $\hat{\mu}_x$ and $\hat{\mu}_c$, respectively.

Recall that $\xi_k$ is a $K$-dimensional vector with 1 at the $k$th dimension and 0 at other dimensions and $I_K$ is a $K \times K$ identity matrix. Let $q_\xi(R^2, \mu, A, a)$ be the $\xi$th quantile of $(1 - R^2), R^2\mu^T\eta \mid \eta^T\eta \leq a$. Theorem 9 below provides asymptotically conservative confidence intervals.

**Theorem 9.** Under regularity conditions,

$$\left[\hat{\xi}_{\text{haj}}^{\text{adj}} + (V_{\text{haj},\tau r}^{\text{adj}} / M)^{1/2} q_{c/2}\{1 - (\hat{R}_x^{\text{adj}})^2, \xi_1, I_K, a\}, \quad \hat{\xi}_{\text{haj}}^{\text{adj}} + (V_{\text{haj},\tau r}^{\text{adj}} / M)^{1/2} q_{1-c/2}\{1 - (\hat{R}_x^{\text{adj}})^2, \xi_1, I_K, a\}\right],$$

$$\hat{\xi}_{\text{ht}}^{\text{adj}} + (V_{\text{ht},\tau c}^{\text{adj}} / M)^{1/2} q_{c/2}\{1 - (\hat{R}_x^{\text{adj}})^2, \xi_1, I_K, a\}, \quad \hat{\xi}_{\text{ht}}^{\text{adj}} + (V_{\text{ht},\tau c}^{\text{adj}} / M)^{1/2} q_{1-c/2}\{1 - (\hat{R}_x^{\text{adj}})^2, \xi_1, I_K, a\}\right],$$

$$\hat{\xi}_{\text{ht}}^{\text{adj}} + (V_{\text{ht},\tau c}^{\text{adj}} / M)^{1/2} q_{c/2}\{1 - (\hat{R}_x^{\text{adj}})^2, \xi_1, I_K, a\}, \quad \hat{\xi}_{\text{ht}}^{\text{adj}} + (V_{\text{ht},\tau c}^{\text{adj}} / M)^{1/2} q_{1-c/2}\{1 - (\hat{R}_x^{\text{adj}})^2, \xi_1, I_K, a\}\right],$$

$$\hat{\xi}_{\text{ht}}^{\text{adj}} + (V_{\text{ht},\tau c}^{\text{adj}} / M)^{1/2} q_{c/2}\{1 - (\hat{R}_x^{\text{adj}})^2, \xi_1, I_K, a\}, \quad \hat{\xi}_{\text{ht}}^{\text{adj}} + (V_{\text{ht},\tau c}^{\text{adj}} / M)^{1/2} q_{1-c/2}\{1 - (\hat{R}_x^{\text{adj}})^2, \xi_1, I_K, a\}\right].$$

29
\[
\left[ \hat{\tau}_{ht} + (\hat{V}_{ht,\tau} / M)^{1/2} q_{k/2} \{ (\hat{R}_{c})^2, \xi_1, I_K, a \}, \right. \\
left. \hat{\tau}_{ht} + (\hat{V}_{ht,\tau} / M)^{1/2} q_{1-\eta/2} \{ (\hat{R}_{c})^2, \xi_1, I_K, a \} \right]
\]
are asymptotically conservative \(1 - \eta\) confidence intervals of \(\tau\) under \(M_x\) and \(M_c\), respectively;

\[
\left[ \hat{\tau}_{ht} + (\hat{V}_{ht,\tau} / M)^{1/2} q_{k/2} \{ (\hat{R}_{c})^2, \hat{\mu}_c, V_{haj,xx} A_c V_{haj,xx}^T, a \}, \right. \\
left. \hat{\tau}_{ht} + (\hat{V}_{ht,\tau} / M)^{1/2} q_{1-\eta/2} \{ (\hat{R}_{c})^2, \hat{\mu}_c, V_{haj,xx} A_c V_{haj,xx}^T, a \} \right]
\]
are asymptotically conservative \(1 - \eta\) confidence intervals of \(\tau\) under \(D_x(A_x)\) and \(D_c(A_c)\), respectively.

### D. Results for cluster rerandomization with cluster-level covariates that are omitted in Section 4.2

We assume that the \(c_i\)'s are orthogonalized by Gram-Schmidt orthogonalization. Let

\[
V_{ht,cc} = \text{diag}(V_{ht,c_1,1}, \ldots, V_{ht,c_K,c_K}), \quad V_{ht,tc} = (V_{ht,t,c_1}, \ldots, V_{ht,t,c_K})
\]
Define the squared multiple correlation for the \(k\)th covariate as \(R_{ck}^2 = V_{ht,tc}^2 (V_{ht,\tau} V_{ht,ck})\). The optimal cluster rerandomization scheme is \(D_c(A^\text{opt}_c) = (M_{ht,\tau} V_{ht,ck}^T A^\text{opt}_c V_{ht,ck}^T, \tau_{ht,c} < a)\) with the optimal diagonal matrix

\[
A^\text{opt}_c = \text{diag}\{ (V_{ht,t,c_1} V_{ht,c_1,c_1}^{-1})^2, \ldots, (V_{ht,t,c_K} V_{ht,c_K,c_K}^{-1})^2 \}.
\]

Corollary 7 below is the counterpart of Corollary 2 in the main text. Recall that

\[
p_K = \frac{2\pi}{K + 2} \left\{ \frac{2\pi^{K/2}}{K! (K/2)} \right\}^{-2/K}
\]

**Corollary 7.** Under regularity conditions with orthogonalized covariates and optimal weighted Euclidean distance, if \(V_{haj,tc} V_{ht,c_k,c_k}^{-1}\)'s are nonzero for all \(k = 1, \ldots, K\), then

\[
\text{var}_a \left\{ M^{1/2} (\hat{\tau}_{ht} - \tau) \mid D_c(A^\text{opt}_c) \right\} = V_{ht,\tau\tau} \left\{ (1 - R_c^2) + K \left( \prod_{k=1}^K R_{ck}^2 \right)^{1/K} p_K \alpha^{2/K} + o(\alpha^{2/K}) \right\},
\]

for a small \(\alpha\).

Similar to Section 4.2, we partition the covariates into \(L\) tiers with \(K_l\) covariates in tier \(l\), for \(l = 1, \ldots, L\) and \(\sum_{l=1}^L K_l = K\). Let \(c[l]\) be the covariates in the \(l\)th tier. Then \(c = (c[1], \ldots, c[L])\).
Within tier \( l \), define \( \hat{\tau}_{ht,c[l]} \) as the Horvitz–Thompson estimator for the covariates, \( V_{ht,c[l]c[l]} \) as its covariance, \( \mathcal{M}_{[l]} \) as the event that the corresponding Mahalanobis distance is smaller than or equal to the threshold \( a_{[l]} \), \( R_{c[p]}^2 \) as the corresponding \( R^2 \), and \( \alpha_{[l]} \) as the asymptotic acceptance rate. The overall asymptotic acceptance rate satisfies \( \alpha = \prod_{l=1}^{L} \alpha_{[l]} \) due to the orthogonalization of the covariates. Corollary 8 below is the counterpart of Corollary 3 for cluster rerandomization with cluster-level covariates.

**Corollary 8.** Under regularity conditions,

\[
\text{var}_a \{ M^{1/2}(\hat{\tau}_m - \tau) \mid \mathcal{M}_{[1]}, \ldots, \mathcal{M}_{[L]} \} = V_{ht,\tau\tau} \left\{ (1 - R_c^2) + \sum_{l=1}^{L} R_{c[p]}^2 p_{K_l} \alpha_{[l]}^{2/K_l} + o(\alpha_{[l]}^{2/K_l}) \right\},
\]

for small \( \alpha_{[l]} \), \( l = 1, \ldots, L \).

Given \( \alpha = \prod_{l=1}^{L} \alpha_{[l]} > 0 \), to minimize the second term in the asymptotic variance in Corollary 8, we must choose

\[
\alpha_{[l]} = \left( c_0 R_{c[p]}^2 p_{K_l} / K_l \right)^{-K_l/2} \quad (l = 1, \ldots, L),
\]

for some positive constant \( c_0 \). Theorem 10 below is the counterpart of Theorem 5 for cluster rerandomization with cluster-level covariates.

**Theorem 10.** Under regularity conditions with orthogonalized covariates, the following inequality holds for any \( \alpha_{[1]}, \ldots, \alpha_{[L]} \) satisfying \( \alpha = \prod_{l=1}^{L} \alpha_{[l]} \):

\[
\sum_{l=1}^{L} R_{c[p]}^2 p_{K_l} \alpha_{[l]}^{2/K_l} \geq K \left( \prod_{k=1}^{K} R_{c[k]}^2 \right)^{1/K} p_K \alpha^{2/K}.
\]

Theorem 10 quantifies the superiority of cluster rerandomization scheme based on the optimal weighted Euclidean distance when the cluster-level covariates are orthogonalized.

**E. A counterexample for Remark 1**

Naturally, we want to compare the optimal \( A_x \) or \( A_c \) with the one used in the Mahalanobis distance. Unfortunately, there could not be a universal result since \( \nu_x(A_{x}^{\text{opt}}) \) or \( \nu_c(A_{c}^{\text{opt}}) \) could be smaller than, equal to, or larger than \( \nu_x(V_{haj,xx}^{-1}) = 1 \) or \( \nu_c(V_{ht,cc}^{-1}) = 1 \), respectively, as shown in the example below.

**Example 1.** Suppose that

\[
V_{haj,xx} = \begin{bmatrix} 4 & \delta \\ \delta & 4 \end{bmatrix}, \quad V_{haj,\tau x} = (1, 1).
\]
Then
\[ \nu_x(A_{x}^{\text{opt}})/\nu_x(V_{\text{haj,xx}}^{-1}) = \left(\frac{4 - \delta}{4 + \delta}\right)^{1/2}. \]

When \( \delta > 0 \), i.e., there is a positive correlation between covariates, \( \nu_x(A_{x}^{\text{opt}}) \) is smaller than \( \nu_x(V_{\text{haj,xx}}^{-1}) \). When \( \delta < 0 \), the opposite result holds.

F. Proofs

F.1. Regularity conditions

This section provides the regularity conditions for the theoretical results. These conditions are required for using the finite population central limit theorem. Let \( ||\cdot||_\infty \) denote the \( \ell_\infty \) norm of a vector.

The regularity conditions below are used for deriving the asymptotic properties of \( \hat{\tau}_{x}^{\text{ht}} \) under classic cluster randomization.

**Condition 1.** As \( M \to \infty \), \( e_1 \) has a limit in \((0,1)\).

**Condition 2.** As \( M \to \infty \),

(i) the finite population variance \( \text{var}_f\{\tilde{Y}(z)\} \) (\( z = 0,1 \)) and covariance \( \text{cov}_f\{\tilde{Y}(0),\tilde{Y}(1)\} \) have finite limiting values, and the limit of \( V_{\text{haj,rr}} \) is positive;

(ii) \( \max_{z=0,1} \max_{1 \leq i \leq M} \{\tilde{Y}_i(z) - \bar{Y}(z)\}^2/M \to 0. \)

Condition 1 indicates that we have enough clusters assigned to both the treatment and control arms. Condition 2 restricts the moments of the potential outcomes. The asymptotic properties of \( \hat{\tau}_{\text{haj}} \) under classic cluster randomization require Condition 1 and Condition 3 below.

**Condition 3.** As \( M \to \infty \),

(i) the finite population variance, \( \text{var}_f\{\tilde{\varepsilon}(z)\} (z = 0,1) \), and covariances, \( \text{cov}_f\{\tilde{\varepsilon}(0),\tilde{\varepsilon}(1)\} \) and \( \text{cov}_f\{\tilde{\varepsilon}(z),\tilde{\omega}\} \), have finite limiting values, and the limit of \( V_{\text{haj,rr}} \) is positive;

(ii) \( M^{-1} \max_{1 \leq i \leq M} (\tilde{\omega}_i - 1)^2 \to 0 \) and \( M^{-1} \max_{z=0,1} \max_{1 \leq i \leq M} \{\tilde{\varepsilon}_i(z)\}^2 \to 0. \)

The asymptotic properties of \( \hat{\tau}_{\text{haj}} \) in Theorems 1–4 and 10, Corollaries 1 and 7–8, and Propositions 1–2 require Conditions 1–2 and Condition 4 below.

**Condition 4.** As \( M \to \infty \),

(i) the finite population covariances, \( \text{cov}_f(C) \) and \( \text{cov}_f\{C,\tilde{Y}(z)\} (z = 0,1) \), and \( A_c \) have finite limiting values, and the limits of \( \text{cov}_f(C) \) and \( A_c \) are nonsingular;
(ii) $M^{-1} \max_{1 \leq i \leq M} \| c_i \|_\infty^2 \to 0$.

The asymptotic properties of $\hat{\tau}_{\text{haj}}$ in Theorems 1–5, Corollaries 1–3, and Propositions 1–2 require Conditions 1, 3, and Condition 5 below.

**Condition 5.** As $M \to \infty$,

(i) the finite population covariances, $\text{cov}_t(\hat{X})$, $\text{cov}_t\{\hat{X}, \hat{\varepsilon}(z)\}$ ($z = 0, 1$), and $\text{cov}_t(\hat{X}, \hat{\omega})$, and $A_x$ have finite limiting values, and the limits of $\text{cov}_t(\hat{X})$ and $A_x$ are nonsingular;

(ii) $M^{-1} \max_{1 \leq i \leq M} \| \hat{\mu}_i \|_\infty^2 \to 0$.

The asymptotic properties of $\hat{\tau}_{\text{ht}}^\text{adj}$ in Theorems 6 and 7–9, Corollaries 4–6, and Proposition 3 require Conditions 1, 2, 4, and Condition 6 below.

**Condition 6.** As $M \to \infty$,

(i) $M^{-1} \max_{1 \leq i \leq M} \| v_i \|_\infty^2 = o(1)$;

(ii) the finite population covariances, $\text{cov}_t(V)$, $\text{cov}_t\{V, \hat{Y}(z)\}$ ($z = 0, 1$), and $\text{cov}_t(V, C)$, have finite limiting values, and the limit of $\text{cov}_t(V)$ is nonsingular;

The asymptotic properties of $\hat{\tau}_{\text{haj}}^\text{adj}$ in Theorems 6 and 7–9 and Proposition 3 require Conditions 1, 3, 5, and Condition 7 below.

**Condition 7.** As $M \to \infty$,

(i) $N^{-1} \sum_{i=1}^{M} \sum_{j=1}^{n_i} w_{ij} \varepsilon_{ij}(z)$ ($z = 0, 1$) converges to a finite vector, and $N^{-1} \sum_{i=1}^{M} \sum_{j=1}^{n_i} w_{ij} w_{ij}^T$ converges to a finite and invertible matrix;

(ii) $\max_{1 \leq i \leq M} \omega_i = o(M^{1/3})$, $N^{-1} \sum_{i=1}^{M} \sum_{j=1}^{n_i} \| w_{ij} \|_4^4 = O(1)$, $M^{-1} \max_{1 \leq i \leq M} \| \hat{\mu}_i \|_\infty^2 = o(1)$, $N^{-1} \sum_{i=1}^{M} \sum_{j=1}^{n_i} \{ Y_{ij}(z) \}^4 = O(1)$ ($z = 0, 1$);

(iii) the finite population covariances, $\text{cov}_t(\hat{W})$, $\text{cov}_t\{\hat{W}, \hat{\varepsilon}(z)\}$ ($z = 0, 1$), $\text{cov}_t\{\hat{W}, \hat{\omega}\}$, and $\text{cov}_t(\hat{W}, \hat{X})$, have finite limiting values, and the limit of $\text{cov}_t(\hat{W})$ is nonsingular.

**F.2. Some preliminary results on weak convergence**

Before proving the main results, we introduce some preliminary results on weak convergence derived by Li et al. (2018). Consider the combination $(\hat{\tau}, \hat{\tau}_*)$ as the estimator of the average treatment effects for the outcomes and covariates, for example, $(\hat{\tau}_{\text{ht}}, \hat{\tau}_{\text{ht,c}})$ and $(\hat{\tau}_{\text{haj}}, \hat{\tau}_{\text{haj,z}})$. Consider a balance criterion $\phi(M^{1/2} \hat{\tau}_*, A)$ which is a binary function, and $A$ is the matrix used to conduct cluster rerandomization. Denote the event that a treatment assignment is acceptable under the balance criterion $\phi(M^{1/2} \hat{\tau}_*, A)$ as $\phi(M^{1/2} \hat{\tau}_*, A) = 1$, and let $\mathcal{G} = \{ \mu : \phi(\mu, A) = 1 \}$ be the acceptance region for $M^{1/2} \hat{\tau}_*$. We write $A > 0$ if $A$ is strictly positive definite. Suppose that Condition 8 below on $\phi(\cdot, \cdot)$ holds.
Condition 8. (i) $\phi(\cdot, \cdot)$ is almost surely continuous;

(ii) if $T_\star \sim \mathcal{N}(0, V_\star)$, then $\text{pr}\{\phi(T_\star, A) = 1\} > 0$ for any $A > 0$, and $\text{var}\{T_\star \mid \phi(T_\star, A) = 1\}$ is a continuous function of $V_\star$;

(iii) $\phi(\mu, A) = \phi(-\mu, A)$, for all $\mu$ and $A > 0$.

In Condition 8, (i) and (ii) impose smoothness constraints on $\phi$ and prevent the acceptance region from being a set of measure zero; (iii) is a symmetry consideration to ensure that relabel the treatment and control units does not change the balance criterion. Cluster rerandomization schemes based on the Mahalanobis distances and weighted Euclidean distances satisfy Condition 8. We denote the variance of $M^{1/2}(\hat{\tau}, \hat{T}_\star)$ as $V$, and we use the same notation to represent its limit:

$$V = \begin{bmatrix} V_{\tau\tau} & V_{\tau\star} \\
V_{\tau\star} & V_{\star\star} \end{bmatrix}.$$ 

Assume that $V$ is strictly positive definite. Let $A_\infty$ be the limit of $A$, and $\mathcal{G}_\infty = \{\mu : \phi(\mu, A_\infty) = 1\}$ be the limit of $\mathcal{G}$. Proposition 4 below is a direct result of Proposition A1 in Li et al. (2018).

**Proposition 4.** Under Condition 8, as $M \to \infty$, if

$$M^{1/2} \left( \begin{array}{c} \hat{\tau} - \tau \\ \hat{T}_\star \end{array} \right) \sim \mathcal{N}(0, V),$$

then

$$M^{1/2} \left( \begin{array}{c} \hat{\tau} - \tau \\ \hat{T}_\star \end{array} \right) \bigg| M^{1/2} \hat{T}_\star \in \mathcal{G} \sim \left( \begin{array}{c} T \\ T_\star \end{array} \right) \bigg| T_\star \in \mathcal{G},$$

where $(T, T_\star^T) \sim \mathcal{N}(0, V)$.

**F.3. Proof of Proposition 1**

We need the following Lemma from Su and Ding (2021).

**Lemma 1.** Under Conditions 1 and 3,

$$M^{1/2} \left[ \hat{\tau}_{\text{bar}} - \left\{ M_1^{-1} \sum_{i=1}^N Z_i \tilde{\varepsilon}_i - M_0^{-1} \sum_{i=1}^N (1 - Z_i) \tilde{\varepsilon}_i \right\} \right] = o_p(1).$$

Su and Ding (2021) proved Lemma 1 under slightly stronger conditions. After carefully examining their proof, we found that it can be easily generalized to the case of our weaker conditions, so we omit the proof of Lemma 1.

34
of Proposition 1. Applying the vector-form finite population central limit theorem developed by Li and Ding (2017) to the scaled cluster-total potential outcomes \( \hat{Y}_i(z) \), \( z = 0,1 \), and cluster-level covariates \( c_i \), we have, under Conditions 1, 2, and 4,

\[
M^{1/2} \left( \frac{\hat{\tau}_{ht} - \tau}{\hat{\tau}_{ht,c}} \right) \sim \mathcal{N} \left( 0, \begin{bmatrix} V_{ht,\tau\tau} & V_{ht,\tau c} \\ V_{ht,c\tau} & V_{ht,cc} \end{bmatrix} \right).
\]

We could get a similar result for the joint asymptotic distribution of \( (\hat{\tau}_{ht}, \hat{\tau}_{ht,x})^T \) after replacing \( \hat{Y}_i(z) - \bar{Y}(z) \) by \( \hat{\varepsilon}_i(z) = \hat{Y}_i(z) - \overline{\omega}_i \bar{Y}(z) \) and applying Lemma 1. Specifically, applying Lemma 1 to each element of \( M^{1/2} (\hat{\tau}_{ht} - \tau, \hat{\tau}_{ht,x})^T \), we have, under Conditions 1 and 3,

\[
M^{1/2} \left( \frac{\hat{\tau}_{ht} - \tau}{\hat{\tau}_{ht,x}} \right) = M^{1/2} \left( \frac{M_1^{-1} \sum_{i=1}^{M} Z_i \hat{\varepsilon}_i - M_0^{-1} \sum_{i=1}^{M} (1 - Z_i) \hat{\varepsilon}_i(0) }{M_1^{-1} \sum_{i=1}^{M} Z_i \hat{\varepsilon}_i - M_0^{-1} \sum_{i=1}^{M} (1 - Z_i) \hat{\varepsilon}_i} \right) + o_p(1).
\]

Under Conditions 1, 3, and 5, applying the vector-form finite population central limit theorem to \( \hat{\varepsilon}_i(z) \), \( z = 0,1 \), and \( \hat{\varepsilon}_i \), we have

\[
M^{1/2} \left( \frac{M_1^{-1} \sum_{i=1}^{M} Z_i \hat{\varepsilon}_i(1) - M_0^{-1} \sum_{i=1}^{M} (1 - Z_i) \hat{\varepsilon}_i(0)}{M_1^{-1} \sum_{i=1}^{M} Z_i \hat{\varepsilon}_i - M_0^{-1} \sum_{i=1}^{M} (1 - Z_i) \hat{\varepsilon}_i} \right) \sim \mathcal{N} \left( 0, \begin{bmatrix} V_{haj,\tau\tau} & V_{haj,\tau x} \\ V_{haj,x\tau} & V_{haj,xx} \end{bmatrix} \right).
\]

By Slutsky’s theorem, the conclusion holds.

\[\square\]

**F.4. Proof of Theorem 1**

Proposition 5 below follows from Propositions 1 and 4.

**Proposition 5.** Under Conditions 1, 3, and 5,

\[
M^{1/2} \left( \frac{\hat{\tau}_{haj} - \tau}{\hat{\tau}_{haj,x}} \right) \mid M^{1/2} \hat{\tau}_{haj,x} \in \mathcal{G}_x \sim \left( \begin{bmatrix} T \\ T_x \end{bmatrix} \right) \mid T_x \in \mathcal{G}_x,
\]

and under Conditions 1, 2, and 4,

\[
M^{1/2} \left( \frac{\hat{\tau}_{ht} - \tau}{\hat{\tau}_{ht,c}} \right) \mid M^{1/2} \hat{\tau}_{ht,c} \in \mathcal{G}_c \sim \left( \begin{bmatrix} T \\ T_c \end{bmatrix} \right) \mid T_c \in \mathcal{G}_c,
\]

where \( (T, T_x^T)^T \sim \mathcal{N}(0, V_{haj}) \) and \( (T, T_c^T)^T \sim \mathcal{N}(0, V_{ht}) \) with

\[
V_{haj} = \begin{bmatrix} V_{haj,\tau\tau} & V_{haj,\tau x} \\ V_{haj,x\tau} & V_{haj,xx} \end{bmatrix}, \quad V_{ht} = \begin{bmatrix} V_{ht,\tau\tau} & V_{ht,\tau c} \\ V_{ht,c\tau} & V_{ht,cc} \end{bmatrix}.
\]

of Theorem 1. The asymptotic distribution of \( M^{1/2} (\hat{\tau}_{ht} - \tau) \mid \mathcal{M}_c \) is a direct result of applying
Theorem 1 of Li et al. (2018) to \( \tilde{Y}_i(z) \), \( z = 0, 1 \), and \( c_i \).

To derive the asymptotic distribution of \( M^{1/2}(\hat{\tau}_{\text{haj}} - \tau) \mid M_x \), similar to the proof of Proposition 1, we have \( \{M^{1/2}(\hat{\tau}_{\text{haj}} - \tau), M^{1/2}\hat{\tau}_{\text{haj},x}, A_x \} \) has the same asymptotic distribution as \( \{T, T_x, A_x \} \) with \( A_x = V_{\text{haj},xx}^{-1} \). Therefore, \( M^{1/2}(\hat{\tau}_{\text{haj}} - \tau) \mid M^{1/2}\hat{\tau}_{\text{haj},x}, A_x \leq a \) has the same asymptotic distribution as \( T \mid T_x A_x T_x \leq a \). Applying Theorem 1 of Li et al. (2018) to \( \hat{\epsilon}_i(z) \), \( z = 0, 1 \), and \( \hat{x}_i \), we have

\[
T \mid T_x A_x T_x \leq a \sim V_{h_{\tau,T}}^{1/2} \{ (1 - R^2_c \epsilon + R_z L_{K,a} \}.
\]

The conclusion follows immediately.

\[ \square \]

F.5. Proof of Corollary 1

of Corollary 1. For the cluster-level covariates \( c_i = (n_i, \hat{x}_i) \), we have

\[
V_{h_{\tau,T}} = (e_1 e_0)^{-1} \text{var} \{ e_1 \tilde{Y}(0) + e_0 \tilde{Y}(1) \},
\]

\[
V_{h_{\tau,T}} R^2_c = (e_1 e_0)^{-1} \text{cov} \{ e_1 \tilde{Y}(0) + e_0 \tilde{Y}(1), C \} \text{cov}(C)^{-1} \text{cov} \{ C, e_1 \tilde{Y}(0) + e_0 \tilde{Y}(1) \}.
\]

Therefore, \( e_1 e_0 V_{h_{\tau,T}} (1 - R^2_c) \) is the variance of the residuals when we regress \( e_1 \tilde{Y}(0) + e_0 \tilde{Y}(1) \) on \( C \) with intercept, i.e.,

\[
e_1 e_0 V_{h_{\tau,T}} (1 - R^2_c) = \min_{\beta \in \mathbb{R}^{K+1}, \beta_0 \in \mathbb{R}} \text{var} \{ e_1 \tilde{Y}(0) + e_0 \tilde{Y}(1) - 1_M \beta_0 - (N/M \tilde{\omega}, \tilde{X}) \beta \},
\]

where \( 1_M \) is an \( M \)-dimensional all-one vector. Similarly, we have

\[
e_1 e_0 V_{h_{\tau,T}} (1 - R^2_c) = \min_{\beta \in \mathbb{R}^{K}, \beta_0 \in \mathbb{R}} \text{var} \{ e_1 \tilde{\epsilon}(0) + e_0 \tilde{\epsilon}(1) - 1_M \beta_0 - \tilde{X} \beta \}
\]

\[ = \min_{\beta \in \mathbb{R}^{K}, \beta_0 \in \mathbb{R}} \text{var} \{ e_1 \tilde{Y}(0) + e_0 \tilde{Y}(1) - (e_1 \tilde{Y}(0) + e_0 \tilde{Y}(1)) \tilde{\omega} - 1_M \beta_0 - \tilde{X} \beta \},
\]

where the second equality follows from \( \tilde{\epsilon}_i(z) = \tilde{Y}_i(z) - \tilde{\omega}_i \tilde{Y}(z) \). Therefore,

\[
V_{h_{\tau,T}} (1 - R^2_c) \leq V_{h_{\tau,T}} (1 - R^2_x),
\]

which completes the proof.

\[ \square \]

F.6. Proof of Theorem 2

of Theorem 2. By Proposition 1,

\[
M^{1/2}(\hat{\tau}_{\text{haj}} - \tau, \hat{\tau}_{\text{haj},c}^T) \sim (T, T_c^T), \quad M^{1/2}(\hat{\tau}_{\text{haj}} - \tau, \hat{\tau}_{\text{haj},x}^T) \sim (T, T_x^T),
\]

36
where \((T, T^c) \sim \mathcal{N}(0, V_{ht})\) and \((T, T^c) \sim \mathcal{N}(0, V_{haj})\). We only give the proof for cluster rerandomization with individual-level covariates, as the proof for cluster rerandomization with cluster-level covariates is similar. By Proposition 5, we have

\[
M^{1/2}(\hat{\eta}_{haj,x} - \tau) \mid \mathcal{D}_x(A_x) = M^{1/2}(\hat{\eta}_{haj,x} - \tau) \mid (M^{1/2}(\hat{\eta}_{haj,x})^T A_x (M^{1/2}(\hat{\eta}_{haj,x}) \leq a
\sim T \mid T^T_x A_x T_x \leq a.
\]

We decompose \(T\) as

\[
T = T - V_{haj,\tau x} V_{haj,xx}^{-1} T_x + V_{haj,\tau x} V_{haj,xx}^{-1} T_x.
\]

Note that \(T - V_{haj,\tau x} V_{haj,xx}^{-1} T_x\) is independent of \(T_x\), and thus, independent of \(V_{haj,\tau x} V_{haj,xx}^{-1} T_x\) and \(T^T_x A_x T_x\). Therefore,

\[
T - V_{haj,\tau x} V_{haj,xx}^{-1} T_x \mid T^T_x A_x T_x \leq a \sim T - V_{haj,\tau x} V_{haj,xx}^{-1} T_x.
\]

By the definition of \(R^2_x\), we have \(R^2_x = V_{haj,\tau x} V_{haj,xx}^{-1} V_{haj,\tau x} / V_{haj,\tau\tau}\), and therefore

\[
\text{var}(T - V_{haj,\tau x} V_{haj,xx}^{-1} T_x) = V_{haj,\tau\tau} - V_{haj,\tau x} V_{haj,xx}^{-1} V_{haj,\tau x} = (1 - R^2_x) V_{haj,\tau\tau}.
\]

Thus,

\[
T - V_{haj,\tau x} V_{haj,xx}^{-1} T_x \sim V_{haj,\tau\tau}^{1/2} (1 - R^2_x)^{1/2} \epsilon.
\]

Since \(V_{haj,xx}^{-1} T_x\) is a \(K\)-dimensional standard normal random vector,

\[
\begin{align*}
V_{haj,\tau x} V_{haj,xx}^{-1} T_x \mid T^T_x A_x T_x & \leq a \\
\sim V_{haj,\tau x} V_{haj,xx}^{-1/2} V_{haj,xx}^{-1/2} T_x \mid (T^T_x V_{haj,xx}^{-1/2} V_{haj,xx}^{-1/2} T_x)^{1/2} (V_{haj,xx}^{-1/2} T_x) \leq a \\
\sim V_{haj,\tau x} V_{haj,xx}^{-1/2} \eta \mid \eta^T V_{haj,xx}^{-1/2} A_x V_{haj,xx}^{-1/2} \eta \leq a \\
\sim V_{haj,\tau\tau}^{1/2} (R^T_x \mu^T_x \eta) \mid \eta^T V_{haj,xx}^{-1/2} A_x V_{haj,xx}^{-1/2} \eta \leq a,
\end{align*}
\]

where \(\eta\) is a \(K\)-dimensional standard normal random vector and is independent of \(\epsilon\) and

\[
\mu^T_x = (V_{haj,\tau x} V_{haj,xx}^{-1} V_{haj,xx}^{-1/2} V_{haj,xx}^{-1/2} V_{haj,\tau x})^{-1/2} V_{haj,\tau x} V_{haj,xx}^{-1/2}.
\]

Therefore,

\[
V_{haj,\tau\tau}^{1/2} \left\{(1 - R^2_x)^{1/2} \epsilon + R^T_x \mu^T_x \eta \mid \eta^T V_{haj,xx}^{-1/2} A_x V_{haj,xx}^{-1/2} \eta \leq a\right\} \sim T \mid T^T_x A_x T_x \leq a,
\]

which implies that

\[
M^{1/2}(\hat{\eta}_{haj} - \tau) \mid \mathcal{D}_x(A_x) \sim V_{haj,\tau\tau}^{1/2} \left\{(1 - R^2_x)^{1/2} \epsilon + R^T_x \mu^T_x \eta \mid \eta^T V_{haj,xx}^{-1/2} A_x V_{haj,xx}^{-1/2} \eta \leq a\right\}.
\]

\(\square\)
F.7. Proof of Proposition 2

First, we introduce some useful lemmas. Lemma 2 below is from Li et al. (2018, Lemma A8).

**Lemma 2.** If $A$ and $B$ are independent, and are both symmetric around zero and unimodal, then $A + B$ is symmetric around zero and unimodal.

Recall that the asymptotic distributions in Theorem 2 are composed of two independent components: a normal random variable and a truncated normal random variable. To simplify the presentation, we say that a random variable is symmetric unimodal if it is symmetric around zero and unimodal. Clearly, the normal random variable is symmetric unimodal. To prove the symmetric unimodality of the truncated normal component, we follow the proof of Li et al. (2020, Proposition 2) using properties of symmetric unimodality of random vectors. The definition of symmetric unimodal random vector follows from Dharmadhikari and Joag-Dev (1988) as an extension of univariate case.

**Definition 1.** For a set $\mathcal{B}$ of distributions on $\mathbb{R}^K$, we say that $\mathcal{B}$ is closed convex if it satisfies two properties: (i) for any distributions $\nu_1, \nu_2 \in \mathcal{B}$ and for any $\lambda \in (0, 1)$, the distribution $(1-\lambda)\nu_1 + \lambda \nu_2 \in \mathcal{B}$, and (ii) a distribution $\nu \in \mathcal{B}$ if there exist a sequence of distributions in $\mathcal{B}$ converging weakly to $\nu$.

For any set $\mathcal{C}$ of distributions, the closed convex hull of $\mathcal{C}$ is the smallest closed convex set containing $\mathcal{C}$. A compact convex set in Euclidean space $\mathbb{R}^K$ is called a convex body if it has a nonempty interior. A set $\mathcal{K} \subset \mathbb{R}^K$ is symmetric if $\mathcal{K} = \{-a : a \in \mathcal{K}\}$.

**Definition 2.** A distribution on $\mathbb{R}^K$ is symmetric unimodal if it is in the closed convex hull of $\mathcal{U}$, where $\mathcal{U}$ is the set of all uniform distributions on symmetric convex bodies in $\mathbb{R}^K$.

Lemmas 3 and 4 below are from Li et al. (2020, Lemma A6) and Li et al. (2020, Lemma A8) respectively.

**Lemma 3.** If $\psi \in \mathbb{R}^K$ is a symmetric unimodal random vector, then for any non-random vector $b \in \mathbb{R}^K$, $b^T\psi$ is a symmetric unimodal random variable.

**Lemma 4.** If a random vector in $\mathbb{R}^K$ has a log-concave density, then it is symmetric unimodal.

Lemma 5 below is new which shows the symmetric unimodality of a truncated normal random vector.

**Lemma 5.** The truncated normal random variable $\rho b^T \eta \mid \eta^T A \eta \leq a$ is symmetric unimodal, where $\eta \sim \mathcal{N}(0, I_K)$, $\rho$ is a non-random scalar, $b$ is a non-random vector, and $A$ is a non-random symmetric positive definite matrix.

**Proof of Lemma 5.** By Lemma 3, it suffices to show that $\eta \mid \eta^T A \eta \leq a$ is symmetric unimodal. The density function of $\eta \mid \eta^T A \eta \leq a$ is

$$g(x) = \frac{1\{x^T A x \leq a\}}{\text{pr}(\eta^T A \eta \leq a)} (2\pi)^{-K/2} \exp \left(-\frac{x^T x}{2}\right),$$

38
\[
\log g(x) = \begin{cases} 
- \log \{\text{pr} (\eta^T A \eta \leq a) \} - (K/2) \log(2\pi) - x^T x/2, & \text{if } x^T A x \leq a, \\
-\infty, & \text{otherwise}. 
\end{cases}
\]

It is straightforward to show that \( \log g(x) \) is concave. By Lemma 4, \( \eta \mid \eta^T A \eta \leq a \) is symmetric unimodal.

Now we can prove the first part of Proposition 2.

**Proposition 2.** We only give the proof for cluster rerandomization with individual-level covariates, as the proof for cluster rerandomization with cluster-level covariates is similar. By Theorem 2, the asymptotic distribution of \( M^{1/2}(\hat{\tau}_{haj} - \tau) \mid M^{1/2} x \hat{\tau}_{haj, xx} A x \hat{\tau}_{haj, xx} \eta \leq a \) is \( A + B \) with

\[
A = V_{haj, \tau \tau}\left(1 - R_x^2 \right)^{1/2} \epsilon, \quad B = V_{haj, \tau \tau} R_x \mu_x^T \eta \mid \eta^T V_{haj, xx} A x V_{haj, xx} \eta \leq a,
\]

where \( \epsilon, \eta_k (k = 1, \ldots, K) \) are independent standard normal random variables and \( \eta = (\eta_1, \ldots, \eta_K)^T \). \( A \) and \( B \) are independent and symmetric unimodal where the symmetric unimodality of \( B \) follows directly from Lemma 5. Thus, by Lemma 2, \( A + B \) is symmetric unimodal.

Next, we prove the second part of Proposition 2. We need the following two Lemmas. The first one is from Das Gupta et al. (1972, Theorem 2.1).

**Lemma 6.** Let

\[
\Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \sigma_{pp} \end{bmatrix}
\]

be a \( p \times p \) positive definite matrix with \( \Sigma_{11} \) being a \((p - 1) \times (p - 1)\) matrix. Let \( x = (x_1, \cdots, x_p)^T \) be a random vector with density function \( |\Sigma_\lambda|^{-1/2} f \left( x \Sigma_\lambda^{-1} x^T \right) \), where

\[
\Sigma_\lambda = \begin{bmatrix} \Sigma_{11} & \lambda \Sigma_{12} \\ \lambda \Sigma_{21} & \sigma_{pp} \end{bmatrix}, \quad 0 \leq \lambda \leq 1.
\]

If \( E \) is a convex symmetric set in \( R^{p-1} \), then \( \text{pr}\{ (x_1, \cdots, x_{p-1}) \in E, |x_p| \leq h \} \) is non-decreasing in \( \lambda \).

The second one is new.

**Lemma 7.** \( \text{pr}\{ (1 - \rho^2)^{1/2} \epsilon + \rho b^T \eta < c \mid \eta^T A \eta \leq a \} \) is a non-decreasing function of \( \rho \), where \( \epsilon \sim \mathcal{N}(0, 1) \) and \( \eta \sim \mathcal{N}(0, I_K) \) are independent, and \( b \) is a non-random vector satisfying \( b^T b = 1 \).

**Lemma 7.** Simple calculation gives

\[
\left( (1 - \rho^2)^{1/2} \epsilon + \rho b^T \eta \right) \sim \mathcal{N} \left( 0, \begin{bmatrix} 1 & \rho b^T A^{1/2} \\ \rho b^T A^{1/2} & A \end{bmatrix} \right).
\]
By Lemma 6, \( \Pr\{(1 - \rho^2)^{1/2} + \rho b^T \eta < c, \eta^T A \eta \leq a\} \) is a non-decreasing function of \( \rho \). The same is true for the conditional probability \( \Pr\{(1 - \rho^2)^{1/2} + \rho b^T \eta < c | \eta^T A \eta \leq a\} \).

The second half of Proposition 2 follows directly from Lemma 7.

F.8. Proof of Theorem 3

Before proving Theorem 3, we introduce two useful lemmas.

**Lemma 8.** Let \( s_K = \frac{2\pi^{K/2}}{\Gamma(K/2)} \) be the surface of a \( K \)-dimensional unit sphere and \( B(a) = \{ x = (x_1, \ldots, x_K) | \|x\|^2 \leq a^2 \} \). Then

\[
\int_{B(a)} x_1^2 \, dx_1 \cdots dx_K = \frac{1}{(K + 2)K} a^{K+2} s_K.
\]

of Lemma 8. By symmetry,

\[
\int_{B(a)} x_1^2 \, dx_1 \cdots dx_K = K^{-1} \int_{B(a)} (x_1^2 + \cdots + x_K^2) \, dx_1 \cdots dx_K.
\]

Because the integrand on the right-hand side is the radius, the above formula reduces to

\[
\frac{s_K}{K} \int_0^a r^2 r^{K-1} \, dr = \frac{1}{(K + 2)K} a^{K+2} s_K.
\]

**Lemma 9.** Under Conditions 1, 3, and 5, the threshold \( a \) in the cluster rerandomization scheme \( D_x(A_x) \) satisfies

\[
a = (2\pi) \det(V_{haj,x})^{1/K} \det(A_x)^{1/K} \left( \frac{s_K}{K} \right)^{-2/K} \alpha^{2/K} + o(\alpha^{2/K}).
\]

Under Conditions 1, 2, and 4, the threshold \( a \) in the cluster rerandomization scheme \( D_c(A_c) \) satisfies

\[
a = (2\pi) \det(V_{ht,cc})^{1/K} \det(A_c)^{1/K} \left( \frac{s_K}{K} \right)^{-2/K} \alpha^{2/K} + o(\alpha^{2/K}).
\]

of Lemma 9. We only give the proof for cluster rerandomization with individual-level covariates, as the proof for cluster rerandomization with cluster-level covariates is similar. Denote the asymptotic distribution of \( (M^{1/2}(\hat{\tau}_{haj} - \tau), M^{1/2}(\hat{\tau}^T_{haj,x}) ) \) as \( (T_{\infty}, T_{x,\infty}^T) \), where \( T_{x,\infty} \) is a \( K \)-dimensional normal
random vector. By the property of normal random vector, we have

$$T_{x,\infty}^T A_x T_{x,\infty} \sim \sum_{k=1}^{K} \lambda_k \eta_k^2,$$

where $\lambda_1, \ldots, \lambda_K$ are the eigenvalues of $V_{haj,xx}^{1/2} A_x V_{haj,xx}^{1/2}$ and $\eta_1, \ldots, \eta_K$ are independent standard normal random variables. Let $\phi(x)$ be the density function of a standard normal random variable, then

$$\Pr\left(\sum_{k=1}^{K} \lambda_k \eta_k^2 \leq a\right) = \int_{\sum_{k=1}^{K} \lambda_k \eta_k^2 \leq a} \prod_{k=1}^{K} \phi(x_k) \, dx_1 \cdots dx_K$$

$$= (2\pi)^{-K/2} \left(\prod_{k=1}^{K} \lambda_k\right)^{-1/2} \int_{B(a^{1/2})} \exp\left(2^{-1} \sum_{k=1}^{K} x_k^2 / \lambda_k\right) dx_1 \cdots dx_K$$

$$= (2\pi)^{-K/2} \left(\prod_{k=1}^{K} \lambda_k\right)^{-1/2} \int_{B(a^{1/2})} \{1 + O(r^2)\} dx_1 \cdots dx_K.$$

The last line follows from $\min_{k=1,\ldots,K} \lambda_k > 0$ and the Taylor expansion,

$$\exp\left(2^{-1} \sum_{k=1}^{K} x_k^2 / \lambda_k\right) = 1 + O\left(2^{-1} \sum_{k=1}^{K} x_k^2 / \lambda_k\right) = 1 + O(r^2), \quad r^2 = \sum_{k=1}^{K} x_k^2.$$

By the volume formula of a $K$-dimensional ball,

$$\alpha = \Pr\left(\sum_{k=1}^{K} \lambda_k \eta_k^2 \leq a\right) = (2\pi)^{-K/2} \left(\prod_{k=1}^{K} \lambda_k\right)^{-1/2} \frac{s_K}{K} a^{K/2} + O(a^{K/2+1}). \quad (8)$$

As $\lambda_k$, $k = 1, \ldots, K$, are eigenvalues of $V_{haj,xx}^{1/2} A_x V_{haj,xx}^{1/2}$, we have

$$\prod_{k=1}^{K} \lambda_k = \det \left(V_{haj,xx}^{1/2} A_x V_{haj,xx}^{1/2}\right) = \det(V_{haj,xx}) \det(A_x).$$

Substitute into (8) and reorganize the terms, we get the desired result.

$\square$

of Theorem 3. We only give the proof for cluster rerandomization with individual-level covariates, as the proof for cluster rerandomization with cluster-level covariates is similar. As $(T_{\infty}, T_{x,\infty}^T)$ is the
Referring to the proof of Theorem 2,
\[
T_\infty | T_{x,\infty}^t A_x T_{x,\infty} \leq a \sim V_{haj,rr}^{1/2} \{ (1 - R_x^2)^{1/2} \epsilon + R_x \mu_x^T \eta | \eta^T V_{haj,xx} A_x V_{haj,xx}^{1/2} \eta \leq a \},
\]
where
\[
\mu_x^t = (\mu_1, \ldots, \mu_K) = V_{haj,rx}^{-1/2} (V_{haj,rx}^{-1} V_{haj,xx} V_{haj,rx})^{1/2}, \quad \eta = (\eta_1, \ldots, \eta_K)^T,
\]
and \(\epsilon, \eta_1, \ldots, \eta_K\) are independent standard normal random variables.

We perform the eigenvalue decomposition as follows: \(V_{haj,xx}^{1/2} A_x V_{haj,xx}^{1/2} = P_x \Lambda_x P_x^T\), where \(\Lambda_x = \text{diag}(\lambda_1, \ldots, \lambda_K)\). Then \(\mu_x^T \eta| \eta^T V_{haj,xx}^{1/2} A_x V_{haj,xx}^{1/2} \eta \leq a\) has the same distribution as \(\mu_x^T P_x \eta| \eta^T \Lambda_x \eta \leq a\).

First, we derive the asymptotic variance of \(\sum_{k=1}^K \zeta_k \eta_k^2 \leq a\) with \(\min_{1 \leq k \leq K} \lambda_k > 0\). Note that

\[
\text{var} \left( \eta_1 \bigg| \sum_{k=1}^K \lambda_k \eta_k^2 \leq a \right) = \alpha^{-1} \int_{\sum_{k=1}^K \lambda_k \eta_k^2 \leq a} x_1^2 \prod_{k=1}^K \phi(x_k) \, dx_1 \cdots dx_K, \quad \text{where} \quad \alpha = \text{pr} \left( \sum_{k=1}^K \lambda_k \eta_k^2 \leq a \right),
\]
and

\[
\int_{\sum_{k=1}^K \lambda_k \eta_k^2 \leq a} x_1^2 \prod_{k=1}^K \phi(x_k) \, dx_1 \cdots dx_K = (2\pi)^{-K/2} \left( \prod_{k=1}^K \lambda_k \right)^{-1/2} \lambda_1^{-1} \int_{B(a^{1/2})} \{ x_1^2 + O(r^4) \} \, dx_1 \cdots dx_K.
\]

The above approximation follows from the Taylor expansion,

\[
x_1^2 \exp \left( 2^{-1} \sum_{k=1}^K x_k^2 / \lambda_k \right) = x_1^2 + O \left( 2^{-1} x_1^2 \sum_{k=1}^K x_k^2 / \lambda_k \right) = x_1^2 + O(r^4), \quad \text{where} \quad r^2 = \sum_{k=1}^K x_k^2.
\]

By Lemma 8,

\[
\int_{\sum_{k=1}^K \lambda_k \eta_k^2 \leq a} x_1^2 \prod_{k=1}^K \phi(x_k) \, dx_1 \cdots dx_K = (2\pi)^{-K/2} \left( \prod_{k=1}^K \lambda_k \right)^{-1/2} \lambda_1^{-1} \frac{1}{K+2} a^{K/2+1} s_K + O(a^{K/2+2}).
\]

Substitute \(a\) with the result of Lemma 9, we have

\[
\text{var} \left( \eta_1 \bigg| \sum_{k=1}^K \lambda_k \eta_k^2 \leq a \right) = p_K \lambda_1^{-1} \left( \prod_{k=1}^K \lambda_k \right)^{1/K} \alpha^{2/K} + o(\alpha^{2/K}).
\]
Similarly, for \( k = 1, \ldots, K \),

\[
\text{var}\left( \eta_k \mid \sum_{k=1}^{K} \lambda_k \eta_k^2 \leq a \right) = p_K \lambda_k^{-1} \left( \prod_{k=1}^{K} \lambda_k \right)^{1/K} \alpha^2/K + o(\alpha^2/K).
\]

Moreover, for \( m \neq n \), \( \eta_m \) and \( \eta_n \) are conditional uncorrelated, then

\[
E\left( \eta_m \eta_n \mid \sum_{k=1}^{K} \lambda_k \eta_k^2 \leq a \right) = E\left\{ \eta_m E\left( \eta_n \mid \eta_m, \sum_{k=1}^{K} \lambda_k \eta_k^2 \leq a \right) \mid \sum_{k=1}^{K} \lambda_k \eta_k^2 \leq a \right\} = E\left( \eta_m \times 0 \mid \sum_{k=1}^{K} \lambda_k \eta_k^2 \leq a \right) = 0.
\]

The last line follows from the fact that given \( \eta_m \) and a symmetric ellipsoidal acceptance region, the conditional distribution of \( \eta_n \) is symmetric. Therefore,

\[
\text{var}\left( \sum_{k=1}^{K} \zeta_k \eta_k \mid \sum_{k=1}^{K} \lambda_k \eta_k^2 \leq a \right) = \sum_{k=1}^{K} \zeta_k^2 \text{var}\left( \eta_k \mid \sum_{k=1}^{K} \lambda_k \eta_k^2 \leq a \right) = p_K \left( \sum_{k=1}^{K} \zeta_k^2 \right) \left( \prod_{k=1}^{K} \lambda_k \right)^{1/K} \alpha^2/K + o(\alpha^2/K).
\]

Note that

\[
\left( \prod_{k=1}^{K} \lambda_k \right)^{1/K} = \det(V_{haj,xx})^{1/K} \det(A_x)^{1/K}, \quad \text{diag}(\lambda_1, \ldots, \lambda_K) = P_x V_{haj,xx}^{1/2} A_x V_{xx}^{1/2} P_x,
\]

\[
(\zeta_1, \ldots, \zeta_K) = V_{haj,xx}^{-1/2} P_x \left( (V_{haj,xx}^{-1} V_{haj,xx} A_x V_{xx}^{-1})^{1/2} \right).
\]

Thus,

\[
\sum_{k=1}^{K} \frac{\zeta_k^2}{\lambda_k} = V_{haj,xx}^{-1/2} P_x \left( (V_{haj,xx}^{-1} V_{haj,xx} A_x V_{xx}^{-1} P_x)^{-1} P_x V_{haj,xx}^{-1/2} V_{haj,xx} A_x V_{xx}^{-1} V_{haj,xx} V_{haj,xx}^{-1} \right) = V_{haj,xx}^{-1} A_x^{-1} V_{haj,xx}^{-1} V_{haj,xx} V_{haj,xx}^{-1} (V_{haj,xx}^{-1} V_{haj,xx} V_{haj,xx}^{-1}).
\]

Therefore,

\[
\text{var}(T_{\infty}^{T} T_{x,\infty}^{T} A_x T_{x,\infty} \leq a) = V_{haj,\tau \tau} \left\{ (1 - R_{x}^2) + R_{x}^2 \text{var}(\mu_x^{T} P_x \eta \mid \eta^{T} A_x \eta \leq a) \right\} = V_{haj,\tau \tau} \left\{ (1 - R_{x}^2) + R_{x}^2 p_K \nu_x(A_x) \alpha^{2/K} + o(\alpha^{2/K}) \right\}.
\]
F.9. Proof of Theorem 4

of Theorem 4. It is convenient to fix \( \prod_{k=1}^{K} w_k = 1 \) and minimize the term that is related to \( w_k \) for \( k = 1, \ldots, K \). Denote \( (b_1, \ldots, b_K)^T = V_{haj,xx} V_{haj,x\tau} \). We only need to minimize

\[
V_{haj,\tau x}^{-1} V_{haj,xx} A_x^{-1} V_{haj,xx} V_{haj,x\tau} = \sum_{k=1}^{K} b_k^2 w_k^{-1}.
\]

Using the inequality of arithmetic and geometric means, we have

\[
\sum_{k=1}^{K} b_k^2 w_k^{-1} \geq K \left( \prod_{k=1}^{K} b_k^2 w_k^{-1} \right)^{1/K} = K \left( \prod_{k=1}^{K} w_k^2 \right)^{1/K}.
\]

The equality holds if and only if

\[
b_1^2 = \cdots = b_K^2 = w_K^2,
\]

which implies \( w_k = c_0 b_k^2 = c_0 (V_{haj,\tau x} V_{haj,xx}^{-1} \xi_k)^2 \) for some constant \( c_0 > 0 \). Then within all positive diagonal matrix, \( \nu_x(A_x) \) reach its minimum at \( A_x^{opt} = \text{diag}(w_1, \ldots, w_K) \) with \( w_k = c_0 (V_{haj,\tau x} V_{haj,xx}^{-1} \xi_k)^2 \) for some constant \( c_0 > 0 \). The proof for \( \nu_c(A_c) \) is similar.

\( \square \)

F.10. Proof of Corollary 2

of Corollary 2. It suffices to show that the optimal weights \( w_k = c_0 R^2_{x_k} / V_{haj,x_k x_k} \), \( k = 1, \ldots, K \), for some constant \( c_0 > 0 \). Denote \( V_{haj,xx} = \text{diag}(V_{haj,x_1 x_1}, \ldots, V_{haj,x_K x_K}) \). Recall that \( \sum_{k=1}^{K} R^2_{x_k} = R_x^2 \) with

\[
R^2_{x_k} = V_{haj,\tau x_k}^2 / (V_{haj,\tau \tau} V_{haj,x_k x_k}).
\]

Then

\[
V_{haj,\tau x} V_{haj,xx}^{-1} = (V_{haj,\tau x_1} V_{haj,xx}^{-1}, \ldots, V_{haj,\tau x_K} V_{haj,xx}^{-1})
\]

\[
= (R_{x_1} V_{haj,\tau \tau}^{1/2} V_{haj,x_1 x_1}^{1/2}, \ldots, R_{x_K} V_{haj,\tau \tau}^{1/2} V_{haj,x_K x_K}^{1/2}).
\]

We minimize the term related to \( A_x \) in \( \nu_x(A_x) \). Note that

\[
V_{haj,\tau x} V_{haj,xx}^{-1} A_x^{-1} V_{haj,xx} V_{haj,x\tau} \det(A_x)^{1/K} \det(V_{haj,xx})^{1/K}
\]

\[
= \sum_{k=1}^{K} R^2_{x_k} V_{haj,\tau \tau} / (V_{haj,x_k x_k} w_k) \left( \prod_{k=1}^{K} w_k V_{haj,x_k x_k} \right)^{1/K}.
\]
\[ \geq KV_{haj,\tau\tau} \left( \prod_{k=1}^{K} R_{X_k}^2 \right)^{1/K}, \]

where the last inequality follows from the inequality of arithmetic and geometric means. Therefore,

\[ \nu_x(A_x) \geq KV_{haj,\tau\tau} \left( \prod_{k=1}^{K} R_{x_k}^2 \right)^{1/K} / (V_{haj,xx}^{-1} V_{haj,x\tau}) = KV_{haj,\tau\tau} \left( \prod_{k=1}^{K} R_{X_k}^2 \right)^{1/K} / R_x^2. \]

The equality holds if and only if

\[ R_{x_1}^2 / (V_{haj,x_1x_1} w_1) = \cdots = R_{x_K}^2 / (V_{haj,x_Kx_K} w_K), \]

which implies \( w_k = c_0 R_{x_k}^2 / V_{haj,x_kx_k} \) for some constant \( c_0 > 0 \).

\[ \square \]

**F.11. Proof of Corollary 3**

of Corollary 3. By Theorem 3 of Li et al. (2018),

\[ M^{1/2}(\hat{\tau}_{haj} - \tau) \mid \mathcal{M}_{[1]}, \ldots, \mathcal{M}_{[L]} \overset{d}{\to} V_{haj,\tau\tau}^{1/2} \left\{ (1 - R_x^2)^{1/2} \epsilon + \sum_{l=1}^{L} R_{x[l]} L_{K_l,a[l]} \right\}, \]

where \( \epsilon \) is a standard normal random variable, and \( \epsilon, L_{K_l,a[l]}, \ldots, L_{K_l,a[l]} \) are jointly independent. Applying our Theorem 1 and 3 with \( K = K_l, \alpha = \alpha[l], V_{haj,\tau\tau} = 1, A_x = V_{haj,xx}^{-1}, \) and \( R_x^2 = 1, \) we have

\[ \var(L_{K_l,a[l]} = p_K \alpha^{2/K_l} + o(\alpha^{2/K_l}). \]

Therefore,

\[ \var_a \{ M^{1/2}(\hat{\tau}_{haj} - \tau) \mid \mathcal{M}_{[1]}, \ldots, \mathcal{M}_{[L]} \} = V_{haj,\tau\tau} \left\{ (1 - R_x^2) + \sum_{l=1}^{L} p_K R_{x[l]}^2 \alpha^{2/K_l} + o(\alpha^{2/K_l}) \right\}. \]

The leading term in \( \var_a \{ M^{1/2}(\hat{\tau}_{haj} - \tau) \mid \mathcal{M}_{[1]}, \ldots, \mathcal{M}_{[L]} \} \) has the following lower bound:

\[ V_{haj,\tau\tau} \left\{ (1 - R_x^2) + \sum_{l=1}^{L} p_K R_{x[l]}^2 \alpha^{2/K_l} \right\} \geq V_{haj,\tau\tau} \left[ (1 - R_x^2) + K \left\{ \prod_{l=1}^{L} \left( \frac{p_K R_{x[l]}^2 \alpha^{2/K_l}}{K_l} \right) K_l \right\}^{1/K} \right] = V_{haj,\tau\tau} \left[ (1 - R_x^2) + K \left\{ \prod_{l=1}^{L} \left( \frac{p_K R_{x[l]}^2 \alpha^{2/K_l}}{K_l} \right) K_l \right\}^{1/K} \right]. \]
The equality holds if and only if
\[ p_{K_1} R^2_{x[1]} \alpha_{[1]}^{2/K_1} / K_1 = \cdots = p_{K_L} R^2_{x[L]} \alpha_{[L]}^{2/K_L} / K_L, \]
which implies that for some constant \( c_0 > 0 \),
\[ \alpha_{[l]} = \left( c_0 R^2_{x[l]} p_{K_l} / K_l \right)^{-K_l/2} \quad (l = 1, \ldots, L). \]

\[ \square \]

F.12. Proof of Theorem 5

To prove Theorem 5, we need Lemma 10 below.

Lemma 10.
\[ p_K = \frac{2\pi}{K + 2} \left\{ \frac{2\pi^{K/2}}{K\Gamma(K/2)} \right\}^{-2/K} \quad (K = 1, 2, \ldots) \]
is decreasing in \( K \).

of Lemma 10. First,
\[ \log p_K = \log(2\pi) - \log(K + 2) - 2\{\log(2/K) + (K/2) \log \pi - \log \Gamma(K/2)\}/K \]
\[ = \log(2\pi) - \log\{\pi(K + 2)\} + (2/K) \log \Gamma(K/2 + 1). \]

Let \( x = K/2 \) and we consider the function
\[ f(x) = -\log\{2\pi(x + 1)\} + (1/x) \log \Gamma(x + 1). \]
It suffices to prove that \( f(x) \) is decreasing in \( x \) for \( x \geq 0 \). Simple calculation gives
\[ f'(x) = -1/(x + 1) + \psi(x + 1)/x - (1/x^2) \log \Gamma(x + 1), \]
where \( \psi(x) = \text{d} \log \Gamma(x)/\text{d}x \) is the Digamma function. Let
\[ g(x) = x^2 f'(x) = -x^2/(x + 1) + x\psi(x + 1) - \log \Gamma(x + 1), \]
We only need to show that \( g(x) \leq 0 \) for \( x \geq 0 \). In fact,
\[ g'(x) = -x(x + 2)/(x + 1)^2 + \psi(x + 1) + x\psi'(x + 1) - \psi(x + 1) \]
\[ = -x(x + 2)/(x + 1)^2 + x\psi'(x + 1). \]
By Alzer (1997, Theorem 1), \( \log x - \psi(x) - 1/x \) is an increasing function for \( x > 0 \). Thus, we have
\[ 1/x + 1/x^2 - \psi'(x) \text{ is positive for } x > 0, \]
which implies that \( \psi'(x + 1) < (x + 2)/(x + 1)^2 \) for \( x \geq 0 \).
Therefore, \( g'(x) \leq 0 \) and \( g(x) \leq g(0) = 0 \) for \( x \geq 0 \).

of Theorem 5. By Lemma 10, \( p_K \) is decreasing in \( K \). Therefore,
\[
\sum_{l=1}^{L} R_{x[l]}^2 p_{K_i} \alpha^{2/K} \geq \left\{ \prod_{l=1}^{L} \left( \frac{p_{K_i} R_{x[l]}^2}{K_l} \right)^{K_l} \right\}^{1/K} \alpha^{2/K} \geq p_K \left\{ \prod_{l=1}^{L} \left( \frac{R_{x[l]}^2}{K_l} \right)^{K_l} \right\}^{1/K} \alpha^{2/K} \]
\[
\geq K p_K \left( \prod_{k=1}^{K} R_{x_k}^2 \right)^{1/K} \alpha^{2/K}.
\]
The last inequality follows from the inequality of geometric and arithmetic means, and
\[
R_{x[l]}^2 = \sum_{k \in [l]} R_{x_k}^2, \quad \left( \frac{R_{x[l]}^2}{K_l} \right)^{K_l} \geq \prod_{k \in [l]} R_{x_k}^2.
\]

F.13. Proof of Theorem 7

Define
\[
\tilde{\tau}_{ht}^{\text{adj}} = M^{-1} \sum_{i=1}^{M} Z_i \{ \tilde{Y}_i(1) - u^T \beta(1) \} - M_0^{-1} \sum_{i=1}^{M} (1 - Z_i) \{ \tilde{Y}_i(0) - v^T \beta(0) \},
\]

and
\[
\tilde{\tau}_{haj}^{\text{adj}} = N^{-1} \sum_{i,j} Z_{ij} \{ Y_{ij}(1) - w^T \beta_w(1) \} - N_0^{-1} \sum_{i,j} (1 - Z_i) \{ Y_{ij}(0) - w^T \beta_w(0) \}.
\]

Lemma 11 below shows that \( \tilde{\tau}_{ht}^{\text{adj}} \) and \( \tilde{\tau}_{haj}^{\text{adj}} \) have the same asymptotic distributions under cluster rerandomization. The same is true for \( \hat{\tau}_{ht}^{\text{adj}} \) and \( \hat{\tau}_{haj}^{\text{adj}} \).

Lemma 11. If Conditions 1, 2, 4, 6 hold, then
\[
M^{1/2}(\hat{\tau}_{ht}^{\text{adj}} - \tilde{\tau}_{ht}^{\text{adj}})|D_c(A_c) = o_p(1).
\]

If Condition 1, 3, 5, 7 hold, then
\[
M^{1/2}(\hat{\tau}_{haj}^{\text{adj}} - \tilde{\tau}_{haj}^{\text{adj}})|D_x(A_x) = o_p(1).
\]

of Lemma 11. By Lemma A7 of Su and Ding (2021), \( M^{1/2}(\hat{\tau}_{ht}^{\text{adj}} - \tilde{\tau}_{ht}^{\text{adj}}) = o_p(1) \), which implies that, for any \( \delta > 0 \),
\[
\Pr \left\{ M^{1/2}(\hat{\tau}_{ht}^{\text{adj}} - \tilde{\tau}_{ht}^{\text{adj}}) > \delta \right\} = o(1).
\]

47
Proposition 1 implies that
\[
\lim_{M \to \infty} \Pr\{D_c(A_c)\} > 0.
\]
Therefore,
\[
\Pr \{|M^{1/2}(\hat{\tau}_{\text{ht}} - \hat{\tau}_{\text{adj}})| > \delta \mid D_c(A_c)\} \leq \Pr \{|M^{1/2}(\hat{\tau}_{\text{ht}} - \hat{\tau}_{\text{adj}})| > \delta\} / \Pr\{D_c(A_c)\} = o(1),
\]
which implies that
\[
M^{1/2}(\hat{\tau}_{\text{ht}} - \hat{\tau}_{\text{adj}}) \mid D_c(A_c) = o_p(1).
\]
Similarly, we can prove the second part of Lemma 11.

F.14. Proof of Corollary 4

of Corollary 4. By Lemma 11, \(M^{1/2}(\hat{\tau}_{\text{ht}} - \tau) \sim M^{1/2}(\hat{\tau}_{\text{ht}} - \tau)\) under cluster rerandomization. When \(c_i = Bv_i\), \(M^{1/2}(\hat{\tau}_{\text{ht}} - \tau)\) is uncorrelated with \(M^{1/2}\hat{\tau}_{\text{ht},c}\). Applying Theorem 2, the conclusion follows immediately.

F.15. Proof of Theorem 8

of Theorem 8. By Theorems 2 and 4 of Su and Ding (2021), we have
\[
M\hat{V}_{LZ} \overset{p}{\to} e^{-1} \text{var}\{\hat{\varepsilon}_{\text{adj}}(1)\} + e^{-1} \text{var}\{\hat{\varepsilon}_{\text{adj}}(0)\} \geq V_{\text{adj},ht,\tau},
\]
\[
M\hat{V}_{HW} \overset{p}{\to} e^{-1} \text{var}\{\hat{\varepsilon}_{\text{adj}}(1)\} + e^{-1} \text{var}\{\hat{\varepsilon}_{\text{adj}}(0)\} \geq V_{\text{adj},ht,\tau}.
\]
As \(\lim_{M \to \infty} \Pr\{D_*(A_*)\} > 0\), for \(* = x, c\), similar to the proof of Lemma 11, we have
\[
M\hat{V}_{LZ} - V_{\text{adj},ht,\tau} \mid D_x(A_x) \geq_p 0, \quad M\hat{V}_{HW} - V_{\text{adj},ht,\tau} \mid D_c(A_c) \geq_p 0.
\]

F.16. Proof of Theorem 6

of Theorem 6. When \(v_i = c_i\) and \(x_{ij} = w_{ij}\), we have \(R_{\text{adj}} = 0, R_{x}^{\text{adj}} \geq 0\), and
\[
V_{\text{adj},ht,\tau}\{1 - (R_{\text{adj}})^2\} = V_{\text{adj},ht,\tau}(1 - R_x^2), \quad V_{\text{adj},ht,\tau}\{1 - (R_{\text{adj}})^2\} = V_{\text{ht,ht,\tau}}(1 - R_c^2).
\]
By Theorem 7, we have
\[
M^{1/2}(\hat{\tau}_{ht}^\text{adj} - \tau) \mid \mathcal{D}_c(A_c) \sim (V_{ht,\tau})^{1/2}(1 - R_c^2)\epsilon,
\]
and
\[
M^{1/2}(\hat{\tau}_{haj}^\text{adj} - \tau) \mid \mathcal{D}_x(A_x) \sim (V_{haj,\tau})^{1/2}\left\{1 - (R_x^\text{adj})^2\right\}^{1/2} \epsilon + R_x^\text{adj} \mu_x^T \eta \mid \eta^T V_{haj,xx} A_x V_{haj,xx}^{1/2} \eta \leq a\right].
\]
Moreover, by Theorem 8, \(M\hat{\tau}_{lz}^\text{adj}\) and \(M\hat{\tau}_{lw}^\text{adj}\) are conservative estimators of \(V_{haj,\tau}\) and \(V_{ht,\tau}\), respectively. The conservativeness of the Wald-type confidence intervals follows from the conservativeness of \(M\hat{\tau}_{lz}^\text{adj}\) and \(M\hat{\tau}_{lw}^\text{adj}\) and Proposition 2. Therefore, (i) and (ii) hold.

When \(c_i = (n_i, \tilde{x}_i^T)^T\), Corollary 1 implies that
\[
V_{haj,\tau}\left\{1 - (R_x^\text{adj})^2\right\} \geq V_{ht,\tau}\left\{1 - (R_c^\text{adj})^2\right\}.
\]
Thus, the normal component of the asymptotic distribution of the cluster-level regression adjustment is more concentrated than that of the individual-level regression adjustment. Moreover, the asymptotic distribution of the individual-level regression adjustment has a truncated normal component while the cluster-level regression adjustment does not. Thus, (iii) holds.

\[\square\]

**F.17. Proof of Corollary 5**

*of Corollary 5.* By Lemma 11, \(M^{1/2}(\hat{\tau}_{ht}^\text{adj} - \tau) \sim M^{1/2}(\tilde{\tau}_{ht}^\text{adj} - \tau)\) under cluster rerandomization. By Proposition 1 of Li and Ding (2020),
\[
\tilde{\tau}_{ht}^\text{adj} - \tau = \hat{\tau}_{ht} - \tau - \text{cov}(\hat{\tau}_{ht}, \hat{\tau}_{ht,v})\{\text{cov}(\hat{\tau}_{ht,v})\}^{-1}\hat{\tau}_{ht,v}.
\]
Since \(v_i = Bc_i\), then \(\hat{\tau}_{ht,v} = B\tilde{\tau}_{ht,c}\). As \(M\text{var}_a(\tilde{\tau}_{ht,c}) = V_{ht,cc}\) and \(M\text{cov}_a(\tilde{\tau}_{ht}, \tilde{\tau}_{ht,c}) = V_{ht,\tau c}\), substituting them into the above equation, we have
\[
\hat{\tau}_{ht}^\text{adj} - \tau \sim \hat{\tau}_{ht} - \tau - V_{ht,\tau c} B^T (BV_{ht,cc} B^T)^{-1}B\tilde{\tau}_{ht,c} = \hat{\tau}_{ht} - \tau - V_{ht,\tau c} V_{ht,cc}^{1/2}\tilde{\tau}_{ht,c} + V_{ht,\tau c} V_{ht,cc}^{1/2}B^T (BV_{ht,cc} B^T)^{-1}B\tilde{\tau}_{ht,c} = \{\hat{\tau}_{ht} - \tau - V_{ht,\tau c} V_{ht,cc}^{1/2}\tilde{\tau}_{ht,c}\} + V_{ht,\tau c} V_{ht,cc}^{1/2}\left\{I_K - V_{ht,cc}^{1/2} B^T (BV_{ht,cc} B^T)^{-1} B V_{ht,cc}^{1/2}\right\} V_{ht,cc}^{1/2}\tilde{\tau}_{ht,c}.
\]
Note that
\[
\text{var}_a\{M^{1/2}(\hat{\tau}_{ht} - \tau - V_{ht,\tau c} V_{ht,cc}^{1/2}\tilde{\tau}_{ht,c})\} = (1 - R_c^2) V_{ht,\tau \tau},
\]
\[
\text{cov}_a\{M^{1/2}(\hat{\tau}_{ht} - \tau - V_{ht,\tau c} V_{ht,cc}^{1/2}\tilde{\tau}_{ht,c}), M^{1/2}\hat{\tau}_{ht,c}\} = 0.
\]
49
Therefore, by Proposition 5, we have
\[
M^{1/2}(\tilde{\tau}_{ht} - \tau) | D_c(A_c) \sim V_{ht,\tau}^{1/2} (1 - R_c^2)^{1/2} \epsilon + V_{ht,\tau}^{-1/2} \left\{ I_K - V_{ht,cc}^{-1/2} (BV_{ht,cc} B^\top)^{-1} B V_{ht,cc}^{1/2} \right\} \eta \mid \eta^\top V_{ht,cc}^{1/2} A_c V_{ht,cc}^{1/2} \eta \leq a,
\]
which concludes the proof.

\[ \square \]

F.18. Proof of Corollary 6

of Corollary 6. Let \( \mu_c^T = (\mu_1, \ldots, \mu_K) = V_{ht,\tau}^{-1/2} / \{V_{ht,cc} V_{ht,cc}^{-1} V_{ht,cc}\}^{1/2} \). It suffices to compare the variances of
\[
(V_{ht,\tau})^{1/2} \{ (1 - R_c^2)^{1/2} \epsilon + R_c \mu_c^T H \eta \mid \eta^\top V_{ht,cc}^{1/2} A_c V_{ht,cc}^{1/2} \eta \leq a \}
\]
and
\[
(V_{ht,\tau})^{1/2} \{ (1 - R_c^2)^{1/2} \epsilon + R_c \mu_c^T \eta \mid \eta^\top V_{ht,cc}^{1/2} A_c V_{ht,cc}^{1/2} \eta \leq a \},
\]
where
\[
H = \begin{bmatrix} 0 & 0 \\ 0 & I_{(K-J) \times (K-J)} \end{bmatrix}.
\]
Due to the conditional uncorrelatedness of \( \eta_m \) and \( \eta_n \) for \( m \neq n \), the difference between the variances of the above two distributions is equal to
\[
V_{ht,\tau} R_c^2 \sum_{k=1}^J \mu_k^2 \text{var}(\eta_k \mid \eta^\top V_{ht,cc}^{1/2} A_c V_{ht,cc}^{1/2} \eta \leq a) \geq 0,
\]
which concludes the proof.

\[ \square \]

F.19. Proof of Theorem 9

Let \( \hat{\beta}_v(1) \) and \( \hat{\beta}_v(0) \) be the coefficients of \( v \) in the least squares fit of \( \tilde{Y}_1 \) on \( (1, v_1) \) under treatment and control arms, respectively. Let \( \hat{\beta}_w(1) \) and \( \hat{\beta}_w(0) \) be the coefficients of \( w \) in the least squares fit of \( Y_{ij} \) on \( (1, w_{ij}) \) under treatment and control arms, respectively. Lemmas 12–14 below show the consistency of the ordinary least squares coefficients, sample means, variances, and covariances under cluster rerandomization. Their unconditional versions can be found in Su and Ding (2021) and Li et al. (2020). The proof is similar to that of Lemma 11, so we omit. Let \( \bar{Y}_z \) be the sample mean of \( Y_{ij} \) under treatment arm \( z \).

Lemma 12. If Conditions 1, 2, 4, 6 hold, then
\[
\hat{\beta}_v(z) - \beta_v(z) \mid D_c(A_c) \overset{p}{\to} 0.
\]
If Condition 1, 3, 5, 7 hold, then

\[
\hat{\beta}_w(z) - \beta_w(z) \mid D_x(A_x) \xrightarrow{p} 0.
\]

**Lemma 13.** If Condition 1, 3, 5, 7 hold, then

\[
\hat{Y}_z - \hat{Y}(z) \mid D_x(A_x) \xrightarrow{p} 0.
\]

**Lemma 14.** If Conditions 1, 2, 4, 6 hold, then

\[
\text{var}_\tau \{\hat{Y}(z)\} - \text{var}_\tau \{\hat{Y}(z)\} \mid D_c(A_x) \xrightarrow{p} 0, \quad \text{cov}_\tau \{\hat{Y}, \hat{Y}\} \mid D_c(A_x) \xrightarrow{p} 0,
\]

\[
\text{cov}_\tau \{\hat{Y}, \hat{Y}\} \mid D_c(A_x) \xrightarrow{p} 0, \quad \text{cov}_\tau \{\hat{Y}, \hat{Y}\} \mid D_c(A_x) \xrightarrow{p} 0,
\]

By the property of projection, Lemma 15 below holds.

**Lemma 15.**

\[
\text{cov}_\tau \{\hat{Y}(1) - \hat{Y}(0), \hat{G}\} \{\text{cov}_\tau (\hat{G})\} - 1 \text{cov}_\tau \{\hat{G}, \hat{Y}(1) - \hat{Y}(0)\} \leq \text{var}_\tau \{\hat{Y}(1) - \hat{Y}(0)\},
\]

\[
\text{cov}_\tau \{\hat{Y}(1) - \hat{Y}(0), C\} \{\text{cov}_\tau (C)\} - 1 \text{cov}_\tau \{C, \hat{Y}(1) - \hat{Y}(0)\} \leq \text{var}_\tau \{\hat{Y}(1) - \hat{Y}(0)\}.
\]

**of Theorem 9.** Recall that

\[
(\hat{R}^*_c)^2 = [e^{-1}_1 \text{var}_\tau \{\hat{Y}(1) \mid C\} + e^{-1}_0 \text{var}_\tau \{\hat{Y}(0) \mid C\} - \text{var}_\tau \{\hat{Y}(1) - \hat{Y}(0) \mid C\}] / \hat{V}_{ht, \tau}^{rad},
\]

\[
(\hat{R}^{\text{rad}}_c)^2 = [e^{-1}_1 \text{var}_\tau \{\hat{Y}(1) \mid C\} + e^{-1}_0 \text{var}_\tau \{\hat{Y}(0) \mid C\} - \text{var}_\tau \{\hat{Y}(1) - \hat{Y}(0) \mid C\}] / \hat{V}_{haj, \tau}^{rad}.
\]

First, we prove that the denominators, \(\hat{V}_{ht, \tau}^{rad}\) and \(\hat{V}_{haj, \tau}^{rad}\), are conservative. Recall that

\[
\hat{V}_{haj, \tau}^{rad} = e^{-1}_1 \text{var}_\tau \{\hat{Y}(1)\} + e^{-1}_0 \text{var}_\tau \{\hat{Y}(0)\} - \text{var}_\tau \{\hat{Y}(1) - \hat{Y}(0) \mid \hat{G}\},
\]

\[
\hat{V}_{ht, \tau}^{rad} = e^{-1}_1 \text{var}_\tau \{\hat{Y}(1)\} + e^{-1}_0 \text{var}_\tau \{\hat{Y}(0)\} - \text{var}_\tau \{\hat{Y}(1) - \hat{Y}(0) \mid C\}.
\]
Note that
\[
\text{v} \text{ar}_f(\tilde{Y}^{\text{adj}}(z)) = \text{v} \text{ar}_{f,z}(\tilde{Y}(z) - \hat{\beta}^T_v(z)V),
\]
\[
\text{v} \text{ar}_f(\tilde{e}^{\text{adj}}(z)) = \text{v} \text{ar}_{f,z}(\tilde{Y}(z) - \tilde{\omega}\tilde{Y}_z - \tilde{\beta}^T_v(z)\tilde{W}) = \text{v} \text{ar}_{f,z}[\tilde{e}(z) - \tilde{\omega}(Y_z - \tilde{Y}(z)) - \tilde{\beta}^T_v(z)\tilde{W}].
\]

Therefore, by Lemmas 12–14, we have
\[
\text{v} \text{ar}_f(\tilde{Y}^{\text{adj}}(z)) \mid \mathcal{D}_c(A_c) \overset{p}{\rightarrow} \text{var}_f(\tilde{Y}^{\text{adj}}(z)), \quad \text{v} \text{ar}_f(\tilde{e}^{\text{adj}}(z)) \mid \mathcal{D}_x(A_x) \overset{p}{\rightarrow} \text{var}_f(\tilde{e}^{\text{adj}}(z)).
\]

Recall that
\[
\text{v} \text{ar}_f(\tilde{e}^{\text{adj}}(1) - \tilde{e}^{\text{adj}}(0) \mid \tilde{G}) = \{c \text{ov}_{f,1}(\tilde{U}, \tilde{G}) - c \text{ov}_{f,0}(\tilde{U}, \tilde{G})\}^{-1}\{c \text{ov}_{f,1}(\tilde{G}, \tilde{U}) - c \text{ov}_{f,0}(\tilde{G}, \tilde{U})\}.
\]

As \(\tilde{G}\) is the union of \(\tilde{X}\) and \(\tilde{W}\),
\[
\text{cov}_{f,z}(\tilde{U}, \tilde{G}) \mid \mathcal{D}_x(A_x) \overset{p}{\rightarrow} \text{cov}_f(\tilde{e}^{\text{adj}}(z), \tilde{G}),
\]
which implies that
\[
\text{v} \text{ar}_f(\tilde{e}^{\text{adj}}(1) - \tilde{e}^{\text{adj}}(0) \mid \tilde{G}) \mid \mathcal{D}_x(A_x) \overset{p}{\rightarrow} \text{cov}_f(\tilde{e}^{\text{adj}}(1) - \tilde{e}^{\text{adj}}(0), \tilde{G})\{\text{cov}_f(\tilde{G})\}^{-1}\text{cov}_f(\tilde{G}, \tilde{e}^{\text{adj}}(1) - \tilde{e}^{\text{adj}}(0)).
\]

By Lemma 15, the right-hand side is smaller than or equal to \(\text{var}_f(\tilde{e}^{\text{adj}}(1) - \tilde{e}^{\text{adj}}(0))\). Similarly, the probability limit of \(\text{v} \text{ar}_f(\tilde{Y}^{\text{adj}}(1) - \tilde{Y}^{\text{adj}}(0) \mid C)\) is smaller than or equal to \(\text{var}_f(\tilde{Y}^{\text{adj}}(1) - \tilde{Y}^{\text{adj}}(0))\).

Therefore, \(\tilde{V}_{\text{haj},\tau\tau}^{\text{adj}}\) is a conservative estimator of \(V_{\text{haj},\tau\tau}^{\text{adj}}\), and \(\tilde{V}_{\text{ht},\tau\tau}^{\text{adj}}\) is a conservative estimator of \(V_{\text{ht},\tau\tau}^{\text{adj}}\).

Second, we prove that the estimated numerators for the multiple correlation coefficients are consistent. Note that
\[
\text{cov}_f(\tilde{Y}^{\text{adj}}(z), C) = \text{cov}_{f,z}\{\tilde{Y}(z) - \hat{\beta}^T_v(z)V, C\},
\]
\[
\text{cov}_f(\tilde{e}^{\text{adj}}(z), \tilde{X}) = \text{cov}_{f,z}\{\tilde{e}(z) - \tilde{\omega}\{\tilde{Y}_z - \tilde{Y}(z)\} - \tilde{\beta}^T_v(z)\tilde{W}, \tilde{X}\} = \text{cov}_{f,z}\{\tilde{e}(z) - \tilde{\omega}\{\tilde{Y}_z - \tilde{Y}(z)\} - \tilde{\beta}^T_v(z)\tilde{W}, \tilde{X}\}.
\]

Therefore, by Lemmas 12–14, we have
\[
\text{cov}_f(\tilde{Y}^{\text{adj}}(z), C) \mid \mathcal{D}_c(A_c) \overset{p}{\rightarrow} \text{cov}_f(\tilde{Y}^{\text{adj}}(z), C), \quad \text{cov}_f(\tilde{e}^{\text{adj}}(z), \tilde{X}) \mid \mathcal{D}_x(A_x) \overset{p}{\rightarrow} \text{cov}_f(\tilde{e}^{\text{adj}}(z), \tilde{X}).
\]

Together with the following property by Lemma 14,
\[
\text{cov}_{f,z}(\tilde{X}) - \text{cov}_f(\tilde{X}) \mid \mathcal{D}_x(A_x) \overset{p}{\rightarrow} 0, \quad \text{cov}_{f,z}(C) - \text{cov}_f(C) \mid \mathcal{D}_c(A_c) \overset{p}{\rightarrow} 0,
\]
we have
\[
e^{-1}\text{v} \text{ar}_f(\tilde{e}^{\text{adj}}(1) \mid \tilde{X}) + e^{-1}_0\text{v} \text{ar}_f(\tilde{e}^{\text{adj}}(0) \mid \tilde{X}) - \text{v} \text{ar}_f(\tilde{e}^{\text{adj}}(1) - \tilde{e}^{\text{adj}}(0) \mid \tilde{X}) \mid \mathcal{D}_x(A_x) \overset{p}{\rightarrow} e^{-1}_1\text{v} \text{ar}_f(\tilde{e}^{\text{adj}}(1) \mid \tilde{X}) + e^{-1}_0\text{v} \text{ar}_f(\tilde{e}^{\text{adj}}(0) \mid \tilde{X}) - \text{v} \text{ar}_f(\tilde{e}^{\text{adj}}(1) - \tilde{e}^{\text{adj}}(0) \mid \tilde{X}),
\]
\[ e_1^{-1} \text{var}_r \{ \tilde{Y}_{\text{adj}}(1) \mid C \} + e_0^{-1} \text{var}_r \{ \tilde{Y}_{\text{adj}}(0) \mid C \} - \text{var}_r \{ \tilde{Y}_{\text{adj}}(1) - \tilde{Y}_{\text{adj}}(0) \mid C \} \mid D_c(A_c) \xrightarrow{p} \]

Thus, the estimated numerators for the multiple correlation coefficients are consistent. Similarly, we can prove the consistency of \( \hat{\mu}_x \) and \( \hat{\mu}_c \). The conclusion follows immediately.

\[ \square \]

F.20. Proof of Corollaries 7 and 8, and Theorem 10

Cluster rerandomization procedures with individual-level covariates and cluster-level covariates have the same form of asymptotic distributions. The proof is just a slight modification of the proof of Corollaries 2, 3, and Theorem 5.