Berry–Esseen bounds for design-based causal inference with possibly diverging treatment levels and varying group sizes

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Abstract

Neyman (1923/1990) introduced the randomization model, which contains the notation of potential outcomes to define causal effects and a framework for large-sample inference based on the design of the experiment. However, the existing theory for this framework is far from complete especially when the number of treatment levels diverges and the group sizes vary a lot across treatment levels. We provide a unified discussion of statistical inference under the randomization model with general group sizes across treatment levels. We formulate the estimator in terms of a linear permutational statistic and use results based on Stein’s method to derive various Berry–Esseen bounds on the linear and quadratic functions of the estimator. These new Berry–Esseen bounds serve as basis for design-based causal inference with possibly diverging treatment levels and diverging dimension of causal effects. We also fill an important gap by proposing novel variance estimators for experiments with possibly many treatment levels without replications. Equipped with the newly developed results, design-based causal inference in general settings becomes more convenient with stronger theoretical guarantees.

Keywords: Central limit theorem; permutation; potential outcome; Stein’s method; randomized experiment

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1. Motivation: randomization-based causal inference

1.1. Existing results

In a seminal paper, Neyman (1923/1990) introduced the notation of potential outcomes to define causal effects. More importantly, he also proposed a framework for statistical inference of causal effects based on the design of the experiment. In particular, Neyman (1923/1990) considered an experiment with \( N \) units and \( Q \) treatment arms, where the number of units under treatment \( q \) equals \( N_q \), with \( \sum_{q=1}^{Q} N_q = N \). Corresponding to treatment level \( q \), unit \( i \) has the potential outcome \( Y_i(q) \), where \( i = 1, \ldots, N \) and \( q = 1, \ldots, Q \). Despite its simplicity, the following completely randomized experiment has been widely used in practice and has generated rich theoretical results. Definition 1 below characterizes the joint distribution of \( Z = (Z_1, \ldots, Z_N) \) under complete randomization, where \( Z_i \in \{1, \ldots, Q\} \) is the treatment indicator for unit \( i \).

Definition 1 (Complete randomization). \( P(Z = z) = \frac{N_1! \cdots N_Q!}{N!} \) for all \( z = (z_1, \ldots, z_N) \) with \( (N_1, \ldots, N_Q) \) units receiving treatment level \((1, \ldots, Q)\), respectively.

Neyman (1923/1990) formulated complete randomization based on an urn model, which is equivalent to Definition 1. Under complete randomization, \( Z \) is from a random permutation of \( N_1 \) 1’s, \( \ldots, N_Q \) Q’s. The experiment reveals one of the potential outcomes, which is the observed outcome \( Y_i = Y_i(Z_i) = \sum_{q=1}^{Q} Y_i(q) \mathbf{1}\{Z_i = q\} \) for each unit \( i \).

In Neyman (1923/1990)’s framework, all potential outcomes are fixed and only the treatment indicators are random according to Definition 1. Scheffé (1959, Chapter 9) called it the randomization model. Under this model, it is conventional to call the resulting inference as randomization inference or design-based inference. It has become increasingly popular in both theory and practice (e.g., Kempthorne 1952; Copas 1973; Robins 1988; Rosenbaum 2002; Hinkelmann and Kempthorne 2007; Freedman 2008b,a; Lin 2013; Dasgupta et al. 2015; Imbens and Rubin 2015; Athey and Imbens 2017; Fogarty 2018b; Guo and Basse 2021).

A central goal in Neyman (1923/1990)’s framework is to use the observed data \((Z_i, Y_i)_{i=1}^{N}\) to make inference of causal effects defined by the potential outcomes. Define

\[
\bar{Y}(q) = N^{-1} \sum_{i=1}^{N} Y_i(q), \quad S(q, q') = (N - 1)^{-1} \sum_{i=1}^{N} (Y_i(q) - \bar{Y}(q))(Y_i(q') - \bar{Y}(q'))
\]

as the average value of the potential outcomes under treatment \( q \) and the covariance of the potential outcomes under treatments \( q \) and \( q' \), respectively. Define the average potential outcome vector as \( \bar{Y} = (\bar{Y}(1), \ldots, \bar{Y}(Q))^\top \in \mathbb{R}^Q \), and define the covariance matrix of the potential outcomes as \( S = (S(q, q'))_{q,q'=1,\ldots,Q} \). The parameter of interest is a linear transformation of \( \bar{Y} \):

\[
\gamma = F^\top \bar{Y}
\]

for a pre-specified \( F = (f_{qh}) \in \mathbb{R}^{Q \times H} \), which is called the contrast matrix when its columns
are orthogonal to \((1, \ldots, 1)^\top\). Despite the simple form of \(\gamma\), it can answer questions from a wide ranges of applications. For instance, Neyman (1923/1990) considered pairwise differences in means, and Dasgupta et al. (2015) and Mukerjee et al. (2018) considered linear combinations of the mean vector. Recently, Li and Ding (2017) unified the literature by studying the properties of the moment estimator for \(\gamma\) under complete randomization. In particular, define the sample mean and variance of the observed \(Y_i(q)\)'s as

\[ \hat{Y}_q = N_q^{-1} \sum_{Z_i=q} Y_i, \quad \hat{S}(q,q) = (N_q - 1)^{-1} \sum_{Z_i=q} (Y_i - \hat{Y}_q)^2, \]

(1) respectively. Define

\[ \tilde{\gamma} = (\tilde{Y}_1, \cdots, \tilde{Y}_Q)^\top \in \mathbb{R}^Q, \quad \tilde{V}_{\tilde{\gamma}} = \text{Diag}\left\{ N_q^{-1} \hat{S}(q,q) \right\}_{q \in [Q]} \in \mathbb{R}^{Q \times Q} \]

(2) as the vector of sample averages and the diagonal matrix of the sample variances across all arms, respectively. Li and Ding (2017) showed that \(\hat{Y}_q\) has mean and covariance

\[ \mathbb{E}\{\tilde{\gamma}\} = \bar{Y}, \quad \text{Var}\left\{ \tilde{\gamma}_q \right\} = V_{\tilde{\gamma}} = \text{Diag}\left\{ N_q^{-1} S(q,q) \right\}_{q \in [Q]} - N^{-1} S, \]

(3) and moreover, \(\tilde{V}_{\tilde{\gamma}}\) is a conservative estimator for \(V_{\tilde{\gamma}}\) in the sense that \(\mathbb{E}\{\tilde{V}_{\tilde{\gamma}}\} - V_{\tilde{\gamma}}\) positive semi-definite. An immediate consequence is that

\[ \tilde{\gamma} = F^\top \tilde{\gamma}, \quad \tilde{\gamma} = F^\top \tilde{V}_{\tilde{\gamma}} F \]

(4) are an unbiased point estimator for \(\gamma\) and a conservative covariance estimator for \(V_{\gamma} = \text{Var}\{\tilde{\gamma}\} = FV_{\tilde{\gamma}} F^\top\), respectively. Li and Ding (2017) also used the established combinatorial or rank central limit theorems (CLTs) (Hájek 1960; Hoeffding 1951; Fraser 1956) to prove the asymptotic Normality of \(\tilde{\gamma}\) and the validity of the associated large-sample Wald-type inference, under certain regularity conditions.

1.2. Open questions

Despite the long history of Neyman (1923/1990)’s randomization model, the theory for randomization-based causal inference is far from complete. Technically, Li and Ding (2017)’s review only covered the first regime (R1) below, and even there, finer results such as Berry–Esseen bounds (BEBs) have not been rigorously established for the most general setting (see Wang and Li (2022) for some recent results of BEBs for treatment-control experiments). For other regimes below, many basic results are still missing in the literature. Table 1 provides a list of important regimes and reviews the established and missing theoretical results. The discussion below gives more details.

(R1) Small \(Q\) and large \(N_q\)’s. In this regime, the number of arms is small and the sample size in each arm is large. Asymptotically, as \(N \to \infty\), we have that \(Q\) is a fixed integer and
Table 1: Theoretical results for multi-armed experiments under the randomization model. The regimes (R1)–(R4) correspond to nearly uniform designs by Definition 2, whereas the regime (R5) corresponds to non-uniform designs by Definition 3.

| Regime | $Q$ | $N_q$ | CLT, variance estimation, and BEB |
|--------|-----|-------|----------------------------------|
| (R1)   | Small | Large | CLT and variance estimation; no BEB |
| (R2)   | Large | Large | Seems similar to (R1) but not studied |
| (R3)   | Large | Small but $N_q \geq 2$ | Not studied |
| (R4)   | Large | $N_q = 1$ | Not studied; variance estimation is nontrivial |
| (R5)   | Mixture of the above | Not studied |

$N_q/N \to \varepsilon_q \in (0,1)$ for all $q = 1, \ldots, Q$. Li and Ding (2017) showed that, under (R1) and some regularity conditions on the potential outcomes, we have

$$V^{-1/2} \gamma \sim \mathcal{N}(0, I_H), \quad N \hat{\gamma} - N\mathbb{E}\{\hat{\gamma}\} = o_p(1),$$

which ensure that the large sample Wald-type inference based on the Normal approximation is conservative. Li and Ding (2017)’s results are asymptotic. An important theoretical question is to quantify the finite-sample properties of $\hat{\gamma}$ by deriving non-asymptotic results.

(R2) Large $Q$ and large $N_q$’s. In this regime, each arm has adequate units for the variance estimation, but the number of arms is also large. Asymptotically, as $N \to \infty$, we have $Q \to \infty$ and $N_q \to \infty$ for all $q = 1, \ldots, Q$. Consequently, the limiting values of some $N_q/N$’s must be 0. The point estimates and variance estimators in (4) are still well-defined in this regime. We might expect that the asymptotic results in (5) still hold because of large $N_q$’s. However, previous theoretical results do not cover this seemingly easy case due to the possibly diverging dimension of $F$.

(R3) Large $Q$ and small $N_q$’s. In this regime, the number of arms is large but the sample size within each arm is small. Asymptotically, as $N \to \infty$, we have $Q \to \infty$ and $2 \leq N_q \leq \pi$ for some fixed $\pi \geq 2$. This regime is well suited for many factorial experiments (see Example 1 below), in which the total number of factor combinations can be much larger than the number of replications in each combination (e.g., Mukerjee and Wu 2006; Wu and Hamada 2011). Although the point estimate and variance estimator in (4) are still well-defined, we do not expect a simple CLT based on the joint asymptotic Normality of $\hat{Y}$ due to the small $N_q$’s. Nevertheless, $\hat{\gamma} = F^\top \hat{Y}$, as a linear transformation of $\hat{Y}$, can still satisfy the CLT for some choice of $F$. This regime is reminiscence of the so-called proportional asymptotics in regression analysis, and even there, statistical inference is still not satisfactory in general (e.g., El Karoui et al. 2013; Lei et al. 2018; El Karoui and Purdom 2018). Technically, we need to analyze $F^\top \hat{Y}$ with the dimension of $\hat{Y}$ proportional to the sample size under the
randomization model. This is a gap in the literature.

(R4) Large \( Q \) and \( N_q = 1 \) for all \( q = 1, \ldots, Q \). This regime is much harder than (R3) because the variance estimator in (4) is not even well defined due to the lack of replications within each arm (e.g., Espinosa et al. 2016). Therefore, we need to answer two fundamental questions. First, does \( F^\top \hat{Y} \) still satisfy the CLT for some \( F \)? Second, how do we estimate the variance of \( F^\top \hat{Y} \)? These two questions are the basis for large-sample Wald-type inference in this regime. Neither has been covered by existing results.

(R5) Mixture of (R1)–(R4). In the most general case, it is possible that the number of treatment levels diverges and the group sizes within different treatment arms vary a lot. Theoretically, we can partition the treatment levels into different types corresponding to the four regimes above. Understanding (R5) relies on understanding (R1)–(R4). Due to the difficulties in (R1)–(R4) mentioned above, a rigorous analysis of (R5) requires deeper understanding of the randomization model. This is another gap in the literature.

For descriptive convenience, we define (R1)–(R4) as nearly uniform designs and (R5) as non-uniform designs, respectively, based on the heterogeneity of the group sizes across treatment arms. Definitions 2 and 3 below make the intuition more precise.

**Definition 2** (Nearly uniform design). There exists a positive integer \( N_0 > 0 \) and absolute constants \( c \leq c_q \leq \bar{c} \), such that \( N_q = c_q N_0 \) with \( c \leq c_q \leq \bar{c} \), for all \( q = 1, \ldots, Q \).

**Definition 3** (Non-uniform design). Partition the treatment arms as \( \{1, \ldots, Q\} = Q_s \cup Q_l \) with detailed descriptions below.

(i) \( Q_l \) contains the arms with large sample sizes. There exists a positive integer \( N_0 \) and absolute constants \( c \leq c_q \leq \bar{c} \), such that \( N_q = c_q N_0 \) with \( c \leq c_q \leq \bar{c} \), for all \( q \in Q_l \).

(ii) \( Q_s \) contains the arms with small sample sizes. There exists a fixed integer \( \bar{\pi} \) such that \( N_q \leq \bar{\pi} \) for all \( q \in Q_s \). Further partition \( Q_s \) as \( Q_s = Q_u \cup Q_r \) where

- \( Q_r \) contains the arms with replications, that is, \( 2 \leq N_q \leq \pi \) for all \( q \in Q_r \);
- \( Q_u \) contains the arms without replications, that is, \( N_q = 1 \) for all \( q \in Q_u \).

For simplicity, we will use \( |Q_*| \) and \( N_* = \sum_{q \in Q_*} N_q \) to denote the number of arms and the sample size in \( Q_* \), respectively, where \( * \in \{s, u, r, l\} \). As a special case of Definition 3, \( |Q_r| = |Q_l| = 0 \) corresponds to unreplicated designs in which each treatment level has only one observation.

We will also use the \( 2^K \) factorial design as a canonical example for many theoretical results throughout. We review the basic setup of the \( 2^K \) factorial design in Example 1 below (Dasgupta et al. 2015; Lu 2016; Zhao and Ding 2022).

**Example 1** (Factorial design). A \( 2^K \) factorial design has \( K \) binary factors which generate \( Q = 2^K \) possible treatment levels. Index the potential outcomes \( Y_i(q) \)’s also as \( Y_i(z_1, \ldots, z_K) \)’s, where \( q = 1, \ldots, Q \) and \( z_1, \ldots, z_K = 0, 1 \). The parameter of interest \( \gamma = F^\top \bar{Y} \) may consist of a subset
of the factorial effects. The contrast matrix $F$ has orthogonal columns and $\pm Q^{-1}$ entries; see Dasgupta et al. (2015) for precise definitions of main effects and interactions.

By definition, the factorial design can either be a nearly uniform design or a non-uniform design, depending on the group sizes across treatment levels. Previous asymptotic results only covered factorial designs under (R1) with fixed $K$ and large sample sizes for all treatment levels. This asymptotic regime can be a poor approximation to finite-sample properties of factorial designs with even a moderate $K$ (for example, if $K = 10$ then $Q = 2^K > 1000$). Based on simulation, Zhao and Ding (2022, Appendix D) showed that CLTs are likely to hold even with diverging $K$ and small sample sizes for all treatment levels. Allowing for a diverging $K$, Li and Ding (2017, Theorem A1) derived the CLT for a single factorial effect under the sharp null hypothesis of no treatment effects for any units whatsoever, i.e., $Y_i(1) = \cdots = Y_i(Q)$ for all $i = 1, \ldots, N$. However, deriving general asymptotic results for the factorial design has been an open problem in the literature.

1.3. Our contributions

Section 1.2 has reviewed various designs and the associated open problems. In this paper, we will give a unified study of all the designs above. We further the literature in the following ways.

First, we formulate the inference problem under the randomization model in terms of linear permutational statistics. This formulation allows us to build upon the existing results in probability theory (Bolthausen 1984; Chatterjee and Meckes 2008) to derive BEBs on the point estimator of the causal effect. In particular, our analysis emphasizes the dependence on the number of treatment levels and the dimension of the causal effects of interest. Importantly, we derive BEBs that can deal with non-uniform designs with varying group sizes.

Second, we establish a novel BEB on quadratic forms of the linear estimator under the randomization model. Importantly, this BEB allows that the number of treatment levels diverges, the sample sizes across treatment levels vary, and the dimension of the causal effects of interest diverges. It serves as the basis for the $\chi^2$ approximation for large-sample Wald-type inference.

Third, we propose variance estimators for unreplicated designs and mixture designs that allow for the group size to be one in many treatment levels. To the best of our knowledge, the variance estimators are new in the literature of design-based causal inference, although they share some features with those in finely stratified survey sampling (e.g., Cochran 1977; Wolter and Wolter 2007; Breidt et al. 2016) and experiments (e.g., Abadie and Imbens 2008; Fogarty 2018a). However, the theoretical analysis of the new variance estimators is much more challenging because of the dependence of the treatment indicators under the randomization model. We also study their probability limits and establish a complete theory that allows for large-sample Wald-type inference.

Fourth, in the process of achieving the above three sets of results, we established some immediate theoretical results that are potentially useful for other problems. For instance, we prove a novel BEB for linear permutational statistic over convex sets, building upon a recent result based on Stein’s method (Fang and Röllin 2015). We also obtain fine results on the sample moments under
the randomization model. Due to the space limit, we relegate them to Appendices A and C in the supplementary material.

1.4. Notation

We use $C$ to denote generic constants that may vary. Let $\Phi(t)$ denote the cumulative distribution function of a standard Normal distribution. For two sequences of numbers, $a_N$ and $b_N$, let $a_N = O(b_N)$ denote $a_N \leq Cb_N$ for some positive constant $C > 0$, and let $a_N = o(b_N)$ denote $a_N/b_N \to 0$ as $N \to \infty$. For a positive integer $N$, define $[N] = \{1, \cdots, N\}$. Let $\mathbf{0}_N$ and $\mathbf{1}_N$ denote, respectively, vectors of all zeros and ones in $\mathbb{R}^N$. For two random variables $X$ and $X'$, we use $X \preceq X'$ or $X' \succeq X$ to represent that $X'$ stochastically dominates $X$, i.e., $\mathbb{P}\{X' \leq t\} \leq \mathbb{P}\{X \leq t\}$ for all $t \in \mathbb{R}$. For any covariance matrix $V$, let $V^\star$ denote the corresponding correlation matrix.

Consider a matrix $M = (M(h,l)) \in \mathbb{R}^{H \times H}$. Let $M(\cdot, l) \in \mathbb{R}^{H \times 1}$ and $M(h, \cdot) \in \mathbb{R}^{1 \times H}$ denote its $l$-th column and $h$-th row, respectively. Let $\varrho_k(M)$ denote its $k$-th largest singular value. Specially, let $\varrho_{\text{max}}(M)$ and $\varrho_{\text{min}}(M)$ denote the largest and smallest singular values, respectively. Define its condition number as the ratio of its largest and smallest singular values: $\kappa(M) = \varrho_{\text{max}}(M)/\varrho_{\text{min}}(M)$. Let $\|M\|_p = (\sum_{h=1}^H \sum_{l=1}^H |M_{hl}|^p)^{1/p}$, $\|M\|_{\text{op}} = (\sum_{l=1}^H \|M(\cdot, l)\|_p^q)^{1/q} = (\sum_{l=1}^H \|M(\cdot, l)\|^q)^{1/q}$, $\|M\|_{\infty} = \max_{h,l} |M_{hl}|$ be, respectively, the Frobenius norm, the operator norm, the $L_{p,q}$ norm and the vectorized $\ell_\infty$ norm.

Design-based results rely crucially on conditions on $M_N(q) = \max_{i \in [N]} |Y_i(q) - \bar{Y}(q)|$, $(q = 1, \ldots, Q)$ which is the maximum absolute deviation from the mean for potential outcome $Y_i(q)$'s. Hájek (1960) used it in proving the CLT for simple random sampling, and Li and Ding (2017) used it in proving CLTs for design-based causal inference. It will also appear frequently in our presentation below.

2. BEBs for the moment estimator under completely randomized experiments

This section presents the BEBs for the moment estimator $\hat{\gamma}$ in (4) under completely randomized experiments. Section 2.1 presents general BEBs for linear projections of $\hat{\gamma}$. Sections 2.2 and 2.3 then apply them to derive useful BEBs for nearly uniform and non-uniform designs, respectively.

2.1. BEBs on the moment estimator

To simplify the presentation, standardize $\tilde{\gamma} = F^T \tilde{Y}$:

$$\tilde{\gamma} = V_{\tilde{\gamma}}^{-1/2}(\tilde{\gamma} - \gamma) \quad \text{with} \quad \mathbb{E}\{\tilde{\gamma}\} = 0 \text{ and } \text{Var}\{\tilde{\gamma}\} = I_H.$$  (6)
The standardization (6) assumes that the covariance matrix \( V_\hat{\gamma} \) is not singular. We assume it for convenience without loss of generality. When the contrast matrix \( F \) has linearly dependent columns and \( V_\hat{\gamma} \) becomes degenerate, we can focus on a subset of linearly independent columns of \( F \).

Our key results are BEBs on linear projections of \( \tilde{\gamma} \). Condition 1 below will facilitate the discussion.

**Condition 1** (Non-degenerate covariance matrix of \( \tilde{\gamma} \)). There exists \( \sigma_F \geq 1 \) such that

\[
F^\top \text{Diag}\{N_q^{-1}S(q,q)\} F \preceq \sigma_F^2 F^\top \hat{\gamma} V_\hat{\gamma} F.
\]  

(7)

Theorem 1 below gives a general BEB for linear projections of \( \tilde{\gamma} \).

**Theorem 1** (BEBs for linear projections of \( \tilde{\gamma} \)). Assume complete randomization. (i) There exists a universal constant \( C > 0 \), such that for any \( b \in \mathbb{R}^H \) with \( \|b\|_2 = 1 \), we have

\[
\sup_{t \in \mathbb{R}} \left| \mathbb{P}\{b^\top \tilde{\gamma} \leq t\} - \Phi(t) \right| \leq C \max_{q \in [Q]} N_q^{-1} M_N(q).
\]

(ii) Further assume Condition 1. There exists a universal constant \( C > 0 \), such that

\[
\sup_{b \in \mathbb{R}^H, \|b\|_2 = 1} \sup_{t \in \mathbb{R}} \left| \mathbb{P}\{b^\top \tilde{\gamma} \leq t\} - \Phi(t) \right| \leq C \max_{i \in [N], q \in [Q]} \min \{I(i,q), II(i,q)\}.
\]

(8)

where

\[
I(i,q) = \sigma_F \frac{\left| Y_i(q) - \overline{Y}(q) \right|}{\sqrt{N_q S(q,q)}}, \quad II(i,q) = \frac{\|F(q,\cdot\)\|_2 \cdot N_q^{-1} |Y_i(q) - \overline{Y}(q)|}{\sqrt{\min \{F^\top \hat{\gamma} V_\hat{\gamma} F\}}}. \tag{9}
\]

The upper bound in Theorem 1(i) depends on the choice of \( b \), whereas the upper bound in Theorem 1(ii) is uniform over all \( b \). The first step of the proof of Theorem 1 is to formulate \( \tilde{\gamma} \) as a linear permutational statistic so that we can apply an existing BEB by Bolthausen (1984). The second step of the proof is to derive upper bounds in terms of I and II in (9) from two different perspectives, which is non-trivial to the best of our knowledge. See Appendix D for technical details. The second step is the key, which makes Theorem 1 applicable in a wide range of designs.

Before discussing the useful consequences of Theorem 1(ii), we first comment on Condition 1, which plays a key role in deriving the upper bound in Theorem 1(ii). Condition 1, coupled with (3), implies that

\[
\sigma_F^{-2} F^\top \text{Diag}\{N_q^{-1}S(q,q)\} F \preceq V_\hat{\gamma} \preceq F^\top \text{Diag}\{N_q^{-1}S(q,q)\} F,
\]

i.e., the covariance matrix \( V_\hat{\gamma} \) is upper and lower bounded by \( F^\top \text{Diag}\{N_q^{-1}S(q,q)\} F \), up to constants. Lemma 1 below gives two sufficient conditions for Condition 1 to aid the interpretation.

**Lemma 1** (Sufficient conditions for Condition 1). (i) Condition 1 holds with \( \sigma_F = 1 \) if the individual causal effects are constant, that is, \( F\{Y_i(q)\}_{q=1}^Q - \overline{Y}\} = 0 \) for all \( i \in [N] \). (ii) Condition 1
holds with $\sigma_F = c\sigma$ if $\max_{q \in [Q]} N_q \leq (1 - c)N$ for some $0 < c < 1$ and the condition number of the correlation matrix corresponding to $V_Y$ is upper bounded by $\sigma^2$.

The sufficient conditions in Lemma 1 are somewhat standard in the literature, especially under (R1). Li and Ding (2017, Corollary 2) gives a CLT under the assumption of constant individual causal effects, which is a special case of Lemma 1(i). Li and Ding (2017, Theorem 5) proves a CLT under the assumption that $S$ has a finite limiting value. When the limit is positive definite, $V_Y$ also converges to a positive definite matrix, which becomes a special case of Lemma 1(ii). The general forms of conditions in Condition 1 and Lemma 1 are more useful for (R2)–(R5).

Now we comment on Theorem 1(ii). The upper bound in (8) depends on the minimum value of two terms. It is convenient to apply these two terms to different treatment arms based on the structure of the design. We elaborate this idea by revisiting (R1) to (R5).

- For (R1) and (R2), because the $N_q$’s are large, we can use term I in (9) and obtain a sufficient condition for a vanishing upper bound.
- For (R3) and (R4), the $N_q$’s are bounded and term I in (9) has constant order. However, term II in (9) is small under mild conditions on $F$. For instance, in the factorial design in Example 1, the following algebraic facts hold:

\begin{align*}
\|F\|_\infty &= Q^{-1}, \quad \|F(q, \cdot)\|_2 = Q^{-1}\sqrt{H}, \quad \varrho_{\min}(F^\top F) = Q^{-1}. \tag{10}
\end{align*}

Combining Condition 1 and (10), we have

\begin{align*}
\varrho_{\min}(F^\top V_Y F) &\geq \sigma_F^{-2} \varrho_{\min}(F^\top \text{Diag}\{N_q^{-1}S(q, q)\} F) \\
&\geq \sigma_F^{-2} \min_{q \in [Q]} \{N_q^{-1}S(q, q)\} \cdot \varrho_{\min}(F^\top F) \\
&= Q^{-1}\sigma_F^{-2} \min_{q \in [Q]} \{N_q^{-1}S(q, q)\}. \tag{11}
\end{align*}

If we assume $\max_{q \in [Q]} M_N(q)^2 \min_{q \in [Q]} S(q, q)$ is of constant order, because the $N_q$’s are bounded, term II in (9) has order $O(\sqrt{H}/Q)$, which is small if $H/Q \to 0$.

- For (R5), we can partition the treatment arms based on the sizes of $N_q$’s to achieve a trade-off between terms I and II in (9). In particular, for non-uniform designs in Definition 3, a natural partition is $[Q] = Q_L \cup Q_S$. On the one hand, the arms in $Q_L$ contain many units, so term I in (9) vanishes asymptotically. On the other hand, $Q_S$ contains many arms which makes term II in (9) small under mild conditions on $F$.

We will provide rigorous results in the next two sections by applying Theorem 1 to obtain useful BEBs for different designs.
2.2. A BEB with a proper contrast in nearly uniform designs

In (R1) with a fixed $Q$ and large $N_q$'s, it is intuitive to have CLTs for linear transformations of $\hat{Y}$ because $\hat{Y}$ itself has a CLT. In other regimes, for instance (R4), CLTs for linear transformations of $\hat{Y}$ are less intuitive. Consider a diverging $Q$ and bounded $N_q$'s. If $F = (1, 0, \ldots, 0) \top \in \mathbb{R}^Q$, then the CLT for $F \top \hat{Y} = \hat{Y}_1$ does not hold due to the bounded sample size in treatment arm 1. As another toy example, if $F = (1_Q, 1_Q) \in \mathbb{R}^{Q \times 2}$, then $F \top \hat{Y}$ has degenerate covariance structure and Theorem 1 cannot be directly applied. Therefore, CLTs should be established for proper contrast matrices. Corollary 1 below gives a positive result on the BEBs for proper contrasts. We first introduce Condition 2 below on $F$.

**Condition 2** (Proper contrast). The contrast matrix $F$ satisfies $\|F\|_\infty \leq cQ^{-1}$ and $\varrho_{\min} \{F \top F\} \geq c'Q^{-1}$ for some constants $c, c' > 0$.

Condition 2 appears to be dependent on the scale of $F$ although the BEB should not depend on the scale of $F$ due to the standardization of $\hat{\gamma}$. We present the above form of Condition 2 to facilitate the discussion of the factorial design in Example 1, in which the scale of $F$ is motivated by scientific questions of interest. When $Q$ is fixed, Condition 2 holds if $F$ has full column rank. So in (R1), Condition 2 does not impose any additional assumptions beyond the standard ones. When $Q$ diverges, Condition 2 rules out sparse $F$ that only results in linear combination of $\hat{Y}$ over a small number of treatment arms. Also, the minimum eigenvalue condition in Condition 2 ensures non-degenerate covariance structure. Example 2 below gives more detailed discussion in the factorial design.

We then give Corollary 1 below.

**Corollary 1** (BEB for nearly uniform designs). Assume complete randomization that satisfies Definition 2, Conditions 1 and 2. There exists a universal constant $C > 0$, such that

$$
\sup_{b \in \mathbb{R}^H, \|b\|_2 = 1} \sup_{t \in \mathbb{R}} |\mathbb{P}\{b \top \hat{\gamma} \leq t\} - \Phi(t)| \leq C \sigma_F \frac{\max_{q \in [Q]} M_N(q)}{\min_{q \in [Q]} S(q, q)} \frac{1}{\sqrt{N}} \sqrt{H}. \tag{12}
$$

We make several comments on Corollary 1. First, technically, we derive the upper bound in Corollary 1 based on the upper bound from term II in (9) in Theorem 1(ii), which is uniform over $b$. Therefore, the upper bound in Corollary 1 preserves the uniformity and does not depend on $b$. Second, the upper bound in (12) reveals the interplay of several parameters: the number of contrasts $H$, the number of units $N$, the scale of the potential outcomes $M_N(q)$, the minimum second moments $\min_{q \in [Q]} S(q, q)$ as well as the structure of $F$. Third, the upper bound in (12) decreases at the rate of $(H/N)^{1/2}$ which can deal with (R1)–(R4).

**Remark 1.** The denominator of (12) depends on $\min_{q \in [Q]} S(q, q)$, which is useful when the variances of the potential outcomes are lower bounded. For the ease of presentation, we did not discuss more complicated cases such as some $S(q, q)$’s are small. We can slightly modify the proof of Corollary 1 to cover scenarios where some $S(q, q)$’s are close or equal to zero.
We conclude this subsection with an example on the nearly uniform factorial design.

**Example 2** (Nearly uniform factorial design). Recall Example 1 and assume it satisfies Definition 2. Let $F \in \mathbb{R}^{Q \times H}$ with $H = K + K(K - 1)/2 = K(K + 1)/2$ be the contrast matrix for all main effects and two-way interactions. Assume Condition 1 and recall (10). Corollary 1 implies

$$
\sup_{b \in \mathbb{R}^H, \|b\|_2 = 1} \sup_{t \in \mathbb{R}} \left| \mathbb{P}\{b^\top \tilde{\gamma} \leq t\} - \Phi(t) \right| \leq C \sigma_F \max_{q \in \mathbb{Q}} \frac{M_N(q)}{\min_{q \in \mathbb{Q}} S(q, q)}^{1/2} \sqrt{\frac{K^2}{N}}. \tag{13}
$$

From (13), we can obtain a sufficient condition for the the upper bound to converge to 0, which implies a CLT of $\tilde{\gamma}$. 

### 2.3. A BEB for non-uniform designs

Now consider the non-uniform design in Definition 3. We can apply Theorem 1 to establish the following BEB for non-uniform designs:

**Corollary 2** (BEB for non-uniform designs). Assume complete randomization that satisfies Definition 3 and Conditions 1 and 2. Also assume

$$Q \geq 2(c^2/c')H|\mathcal{Q}_l| \tag{14}$$

recalling the constants $c$ and $c'$ in Condition 2. There exists a universal constant $C > 0$, such that

$$
\sup_{b \in \mathbb{R}^H, \|b\|_2 = 1} \sup_{t \in \mathbb{R}} \left| \mathbb{P}\{b^\top \tilde{\gamma} \leq t\} - \Phi(t) \right| \leq C \sigma_F \max_{q \in \mathbb{Q}_l} \frac{M_N(q)}{\min_{q \in \mathbb{Q}_l} S(q, q)}^{1/2} \cdot \sqrt{\frac{H}{N}}. \tag{15}
$$

There are two key steps in applying Theorem 1 to prove Corollary 2. The first step is to partition $Q$ into $\mathbb{Q}_s \cup \mathbb{Q}_l$ based on the size of the arms. The second step is to simplify the denominator of term II of (8). The obtained upper bound (15) is uniform over all $b$. Moreover, it depends on the sizes of the treatment arms in a subtle way. On the one hand, for $q \in \mathbb{Q}_l$, the $N_q$’s are large, so the first part of (15) converges to zero if the following “local” condition holds for all $q \in \mathbb{Q}_l$:

$$
\frac{M_N(q)^2}{S(q, q)} = o(N_q).
$$

On the other hand, for $q \in \mathbb{Q}_s$, the $N_q$’s are small, but the second part of (15) still converges to zero if the following “global” condition holds:

$$
\frac{\max_{q \in \mathbb{Q}_s} M_N(q)^2}{\min_{q \in \mathbb{Q}_s} S(q, q)} = o \left( \frac{H}{N_s} \right).
$$

We conclude this section with an example on the non-uniform factorial design.
Example 3 (Non-uniform factorial design). Recall Example 1. Assume the baseline arm $q = 1$ contains a large number of units possibly due to lower cost while the other arms have $N_q \leq n$ for some fixed $n$. This gives a non-uniform design by Definition 3 with $Q_l = \{1\}$ and $Q_s = \{2, \ldots, Q\}$. Let $F \in \mathbb{R}^{Q \times H}$ with $H = K(K + 1)/2$ be the contrast matrix for all main effects as well as two-way interactions. Assume Condition 1 and recall (10). Applying Corollary 2, we have

$$\sup_{b \in \mathbb{R}^H, \|b\|_2 = 1} \sup_{t \in \mathbb{R}} \left| \mathbb{P}\{b^\top \gamma \leq t\} - \Phi(t) \right| \leq C_{\sigma_F} \max \left\{ \frac{M_N(1)}{\sqrt{N_1 S(1,1)}}, \frac{\max_{q \geq 2} M_N(q)}{\min_{q \geq 2} S(q,q)} \right\}^{1/2} \sqrt{\frac{K^2}{N_s}}. \quad (16)$$

From (16), if $K \to \infty, N_1 \to \infty$, and

$$\frac{M_N(1)}{\sqrt{S(1,1)}} = o(N_1^{1/2}), \quad \frac{\max_{q \geq 2} M_N(q)}{\min_{q \geq 2} S(q,q)}^{1/2} = o(N_s^{1/2}/K),$$

then the upper bound in (16) vanishes asymptotically.

3. Design-based causal inference

Now we turn to the central task of design-based causal inference under complete randomization. We focus on the large-sample Wald-type inference based on the quadratic form

$$\hat{T} = (\hat{\gamma} - \gamma)^\top \hat{V}_\gamma^{-1}(\hat{\gamma} - \gamma),$$

recalling the point estimator $\hat{\gamma}$ and the variance estimator $\hat{V}_\gamma$ in (4). In (R1) with fixed $(Q, H)$ and large $N_q$’s, the standard asymptotic argument suggests that we can use $q_\alpha$, the upper $\alpha$-quantile of $\chi^2(H)$, as the critical value for the the quadratic form. For simplicity, we say that the corresponding confidence set is asymptotically valid if $\lim_{N \to \infty} \mathbb{P}\{\hat{T} \leq q_\alpha\} \geq 1 - \alpha$.

The rigorous theoretical justification for the above Wald-type inference procedure typically follows from two steps:

(Step 1) First, analyze the asymptotic distribution of the corresponding quadratic form with the true covariance matrix

$$T = (\hat{\gamma} - \gamma)^\top V_\gamma^{-1}(\hat{\gamma} - \gamma). \quad (17)$$

(Step 2) Second, construct a consistent or conservative estimator $\hat{V}_\gamma$ for the true covariance matrix $V_\gamma$.

Under regime (R1), both Steps 1 and 2 have rigorous theoretical justification ensured by (5). Beyond (R1), it is challenging to derive the asymptotic distribution of the quadratic form in Step 1 especially when $H$ and thus the degrees of freedom of $T$ diverge. To achieve the requirement
in Step 1, we use results based on Stein’s method to derive BEBs on quadratic forms of linear permutational statistics. To avoid excessive notation, we present the results that are most relevant to our inference problem in the main paper and relegate more general yet more complicated results to Appendices A and C. Moreover, the sample variances $\hat{S}(q, q)$’s and thus the variance estimator $\hat{V}_\gamma$ in (4) are not even well defined when some treatment arms do not have replications of the outcome. Without replications in all arms, we must find an alternative form of $\hat{V}_\gamma$ to estimate $V_\gamma$. This is a salient problem for (R4) and (R5). Finally, in all regimes (R1)–(R5), we need to study the properties of $\hat{V}_\gamma$ to achieve the requirement in Step 2.

Due to the different levels of technical complexities, we divide this section into three subsections. Section 3.1 discusses nearly uniform designs with replications in all arms. Section 3.2 discusses unreplicated designs. Section 3.3 discusses the general non-uniform designs. In every subsection, we first present a BEB on the quadratic form in Step 1, then present the properties of the covariance estimator $\hat{V}_\gamma$, and finally present the formal result to justify the Wald-type inference.

To facilitate the discussion, we introduce the following notation

$$T_0 = \xi_H^T \xi_H \quad \text{where} \quad \xi_H \sim N(0, I_H)$$

for a $\chi^2(H)$ random variable with possibly diverging degrees of freedom. It has mean $H$ and variance $2H$. Both $\hat{T}$ and $T$ are related to $T_0$. Moreover, we introduce the following moment condition on the potential outcomes.

**Condition 3** (Bounded fourth moment of the potential outcomes). There exists a $\Delta > 0$ such that

$$\max_{q \in [Q]} N^{-1} \sum_{i=1}^N \{Y_i(q) - \overline{Y}(q)\}^4 \leq \Delta^4.$$ 

### 3.1. Nearly uniform design with replications in all arms

In this subsection, we study the Wald-type inference for nearly uniform designs given by Definition 2. First, we present a BEB for $T$ in (17) in Theorem 2 below.

**Theorem 2** (BEB for the quadratic form $T$ for nearly uniform designs with replications). Assume complete randomization that satisfies Definition 2. Assume Conditions 1 and 2. There exists a universal constant $C > 0$, such that

$$\sup_{t \in \mathbb{R}} |P(T \leq t) - P(T_0 \leq t)| \leq \frac{C \max_{q \in [Q]} M_N(q)^3}{\min_{q \in [Q]} S(q, q)^{3/2}} \cdot \frac{H^{19/4}}{N^{1/2}}.$$ 

(18)

Theorem 2 bounds the difference between $T$ and $T_0$ with possibly diverging $H$. Its upper bound is more useful when $H^{19/2}/N \to 0$, which restricts the number of contrasts of interest. The condition $H^{19/2}/N \to 0$ holds naturally in the factorial design in Example 1 under regime (R4) if only the main effects and two-way interactions are of interest with $H = O(K^2) = O((\log N)^2)$.

Second, we discuss variance estimation. Recall $\hat{S}(q, q)$ and $\hat{V}_\gamma$ be defined as in (1) and (2). Consider the point estimator $\hat{\gamma}$ and covariance estimator $\hat{V}_\gamma$ in (4). We have Theorem 3 below.
Theorem 3 (Variance estimation in nearly uniform designs). Consider designs that satisfies Definition 2 with \( \min_{q \in [Q]} N_q \geq 2 \). Assume Condition 3.

(i) \( \mathbb{E}\{\hat{V}_\gamma\} \succeq V_\gamma \).

(ii) \( \|\hat{V}_\gamma - \mathbb{E}\{\hat{V}_\gamma\}\|_\infty^2 = O_p \left( \|F\|_\infty Q^4 N^{-3} \Delta^4 H^2 \right) \).

(iii) \( \|\hat{V}_\gamma - \mathbb{E}\{\hat{V}_\gamma\}\|_{op}^2 = O_p \left( \|F\|_\infty Q^4 N^{-3} \Delta^4 H^4 \right) \).

Theorem 3(i) reviews that the covariance estimator \( \hat{V}_\gamma \) is conservative, which is well-known in design-based causal inference (Neyman 1923/1990; Imbens and Rubin 2015; Li and Ding 2017).

Theorem 3(ii) and (iii) are novel results on the stochastic orders of the estimation error of the covariance estimator in \( L_\infty \) norm and operator norm, respectively. In Example 1 of the factorial design with \( \|F\|_\infty = O(Q^{-1}) \), if \( \Delta \) is constant, then Theorem 3 simplifies to

\[
N\|\hat{V}_\gamma - \mathbb{E}\{\hat{V}_\gamma\}\|_\infty = O_p \left( H/N^{1/2} \right), \quad N\|\hat{V}_\gamma - \mathbb{E}\{\hat{V}_\gamma\}\|_{op} = O_p \left( H^2/N^{1/2} \right).
\]

The estimation error shrinks to zero quickly if only the main effects and two-way interactions are of interest. The results in Theorem 3 suffice for inference, and we relegate the finer probability tail bound for \( \hat{V}_\gamma \) to the supplementary material.

Third, we present formal results on inference. To simplify the presentation, we impose Condition 4 below.

Condition 4. (i) The absolute value of the centered potential outcomes are upper bounded by a constant \( \nu > 0 \). (ii) The variance of the potential outcomes are lower bounded a constant \( S > 0 \).

The upper boundedness in potential outcomes in Condition 4(i) is not necessary but convenient for the theory. We can relax it to allow for light tails of the potential outcomes. Similarly, the lower boundedness in Condition 4(ii) can be replaced by more general requirement such as light-tailed potential outcomes. We omit the results due to the technicalities.

Theorem 4 below justifies the Wald-type inference under the nearly uniform design with replications, where \( H \) can be either fixed or diverging.

Theorem 4 (Wald-type inference under replicated nearly uniform design). Consider the nearly uniform design given by Definition 2 with \( \min_{q \in [Q]} N_q \geq 2 \). Assume Conditions 1-4. Define \( W_N = V_\gamma^{1/2} \mathbb{E}\left\{\hat{V}_\gamma\right\}^{-1} V_\gamma^{1/2} \in \mathbb{R}^{H \times H} \). Let \( N \to \infty \).

(i) For a fixed \( H \), assume there exists a \( W_\infty \in \mathbb{R}^{H \times H} \) such that \( \lim_{N \to \infty} W_N = W_\infty \). Use \( \mathcal{L} \) to denote the distribution of \( \xi_H^\top W_\infty \xi_H \), where \( \xi_H \sim N(0, I_H) \). We have

\[
(\hat{\gamma} - \gamma)^\top \hat{V}_\gamma^{-1}(\hat{\gamma} - \gamma) \sim \mathcal{L}
\]

and \( \mathcal{L} \preceq \chi^2(H) \). Moreover, the Wald-type confidence set is asymptotically valid.
(ii) For a diverging $H$ with $H \to \infty$ and $H^{19/4}N^{-1/2} \to 0$, we have

$$\frac{(\hat{\gamma} - \gamma)^\top \hat{V}_{\hat{\gamma}}^{-1}(\hat{\gamma} - \gamma) - \text{Tr}(W_N)}{\sqrt{2\text{Tr}(W_N^2)}} \xrightarrow{} \mathcal{N}(0, 1).$$

Moreover, the Wald-type confidence set is asymptotically valid.

Theorem 4(i) reviews the known result for (R1) with a fixed $H$. Theorem 4(ii) is a novel result that allows for diverging $Q$ and $H$. It relies crucially on the BEB on the quadratic form $T$ in Theorem 2 and the stochastic properties of $\hat{V}_{\hat{\gamma}}$ in Theorem 3.

### 3.2. Unreplicated design

In this subsection, we study inference for unreplicated designs with $N_q = 1$ for $q = 1, \ldots, Q$. On the one hand, the BEB on $T$ is identical to that in Theorem 2. We give the formal result in Theorem 5 below for completeness.

**Theorem 5** (BEB for the quadratic form in unreplicated designs). Assume complete randomization with $N_q = 1$ for $q = 1, \ldots, Q$. Assume Conditions 1 and 2. The BEB (18) holds.

On the other hand, covariance estimation without replications is a fundamentally challenging problem as reviewed in Section 1. The commonly-used covariance estimator $\hat{V}_{\hat{\gamma}}$ in (4) is not well defined. We must construct a new estimator. In unreplicated designs, the observed allocation $Z_i$ and the arm $q$ has a one-to-one correspondence. Hence we can denote the single observed outcome in arm $q$ by $Y_q$. The point estimator still has the form $\hat{\gamma} = F^\top \hat{Y}$ where $\hat{Y} = (Y_1, \ldots, Y_Q)^\top$ is simply the observed outcome vector. Without replications, we cannot calculate $\hat{S}(q, q)$ based on only the single observation within arm $q \in Q_v = \{1, \ldots, Q\}$. With a little abuse of notation, we still consider the covariance estimator of the form:

$$\hat{V}_{\hat{\gamma}} = F^\top \hat{V}_{\hat{\gamma}}^F,$$

where $\hat{V}_{\hat{\gamma}}^F$ is a $Q \times Q$ diagonal matrix. The key is to construct its diagonal elements $\hat{V}_{\hat{\gamma}}^F(q, q)$ for all $q$’s.

To obtain substitutes for $\hat{S}(q, q)$, we must borrow information across treatment arms. This motivates us to consider the following grouping strategy.

**Definition 4** (Grouping). Partition $Q_v$ as $Q_v = \bigcup_{g=1}^G Q_{u,g}$ where $Q_{u,g} \cap Q_{u,g'} = \emptyset$ for all $g \neq g'$ and $|Q_{u,g}| \geq 2$ for all $g \in [G]$. The partition does not depend on the observed data.

Definition 4 does not allow for data-dependent grouping, which can cause theoretical complications. Examples 4 and 5 below are special cases of Definition 4. By the construction in Definition 4, the $Q_{u,g}$’s have no overlap, so we can also use $\langle g \rangle$ to denote $Q_{u,g}$ and $\mathcal{G} = \{\langle g \rangle\}_{g=1}^G$ to denote the grouping strategy without causing confusions. Moreover, $|\langle g \rangle|$ must be larger than or equal to two.
so that there are at least two treatment levels in each \( \langle g \rangle \). In general, we use \( \langle g \rangle_q \) to indicate the group \( \langle g \rangle \) that contains arm \( q \), but when no confusions would arise, we also simplify the notation to \( \langle g \rangle \) if the corresponding \( q \) is clear from the context.

Define

\[
\hat{Y}_{\langle g \rangle} = \frac{1}{|\langle g \rangle|} \sum_{q \in \langle g \rangle} Y_q,
\]

as the group-specific average, and construct

\[
\hat{V}_{\hat{Y}}(q,q) = \mu_{\langle g \rangle} (Y_{q} - \hat{Y}_{\langle g \rangle})^2, \quad \text{if } q \in \langle g \rangle
\]

as the \( q \)th diagonal element of \( \hat{V}_{\hat{Y}} \), where

\[
\mu_{\langle g \rangle} = (1 - 2N^{-1})^{-1}(1 - |\langle g \rangle|^{-1})^{-2}
\]

is a correction factor that is motivated by the theory below. Although the mean of \( \hat{Y}_{\langle g \rangle} \) has a simple formula, the mean of \( \hat{V}_{\hat{Y}}(q,q) \) has a cumbersome form. We present an lower bound of \( E\{\hat{V}_{\hat{Y}}(q,q)\} \) below and relegate the complete formula to the supplementary material. The results require Condition 5 below on the largest eigenvalue of the population correlation of the potential outcomes in group \( \langle g \rangle \), defined as

\[
\varrho_{\langle g \rangle} = \varrho_{\max}\{(S^*(q,q'))_{q,q' \in \langle g \rangle}\}.
\]

\textbf{Condition 5} (Bound on \( \varrho_{\langle g \rangle} \)). \( N - \varrho_{\langle g \rangle} - (|\langle g \rangle| - 1) \geq 0 \) for all \( g \in \mathcal{G} \).

Condition 5 reflects a trade-off between \( N \), \( \langle g \rangle \) and \( \varrho_{\langle g \rangle} \). It is more likely to hold with smaller correlations between arms within the same group and smaller subgroup sizes. By a natural bound \( \rho_{\langle g \rangle} \leq |\langle g \rangle| \), Condition 5 holds if \( |\langle g \rangle| \leq (N + 1)/2 \) for all \( g \in \mathcal{G} \). Examples 4 and 5 below satisfy Condition 5 automatically. With Condition 5, we can present Lemma 2 below.

\textbf{Lemma 2} (Sample mean and variance under grouping). Assume grouping \( \mathcal{G} \). We have

\[
E\left\{\hat{Y}_{\langle g \rangle}\right\} = Y_{\langle g \rangle}, \quad \text{where } Y_{\langle g \rangle} = \frac{1}{|\langle g \rangle|N} \sum_{g \in \langle g \rangle} \sum_{i=1}^{N} Y_i(q) = \frac{1}{|\langle g \rangle|} \sum_{q \in \langle g \rangle} Y(q).
\]

Further assume Condition 5. We have

\[
E\{\hat{V}_{\hat{Y}}(q,q)\} \geq S(q,q) + \Omega(q,q) + \mu_{\langle g \rangle} (\hat{Y}(q) - Y_{\langle g \rangle})^2,
\]

where

\[
\text{term III} \quad \text{and} \quad \text{term IV}
\]

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where
\[
\Omega(q, q) = \mu_{(g)} |g|^{-2}
\left(1 - \frac{g(q)}{N} - \frac{|g| - 1}{N}\right)
\sum_{q' \in (g), q' \neq q} S(q', q') \geq 0.
\] (23)

By Lemma 2, \(\hat{V}_\chi(q, q)\), as an estimator for \(S(q, q)\), is conservative, and the conservativeness depends on the variation of other arms \(q'\) that belong to \(\langle g \rangle_q\) (term III) and the between-arm heterogeneity in means within \(\langle g \rangle_q\) (term IV). We comment on some special cases below.

- If we assume homogeneity in means within subgroups, i.e.,
\[
\bar{y}(q) = \bar{y}_{\langle g \rangle}, \text{ for all } q \in \langle g \rangle,
\] (24)
then term IV vanishes.

- If we assume homoskedasticity across treatment arms within the same subgroup, i.e.,
\[
S(q, q) = S(q', q'), \text{ for all } q, q' \in \langle g \rangle,
\] (25)
then term III becomes
\[
\Omega(q, q) = \mu_{(g)}(|g| - 1)|g|^{-2}
\left(1 - \frac{g(q)}{N} - \frac{|g| - 1}{N}\right) S(q, q).
\] (26)

Then we can combine (26) with \(S(q, q)\) and use a smaller correction factor
\[
\mu'_{(g)} = (1 - |g|^{-1})^{-1}\{(1 - |g|^{-1})(1 - 2N^{-1}) + |g|^{-1}(1 - (2|g| - 1)/N)\}^{-1} \leq \mu_{(g)}
\]
to reduce the conservativeness of variance estimation.

- If we assume the strong null hypothesis within subgroups, i.e.,
\[
Y_i(q) = Y_i(q'), \text{ for all } i \in [N] \text{ and } q, q' \in \langle g \rangle,
\]
then both (24) and (25) hold. Applying the correction factor \(\mu'_{(g)}\), we can show \(\mathbb{E}\{\hat{V}_\chi(q, q)\} = S(q, q)\).

Lemma 2 suggests that ideally, we should group treatment arms based on the prior knowledge on the means and variances of the potential outcomes. While more general grouping strategies are possible, we give two examples for their simplicity of implementation. Both target the factorial design in Example 1.

**Example 4** (Pairing by the lexicographic order). Recall Example 1. We order the observations based on the lexicographical order of their treatment levels, then group the \((2k - 1)\)-th level with
the \((2k)\)-th level \(1 \leq k \leq 2^{K-1}\). When \(K = 3\), the grouping reduces to
\[
\langle 1 \rangle = \{(000), (001)\}, \quad \langle 2 \rangle = \{(010), (011)\}, \quad \langle 3 \rangle = \{(100), (101)\}, \quad \langle 4 \rangle = \{(110), (111)\}.
\]
If the last factor has small effect on the outcome, then we expect small differences of the mean potential outcomes within grouping. As a sanity check, Condition 5 holds under this grouping strategy.

**Example 5** (Grouping based on a subset of the factors). Recall Example 1 again. If we have the prior knowledge that \(K_0 < K\) factors are the most important ones, we can group the treatment levels based on these factors. Without loss of generality, assume that the first \(K_0\) factors are the important ones. In particular, we can create \(G = 2^{K_0} < Q\) groups, with each group \(\langle g \rangle\) corresponding to treatment levels with the same important factors. Example 4 above is a special with the first \(K - 1\) factors as the important ones. Also, Condition 5 holds under this grouping strategy.

Now we turn to theoretical analysis of (20). Its properties depend on how successful the grouping \(G\) is, quantified by Condition 6 below.

**Condition 6** (Bound on the within-group variation in potential outcome means). There exists a \(\zeta > 0\), such that
\[
\max_{g \in [G]} \max_{q \in \langle g \rangle} |\bar{Y}(q) - \bar{Y}_{\langle g \rangle}| \leq \zeta.
\]

The \(\zeta\) in Condition 6 bounds the between-arm distance of the mean potential outcomes under grouping \(G\). It plays a key role in Theorem 6 below.

**Theorem 6** (Variance estimation for unreplicated designs). Consider designs that satisfy Definition 3 and the covariance estimator in (20).

(i) Assume Condition 5. We have
\[
\mathbb{E}\{\hat{V}_F\} = V_F + \Omega + \text{Diag}\{\mu_{\langle g \rangle}(\bar{Y}(q) - \bar{Y}_{\langle g \rangle})^2\}_{q \in Q_0} + N^{-1}(\Theta + S)
\]
with \(\Omega = \text{Diag}\{\Omega(q, q)\}_{q \in Q_0}\) and \(\Theta = \text{Diag}\{\Theta(q, q)\}_{q \in Q_0}\), where the \(\Omega(q, q)\)'s are defined in (23) and the \(\Theta(q, q)\)'s are bounded by \(0 \leq \Theta(q, q) \leq 5\mu_{\langle g \rangle} \max_{q' \in \langle g \rangle} S(q', q')\). Therefore,
\[
\mathbb{E}\{F^\top \hat{V}_F F\} \preceq V_\gamma.
\]

(ii) Assume Conditions 3 and 6. We have
\[
\|\hat{V}_\gamma - \mathbb{E}\{\hat{V}_\gamma\}\|_\infty^2 = O_P \left\{ \left( \max_{g \in [G]} \mu_{\langle g \rangle} \right)^2 \|F\|_\infty^4 \Delta^2 (\Delta + \zeta^2) NH^2 \right\}.
\]

(iii) Assume Conditions 3 and 6. We have
\[
\|\hat{V}_\gamma - \mathbb{E}\{\hat{V}_\gamma\}\|_{op}^2 = O_P \left\{ \left( \max_{g \in [G]} \mu_{\langle g \rangle} \right)^2 \|F\|_\infty^4 \Delta^2 (\Delta + \zeta^2) NH^4 \right\}.
\]
Theorem 6(i) demonstrates that based on (20), the covariance estimator \( \hat{V}_\gamma \) is conservative for \( V_\gamma \), which implies that \( F^\top \hat{V}_\gamma F \) is conservative for the true covariance matrix of \( \hat{\gamma} \). The conservativeness, however, has a more complex pattern compared to the setting with replications within all arms (Neyman 1923/1990; Imbens and Rubin 2015; Li and Ding 2017). Theorem 6(i) shows three sources of conservativeness. The first part, captured by \( \Omega \), is due to the between-arm heteroskedasticity within each subgroup. However, it is fundamentally difficult to estimate each \( S(q, q') \) without replications. The second part, captured by \( \text{Diag} \{ \mu_\langle g \rangle (Y(q) - Y_\langle g \rangle)^2 \}_{q \in [Q]} \), is due to the between-arm heterogeneity in means within each subgroup. The part will be small if the grouping strategy ensures that the grouped arms have similar population average of potential outcomes. The third part, captured by \( N^{-1}(\Theta + S) \), is due to the difficulty of estimating \( S \) and in particular, the off-diagonal terms of \( S \). The difficulty of estimating \( S \) has been well documented ever since Neyman (1923/1990) even in experiments with replications in each arm. It is possible to reduce this part but it requires additional assumptions, for example, the individual causal effects are constant.

Theorem 6(ii) and (iii) give the stochastic order of the estimation error of the covariance estimator \( \hat{V}_\gamma \) under the \( L_\infty \) norm and operator norm, respectively. If \( \max_{g \in [G]} \mu_\langle g \rangle, \Delta \) and \( \zeta \) are all constants, then

\[
N\| \hat{V}_\gamma - \mathbb{E}\{\hat{V}_\gamma\}\|_\infty = O_P(H/N^{1/2}), \quad N\| \hat{V}_\gamma - \mathbb{E}\{\hat{V}_\gamma\}\|_{op} = O_P(H^2/N^{1/2}),
\]

which gives sufficient conditions on \( H \) to ensure the convergence of \( \hat{V}_\gamma \) in \( L_\infty \) norm and operator norm, respectively.

Finally, equipped with the BEB on the quadratic form \( T \) in (17) and the conservative variance estimator studied in Theorem 6, it is immediate to establish Theorem 7 below for inference, which parallels Theorem 4.

**Theorem 7** (Wald-type inference under unreplicated design). Consider the unreplicated design with \( N_q = 1 \) for all \( q = 1, \ldots, Q \). Assume Conditions 1–6. Then the conclusion of Theorem 4 holds if we use the covariance estimator in (20).

### 3.3. Non-uniform design

In this section, we consider non-uniform designs in Definition 3. First, we show a BEB on \( T \) in (17) in Theorem 8 below.

**Theorem 8** (Quadratic form BEB for non-uniform designs). Assume complete randomization that satisfies Definition 2. Assume Conditions 1, 2, (14) and \( N = O(Q) \). There exists a universal constant \( C > 0 \), such that

\[
\sup_{t \in \mathbb{R}} |\mathbb{P}(T \leq t) - \mathbb{P}(T_0 \leq t)| \leq C \frac{\max_{g \in [G]} M_N(g)^3}{\min_{q \in Q_s} S(q, q)} \frac{H^{19/4}}{N^{1/2}} \cdot \frac{N^{3/2}}{N^{1/2}}.
\]

Theorem 8 assumes \( N \) has the same order as \( Q \), which is helpful to establish the root \( N \) convergence of BEB. We can relax it if we only need the CLT rather than the BEB with . For
the ease of presentation, we omit the general results. A subtle feature of the upper bound in (27) is that \( \max_{q \in [Q]} M_N(q) \) is the maximum value of the \( M_N(q) \)'s over all treatment arms whereas \( \min_{q \in Q_S} S(q, q) \) is the minimum value of the \( S(q, q) \)'s over treatment arms in \( Q_S \) only.

Second, we construct a covariance estimator. It is a combination of the covariance estimators discussed in Sections 3.1 and 3.2. For the treatment arms with replications, we can calculate sample variances of the potential outcomes based on the observed data. For the treatment arms without replications \( Q_u \), we need the grouping strategy in Definition 4. Therefore, we construct a diagonal covariance estimator \( \hat{V}_Y \) with the \( q \)-th diagonal term

\[
\hat{V}_Y(q, q) = \begin{cases} 
\mu_{(g)}(Y_q - \hat{Y}_{(g)})^2, & q \in Q_U \\
\hat{S}(q, q), & q \in Q_R \cup Q_L.
\end{cases}
\]

In a matrix form, it is equivalent to

\[
\hat{V}_Y = \begin{pmatrix}
\hat{V}_{Y,u} & 0 & 0 \\
0 & \hat{V}_{Y,r} & 0 \\
0 & 0 & \hat{V}_{Y,l}
\end{pmatrix},
\]

where \( \hat{V}_{Y,u} \), \( \hat{V}_{Y,r} \), \( \hat{V}_{Y,l} \) corresponds to the diagonal covariance estimators for treatment arms \( Q_u \), \( Q_r \), \( Q_l \), respectively. Partition the contrast matrix \( F \) accordingly as

\[
F = \begin{pmatrix} F_S \\ F_U \\
F_R \\
F_L \end{pmatrix} \quad \text{where} \quad F_S = \begin{pmatrix} F_U \\ F_R \end{pmatrix}.
\]

Construct the final covariance estimator below:

\[
\hat{V}_\gamma = F^T \hat{V}_Y F = F_U^T \hat{V}_{Y,u} F_U + F_R^T \hat{V}_{Y,r} F_R + F_L^T \hat{V}_{Y,l} F_L.
\]

The decomposition in (29) allows us to characterize the statistical properties of \( \hat{V}_Y \) by combining the results from Sections 3.1 and 3.2.

**Theorem 9** (Covariance estimation for non-uniform designs). Consider designs in Definition 3 and the covariance estimator in (29). Assume Conditions 3, 5, and 6. Assume \( \max_{g \in [G]} \mu_{(g)}, \Delta \) and \( \zeta \) are constants.

(i) \( \mathbb{E}\{\hat{V}_\gamma\} \succeq V_\gamma \).

(ii) We have

\[
\|\hat{V}_\gamma - \mathbb{E}\{\hat{V}_\gamma\}\|_\infty^2 = O_P(\|F_U\|_\infty^4|Q_U|H^2 + \|F_R\|_\infty^4|Q_R|H^2 + \|F_L\|_\infty^4|Q_L|N^{-3}L_3 H^2).
\]

(iii) We have

\[
\|\hat{V}_\gamma - \mathbb{E}\{\hat{V}_\gamma\}\|_{op}^2 = O_P(\|F_U\|_\infty^4|Q_U|H^4 + \|F_R\|_\infty^4|Q_R|H^4 + \|F_L\|_\infty^4|Q_L|N^{-3}L_3 H^4).
\]
In Theorem 9, we assume \( \max_{g \in G} \mu(g) \), \( \Delta \) and \( \zeta \) to be constants to simplify the presentation. Without this assumption, we can derive results similar to those in Theorem 6 but relegate finer results to the supplementary material. Theorem 9(i) shows the conservativeness of \( \hat{V}_\gamma \) as a direct consequence of Theorems 3(i) and 6(i). Theorem 9(ii) and (iii) show the stochastic order of the estimation error of \( \hat{V}_\gamma \) in \( L_\infty \) norm and operator norm, respectively. We only discuss Theorem 9(ii) below. If \( \|F\|_\infty = O(Q^{-1}) \) as in the factorial design in Example 1, it reduces to

\[
\|\hat{V}_\gamma - \mathbb{E}\{\hat{V}_\gamma\}\|_\infty = O_P\left(Q^{-2}H\left(|Q_U|^{1/2} + |Q_R|^{1/2} + |Q_L|^2N^{-3/2}_L\right)\right).
\]

Therefore, if \( N \) and \( Q \) are of the same order, then \( N\|\hat{V}_\gamma - \mathbb{E}\{\hat{V}_\gamma\}\|_\infty = O_P(HN^{-1/2}) \). Besides, when one or two of \( Q_U, Q_R, Q_L \) are small or absent, the stochastic orders in Theorem 9 still hold because the large terms in (30) will dominate the rest. In particular, if \( |Q_U| = |Q_R| = 0 \), then \( \|\hat{V}_\gamma - \mathbb{E}\{\hat{V}_\gamma\}\|_\infty = O_P(HN^{-3/2}_u) \), which gives the same rate as Theorem 3. If \( |Q_L| = 0 \), then we should interpret \( 0 \cdot \infty = 0 \) in Theorem 9(ii) to obtain \( \|\hat{V}_\gamma - \mathbb{E}\{\hat{V}_\gamma\}\|_\infty = O_P(HQ^{-3/2}) = O_P(HN^{-3/2}_s) \), which also agrees with Theorem 3.

Finally, the BEB on the quadratic form \( T \) and the conservativeness of the covariance estimator ensure Theorem 10 below for inference.

**Theorem 10** (Wald-type inference under non-uniform designs). Consider the non-uniform design in Definition 3 with (14) and \( N = O(Q) \). Assume Conditions 1–6. Then the conclusions of Theorem 4 holds if we use the covariance estimator in (29).

This concludes our discussion of design-based causal inference with possibly diverging number of treatment levels and varying group sizes across treatment levels.

### 4. Simulation

In this section, we will evaluate the finite-sample properties of the point estimates and the proposed variance estimator in factorial experiments. We mainly consider non-uniform designs because there have been extensive numerical studies for nearly uniform designs before.

#### 4.1. Practical implementation

For illustration purposes, we focus on conducting inference for the main effects in non-uniform factorial designs. To do this, we need grouping strategies to implement the proposed variance estimator (28). As we discussed in Section 3.2, the structure of factorial designs can provide some practical guidance on the choice of grouping strategy. Besides, our theoretical results in Theorem (6) also give insights in reducing the conservativeness of the variance estimator. In our simulation, we will compare three variance estimation strategies:

(i) **Pairing according to the lexicographical order.** This corresponds to our discussion in Example 4. If arms with similar factor combinations have close means, pairing based on the
lexicographical order can guarantee small between-arm discrepancy in means and reduce the conservativeness.

Moreover, pairing strategies have another benefit in factorial experiments. We can use a smaller correction factor \( \tilde{\mu}_{\langle g \rangle} \) for variance estimation if our goal is to conduct inference marginally (i.e. build confidence intervals on each of \( \gamma_h \) separately). The reason is that, while it is hard to control the \( \Omega \) matrix in Theorem 6(i) in general, we can control the diagonals of \( F_u^T \Omega F_u \) because \( F_u \) has element \( \pm Q^{-1} \). We can get more intuition by noticing that \( \sum_{q' \in \langle g \rangle, q' \neq q} S(q', q') \) is the core of \( \Omega(q, q) \) and that the following algebraic fact holds under pairing:

\[
\sum_{q \in Q_u} \sum_{q' \in \langle g \rangle, q' \neq q} S(q', q') = \sum_{q \in Q_u} S(q, q). \tag{31}\]

The identity (31) enables us to transform the diagonals of \( F_u^T \Omega F_u \) from a source of conservativeness to the part of the true variance. Hence it allows us to choose a smaller correction factor:

\[
\tilde{\mu}_{\langle g \rangle} = (1 - |\langle g \rangle|^{-1})^{-1}(1 - 3N^{-1})^{-1} = 2(1 - 3N^{-1})^{-1},
\]

which is approximately one half of \( \mu_{\langle g \rangle} = 4(1 - 2N^{-1})^{-1} \) in (21) when \( N \) is large.

(ii) **Regression-based variance estimation with the target factors as regressors.** Regression-based approach is a commonly used strategy for analyzing factorial experiments. For non-uniform designs, Zhao and Ding (2022) pointed out ordinary least squares (OLS) with unsaturated model specifications can give biased point estimates and variance estimator. Instead, one should apply weighted least squares (WLS) and the sandwich variance estimation.

(iii) **Regression-based variance estimation with the target factors and their high order interactions as regressors.** This strategy differs from strategy (ii) in whether the interactions are included. If all possible two-way interactions of the target factors are specified in the regression model and the true \( k \)-way (\( k \geq 3 \)) interactions are zero, then this strategy is equivalent to the general factor-based grouping strategy introduced in Example 5.

In next section, we will provide more details on implementing the above strategies in simulation.

### 4.2. Simulation settings

We set up a \( 2^{10} \) non-uniform experiment (\( K = 10 \)) according to Definition 3, with the basic parameters specified as follows:

- unreplicated arms: \( |Q_u| = 660 \) and \( N_q = 1 \) for each \( q \in Q_u \).
- replicated small arms: \( |Q_r| = 350 \) and \( N_q = 2 \) for each \( q \in Q_r \).
large arms: $|Q_l| = 14$ and $N_q = 30$ for each $q \in Q_l$.

The above setup results in a population with $N = 1780$ units. Generate the potential outcomes independently from a shifted exponential distribution:

$$Y_i(q) \sim \text{EXP}(\lambda_q) - 1/\lambda_q + \mu_q,$$

where $\lambda_q$ are randomly set as 1 or 2 with equal probability to induce heteroskedasticity. We generate two sets of $\mu_q$ and set up two numerical studies, one with small factorial effects and the other with large effects. In both experiments, the main effects for factor $F_k$ with $k = 1, 4, 7, 10$ are set as zero. A random subset of two-way of interactions are set as zero as well. All the $k$-way ($k \geq 3$) interactions are zero. We run simulation for two studies below.

**Study 1.** Generated the nonzero main effects and two-way interactions from $\text{Unif}([-0.5, -0.1] \cup [0.1, 0.5])$.

**Study 2.** Generated the nonzero main effects from $\text{Unif}([-1, -0.5] \cup [0.5, 1])$. Generated the nonzero two-way interactions in the same way as Study 1.

In each study, we focus on estimating the main factorial effects for factor $F_{2l}$ for $l = 1, \ldots, 5$. We apply the point estimates $\hat{\gamma}$ in (4) and compare three variance estimation strategies discussed in Section 4.1 above:

1. **LEX:** We use the grouping strategy based on pairing by the lexicographical order.

2. **WLS$_0$:** We use the sandwich variance estimators based on WLS with the target factors:

$$Y \sim F_2 + F_4 + F_6 + F_8 + F_{10},$$

with weights $w_i = N^{-1}Z_i$.

3. **WLS$_1$:** We use the sandwich variance estimators based on WLS with the target factors and their two-way interactions:

$$Y \sim F_2 + F_4 + F_6 + F_8 + F_{10} + \text{Interaction}_2(F_2, F_4, F_6, F_8, F_{10}),$$

with weights $w_i = N^{-1}Z_i$.

**4.3. Simulation results**

We repeat 1000 times for each study. Figure 1 shows the violin plots of the differences between the point estimates and the true parameters. Table 2 compares the aforementioned variance estimators based on two criteria: coverage rate of 95% confidence intervals and rejection rate of the null that the main effects are zero, which corresponds to the “Coverage” column and the “Rejection” column, respectively.

Figure 1 shows that, even in a highly non-uniform design, the point estimates are centered around the truth and asymptotic Normality holds when the total population $N$ is sufficiently large. Table 2 shows that the constructed confidence intervals based on all three variance estimators are
valid and robust for both small effects and large effects settings. The variance estimator based on pairing is less conservative than the sandwich variance estimator, because the between group variation induced by grouping tends to be smaller with finer groups (see Theorem 6 and the relevant discussion). For the sandwich variance estimator, including more terms into the regression can mitigate the conservativeness. In terms of the rejection rate, when the true effect size $|\gamma|$ is large (say $|\gamma| \geq 3(\text{Var}\{\hat{\gamma}\})^{1/2}$), the power of the tests are high in spite of the conservativeness of the variance estimation. However, if the effects are too small, the rejection rate could be negatively impacted. For example, in Study 1, the true main effect for factor $F_6$ is $\gamma_6 = 0.058$ (around $2.6 \ast (\text{Var}\{\hat{\gamma}_6\})^{1/2}$). From Table 2, the rejection rates of all methods for the null $|\gamma_6| = 0$ are smaller than 1, suggesting that the tests are underpowered.

![Graph](image)

(a) Non-uniform experiment under Study 1 with small effects  
(b) Non-uniform experiment under Study 2 with large effects

Figure 1: Violin plots of the differences between the estimators and true parameters for the five target effects. Figure 1(a) corresponds to Study 1 and Figure 1(b) corresponds to Study 2, respectively.

5. Discussion

We focused on scalar outcomes. Results for vector outcomes are also important in both theory and practice. Li and Ding (2017) reviewed CLTs and many applications with vector outcomes under the regime of a fixed number of treatment levels and large sample sizes within all treatment levels. We include an extension of the BEB for vector outcomes under a general regime; see Section C.5 in the supplementary material.

Asymptotic results for design-based inference are often criticized because the population of interest is finite but the asymptotic theory requires a growing sample size. Establishing BEBs
Table 2: Coverage and rejection rates based on three variance estimators

| Effects | Coverage | Rejection |
|---------|----------|-----------|
|         | LEX  | WLS-0 | WLS-1 | LEX  | WLS-0 | WLS-1 |
| Study 1 |      |       |       |      |       |       |
| $F_2$   | 0.963 | 0.977 | 0.973 | 1.000 | 1.000 | 1.000 |
| $F_4$   | 0.968 | 0.980 | 0.976 | 0.026 | 0.015 | 0.018 |
| $F_6$   | 0.974 | 0.985 | 0.982 | 0.665 | 0.600 | 0.622 |
| $F_8$   | 0.974 | 0.984 | 0.982 | 1.000 | 1.000 | 1.000 |
| $F_{10}$| 0.973 | 0.985 | 0.980 | 0.032 | 0.016 | 0.018 |
| Study 2 |      |       |       |      |       |       |
| $F_2$   | 0.977 | 0.996 | 0.995 | 1.000 | 1.000 | 1.000 |
| $F_4$   | 0.970 | 0.996 | 0.995 | 0.030 | 0.004 | 0.005 |
| $F_6$   | 0.969 | 0.994 | 0.993 | 1.000 | 1.000 | 1.000 |
| $F_8$   | 0.974 | 0.994 | 0.993 | 1.000 | 1.000 | 1.000 |
| $F_{10}$| 0.969 | 0.996 | 0.995 | 0.031 | 0.004 | 0.005 |

is an important theoretical step to characterize the finite-sample performance of the statistics. Alternatively, it is also desirable to derive non-asymptotic concentration inequalities for the estimators under the randomization model. This requires deeper understandings of sampling without replacement and permutational statistics. We leave it to future research.

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**Supplementary material.** The supplementary material contains additional results on general linear permutational statistics, randomization-based inference, and all the technical proofs.

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Supplementary materials

Appendix A reviews existing and develops new BEBs for linear permutational statistics. Appendix B gives the proofs of the results in Appendix A. Appendix C presents additional results for design-based causal inference. Appendix D gives the proofs of the results in the main paper and Appendix C.

In addition to the notation used in the main paper, we need additional notation. For a positive integer $N$, let $S_N$ denote the set of permutations over $[N]$. We use $\pi \in S_N$ to denote a permutation, which is a bijection from $[N]$ to $[N]$ with $\pi(i)$ denoting the integer on index $i$ after permutation. We also use the same notation $\pi$ to denote a random permutation, which is uniformly distributed over $S_N$.

For a matrix $M = (M(h,l)) \in \mathbb{R}^{H \times H}$, define its column, row and all-entry sums as
\[
M(+,l) = \sum_{h=1}^{H} M(h,l), \quad M(h,+) = \sum_{l=1}^{H} M(h,l), \quad M(+,+) = \sum_{h=1}^{H} \sum_{l=1}^{H} M(h,l),
\]
respectively. For two matrices $M, M' \in \mathbb{R}^{H \times H}$, define the trace inner product as
\[
\langle M, M' \rangle = \text{trace}(M^T M') = \sum_{h=1}^{H} \sum_{l=1}^{H} M_{hl} M'_{hl}.
\]
Vectorize $M$ as $\text{vec}(M)$ by stacking its column vectors. We will use the following basic result on matrix norms:
\[
\|M\|_{\text{op}} \leq H \|M\|_{\text{\infty}}. \tag{S1}
\]

A. General combinatorial Berry–Esseen bounds for linear permutational statistics

Appendix A presents general BEBs on multivariate linear permutational statistics. Section A.1 provides a unified formulation for linear permutational statistics, which includes the point estimates in the main paper as a special case. Section A.2 discusses BEBs for linear projections of multivariate permutational statistics. Section A.3 provides dimension-dependent BEBs over convex sets, which are the basic tools for proving the BEBs for the quadratic forms of linear permutational statistics.

A.1. Multivariate permutational statistics

To analyze estimates of the form (4), we need a general formulation of multivariate permutational statistics. Let $P \in \mathbb{R}^{N}$ be a random permutation matrix, which is obtained by randomly permuting the columns (or rows) of the identity matrix $I_N$. Also define $M_1, \ldots, M_H$ as $H$ deterministic $N \times N$
matrices. We want to study the random vector (Chatterjee and Meckes 2008)

\[
\Gamma = (\text{Tr}(M_1P), \ldots, \text{Tr}(M_HP))^\top.
\]  

(S2)

Each random permutation matrix \(P\) can also be represented by a random permutation \(\pi\). Then

\[
\text{Tr}(M_hP) = \sum_{i=1}^N M_h(i, \pi(i)), \quad (h = 1, \ldots, H).
\]

Example S1 below revisits complete randomization.

**Example S1** (Revisiting complete randomization). Under complete randomization, the treatment vector \(Z = (Z_1, \cdots, Z_N)\) has a correspondence with \(P\). As a toy example, consider an experiment with \(Q = 2, N_1 = 1\) and \(N_2 = 2\). One can label the rows and columns of \(P\) as follows:

\[
\begin{pmatrix}
1 & 2 & 3 \\
q = 1 & 0 & 1 \\
q = 2 & 1 & 0 \\
q = 2 & 0 & 1 \\
\end{pmatrix}
\]

The pattern of 1’s indicates exactly the treatment allocation. Generally, if we let the rows of \(P\) represent the treatment arms and view the columns as indicator vectors of individuals, a permutation over the columns means a pattern of treatment allocation for all units. We can use (S2) to reformulate the sample mean vector \(\hat{Y}\) as \(\Gamma = (\Gamma_1, \ldots, \Gamma_Q)^\top\), where \(\Gamma_q = \text{Tr}(M_qP)\) with

\[
M_q = \begin{pmatrix}
Z = 1 & \cdots & Z = q & \cdots & Z = Q \\
1 & 0_{N_1} & \cdots & N_q^{-1}Y_1(q) \cdot 1_{N_q}^\top & \cdots & 0_{NQ}^\top \\
2 & 0_{N_1} & \cdots & N_q^{-1}Y_2(q) \cdot 1_{N_q}^\top & \cdots & 0_{NQ}^\top \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\
N & 0_{N_1} & \cdots & N_q^{-1}Y_N(q) \cdot 1_{N_q}^\top & \cdots & 0_{NQ}^\top \\
\end{pmatrix}.
\]  

(S3)

Lemma S1 below gives the mean and covariance of \(\Gamma\):

**Lemma S1** (Mean and covariance of \(\Gamma\)).

(i) For random permutation matrix \(P\), we have

\[
\mathbb{E}\{P(:,i)\} = \frac{1}{N}1_N, \quad \mathbb{E}\{P(:,i)P(:,i)^\top\} = \frac{1}{N}I_N
\]  

(S4)

for all \(i\), and

\[
\mathbb{E}\{P(:,i)P(:,j)^\top\} = \frac{1}{N(N-1)}(1_{N \times N} - I_N)
\]  

(S5)
for \( i \neq j \).

(ii) For the random vector \( \Gamma \) defined in (S2), we have

\[
E\{\Gamma_h\} = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} M_h(i, j)
\]

(S6)

for all \( h \), and

\[
E\{\Gamma_h \Gamma_l\} = \frac{1}{N-1} \langle M_h, M_l \rangle + \frac{1}{N(N-1)} M_h(+, +) M_l(+, +) - \frac{1}{N(N-1)} \sum_{k=1}^{N} M_h(+, k) M_l( +, k) - \frac{1}{N(N-1)} \sum_{k=1}^{N} M_h(k, +) M_l(k, +).
\]

(S7)

for \( h \neq l \).

Special cases of Lemma S1 have appeared in some previous works under certain simplifications. For example, Hoeffding (1951) computed the mean and variance for scalar \( \Gamma \) with \( H = 1 \). Chatterjee and Meckes (2008) did the calculation under the conditions of zero row and column sums as well as orthogonality of the population matrices. Bolthausen and Gotze (1993) relaxed the constraints of orthogonality and presented the covariance formula only under the zero column sum condition.

As an application, we can obtain the mean and covariance of \( \hat{Y} \):

**Example S2** (Mean and covariance matrix of \( \hat{Y} \)). Based on (S3), we can verify that

\[
\langle M_q, M_l \rangle = 0, \text{ if } q \neq l.
\]

Using (S6), we can compute

\[
E\{\Gamma_q\} = \frac{1}{N} \sum_{i=1}^{N} Y_i(q),
\]

and

\[
E\{(\Gamma_q - E\Gamma_q)^2\} = \left( \frac{1}{N_q} - \frac{1}{N} \right) S(q, q),
\]

\[
E\{(\Gamma_q - E\Gamma_q)(\Gamma_l - E\Gamma_l)\} = -\frac{1}{N} S(q, l).
\]

From now on, for the ease of discussion, we assume Condition S1 below:

**Condition S1** (Standardized orthogonal structure of \( M_h \)’s). For each \( h \in [H] \), the row and column sums of \( M_h \) are zero and

\[
\text{Tr}(M_h^\top M_h) = N - 1.
\]

S3
The $M_h$'s are mutually orthogonal with respect to the trace inner product:

$$\text{Tr}(M_h^\top M_l) = 0, \text{ for } h \neq l.$$ 

Lemma S2 below ensures that imposing Condition S1 causes no loss of generality.

**Lemma S2** (Reformulation of the multivariate permutational statistics). Let $P$ be a random $N \times N$ permutation matrix, and $M_1, \ldots, M_H$ be $H$ deterministic $N \times N$ matrices. Let $\mathbb{E}\{\Gamma\}, V = \text{Var}\{\Gamma\}, V^* = \text{Corr}(\Gamma)$ be respectively the expectation, covariance and correlation of $\Gamma$ defined in (S2). Let $\tilde{V} = V^{-1/2}$. Define the $\{M'_h\}_{h=1}^H$ as

$$M'_h(i, j) = M_h(i, j) - N^{-1}M_h(i, +) - N^{-1}M_h(+, j) + N^{-2}M_h(+, +),$$

and then define the $\{M''_h\}_{h=1}^H$ as

$$M''_h(i, j) = \sum_{l=1}^H \tilde{V}_{hl}M'_l(i, j).$$

(i) $M''_1, \ldots, M''_H$ satisfy Condition S1 and

$$V^{-1/2}(\Gamma - \mathbb{E}\{\Gamma\}) = (\text{Tr}(M''_1 P), \ldots, \text{Tr}(M''_H P))^\top.$$

(ii) We have

$$\max_{h \in [H]} \max_{i, j \in [N]} |M''_h(i, j)| \leq \rho_{\min}(V)^{-1/2} \sqrt{H} \max_{h \in [H]} \max_{i, j \in [N]} |M'_h(i, j)|. \quad \text{(S8)}$$

**A.2. BEBs for linear projections**

In this subsection, we establish BEBs for linear permutational statistics. Bolthausen (1984) established a BEB for univariate permutational statistics, which is a basic tool for our proofs.

**Lemma S3** (Main theorem of Bolthausen (1984)). There exists an absolute constant $C > 0$, such that

$$\sup_{t \in \mathbb{R}}|\mathbb{P}\{\Gamma_1 \leq t\} - \Phi(t)| \leq C \frac{\sum_{i, j \in [N]} |M_1(i, j)|^3}{N^2}.$$ 

We can use Lemma S3 to prove Theorem S1 below.

**Theorem S1.** Assume Condition S1. Let $b \in \mathbb{R}^H$ be a vector with $\|b\|_2 = 1$. Then there exists an absolute constant $C > 0$, such that

$$\sup_{t \in \mathbb{R}}|\mathbb{P}\{b^\top \Gamma \leq t\} - \Phi(t)| \leq C \max_{i, j \in [N]} \left| \sum_{h=1}^H b_h M_h(i, j) \right|.$$
The proof of Theorem S1 is straightforward based on the theorem of Bolthausen (1984). It is more interesting to compute the upper bound in specific examples, which we will do in Appendix C. Theorem S1 is a finite-sample result. It implies a CLT when the upper bound vanishes:

$$\max_{i,j \in [N]} \left| \sum_{h=1}^{H} b_h M_h(i,j) \right| \to 0, \text{ as } N \to \infty.$$  \hspace{1cm} (S9)

We can further upper bound the left hand side of (S9):

$$\max_{i,j \in [N]} \left| \sum_{h=1}^{H} b_h M_h(i,j) \right| \leq \max_{i,j \in [N], h \in [H]} |M_h(i,j)| \cdot \|b\|_1 \leq \sqrt{H} \max_{i,j \in [N], h \in [H]} |M_h(i,j)|.$$

Hence Theorem S1 reveals a trade-off between $H$ and $\max_{i,j \in [N], h \in [H]} |M_h(i,j)|$. Alternatively, we can use the Cauchy-Schwarz inequality to obtain another bound:

$$\max_{i,j \in [N]} \left| \sum_{h=1}^{H} b_h M_h(i,j) \right| \leq \max_{i,j \in [N]} \left\{ \sum_{h=1}^{H} |M_h(i,j)|^2 \right\}^{1/2} \cdot \|b\|_2 \leq \max_{i,j \in [N]} \left\{ \sum_{h=1}^{H} |M_h(i,j)|^2 \right\}^{1/2}.$$

which can be a better bound for some $M_q$'s.

Besides, the combinatorial CLT of Hoeffding (1951, Theorem 3) establishes the following sufficient condition for $b^\top \Gamma$ converging to a standard Normal distribution:

**Lemma S4** (Combinatorial CLT by Theorem 3 of Hoeffding (1951)). $b^\top \Gamma$ is asymptotically Normal if

$$\max_{i,j \in [N]} \left\{ \sum_{h=1}^{H} b_h M_h(i,j) \right\}^2(N^{-1} \sum_{i,j \in [N]} \left\{ \sum_{h=1}^{H} b_h M_h(i,j) \right\}^2) \to 0.$$  \hspace{1cm} (S10)

Under Condition S1, we have

$$\sum_{i,j \in [N]} \left\{ \sum_{h=1}^{H} b_h M_h(i,j) \right\}^2 = N - 1.$$

Hence (S10) is equivalent to (S9). But from Theorem S1, (S10) implies not only convergence in distribution, but also an upper bound on the convergence rate in the Kolmogorov distance.

### A.3. A permutational BEB over convex sets

With independent random variables, the BEBs over convex sets match the optimal rate $N^{1/2}$ (Nagaev 1976; Bentkus 2005). We achieve the same order for linear permutational statistics by using a result based on Stein’s method (Fang and Röllin 2015).
**Definition S1** (Exchangeable pair). \((\Gamma, \Gamma')\) is an exchangeable pair if \((\Gamma, \Gamma')\) and \((\Gamma', \Gamma)\) have the same distribution.

**Definition S2** (Stein coupling, Definition 2.1 of Fang and Röllin (2015)). A triple of square integrable \(H\)-dimensional random vectors \((\Gamma, \Gamma', G)\) is called a \(H\)-dimensional Stein coupling if

\[
E\{G^\top f(\Gamma') - G^\top f(\Gamma)\} = E\{\Gamma^\top f(\Gamma)\}
\]

for all \(f : \mathbb{R}^H \to \mathbb{R}^H\) provided that the expectations exist.

Fang and Röllin (2015, Remark 2.3) made a connection between Definitions S1 and S2, shown below.

**Lemma S5** (Remark 2.3 of Fang and Röllin (2015)). If \((\Gamma, \Gamma')\) is an exchangeable pair and \(E(\Gamma' - \Gamma | \Gamma) = -\Lambda \Gamma\) for some invertible \(\Lambda\), then \((\Gamma, \Gamma', \frac{1}{2} \Lambda^{-1}(\Gamma' - \Gamma))\) is a Stein coupling.

Fang and Röllin (2015) established the following BEB based on multivariate Stein coupling.

**Lemma S6** (Theorem 2.1 of Fang and Röllin (2015)). Let \((\Gamma, \Gamma', G)\) be a \(H\)-dimensional Stein coupling. Assume \(\text{Cov}(\Gamma) = I_H\). Let \(\xi_H\) be an \(H\)-dimensional standard Normal random vector. With \(D = \Gamma' - \Gamma\), suppose that there are positive constants \(\alpha\) and \(\beta\) such that \(\|G\|_2 \leq \alpha\) and \(\|D\|_2 \leq \beta\). Then there exists a universal constant \(C\), such that

\[
\sup_{A \in \mathcal{A}} |P\{\Gamma \in A\} - P\{\xi_H \in A\}| 
\leq C(H^{7/4} \alpha \|D\|_2^2 + H^{1/4} \beta + H^{7/8} \alpha^{1/2} B_1^{1/2} + H^{3/8} B_2 + H^{1/8} B_3^{1/2}),
\]

where

\[
B_1^2 = \text{Var}\{E(\|D\|_2^2 | \Gamma)\},
\]

\[
B_2^2 = H \sum_{h=1}^H \sum_{l=1}^H \text{Var}\{E(G_h D_l | \Gamma)\},
\]

\[
B_3^2 = H \sum_{h=1}^H \sum_{l=1}^H \sum_{m=1}^H \text{Var}\{E(G_h D_l D_m | \Gamma)\}.
\]

Our construction of exchangeable pairs for linear permutational statistics is motivated by Chatterjee and Meckes (2007). For \(\Gamma\), construct a coupling random vector \(\Gamma'\) by performing a random transposition to the original pattern of permutation. Here a random transposition is defined as follows:

**Definition S3** (Random transposition). The set of transpositions \(\mathcal{T}_N = \{(t_1 t_2)\}\) is defined as the subset of permutations over \([N]\) which only switches two indices \(t_1\) and \(t_2\) among \(\{1, \ldots, N\}\) while keeping the other fixed. A random transposition \(\tau\) takes a uniform distribution on \(\mathcal{T}_N\).
If a random transposition $\tau$ and a random permutation $\pi$ are independent, their composite $\pi' = \tau \circ \pi$ is also a random permutation over $[N]$. As we discussed in Section A.1, $\pi$ and $\pi'$ can be represented as random permutation matrices $P$ and $P'$. Let

$$\Gamma' = (\text{Tr}(M_1 P'), \ldots, \text{Tr}(M_H P'))^\top.$$  \hfill (S11)

Now $(\Gamma, \Gamma')$ is an exchangeable pair and has the following basic property.

**Lemma S7** (Lemma 8 of Chatterjee and Meckes (2007)).  
$$\mathbb{E}\{\Gamma' - \Gamma \mid \pi\} = -\frac{2}{N-1} \Gamma.$$  

By Lemmas S5 and S7, $(\Gamma, \Gamma', -\frac{N-1}{4}(\Gamma - \Gamma'))$ with $G = -\frac{N-1}{4}(\Gamma - \Gamma')$ is a Stein coupling.

We prove the following result based on Lemma S6:

**Theorem S2** (Permutational BEB over convex sets). Assume $|M_h(i,j)| \leq B_N$ for $h \in [H]$ and $i,j \in [N]$. Assume Condition S1. Then there exists a universal constant $C > 0$, such that

$$\sup_{A \in \mathcal{A}} |\mathbb{P}\{\Gamma \in A\} - \mathbb{P}\{\xi_H \in A\}| \leq C \frac{H^{13/4} N B_N^2 + C H^{13/4} N^{1/4} B_N^{3/2} + C H^{11/8} N^{1/2} B_N^2}{N^{1/2}}.$$  \hfill (S12)

When $B_N = O(N^{-1/2})$, the upper bound (S12) becomes

$$\sup_{A \in \mathcal{A}} |\mathbb{P}\{\Gamma \in A\} - \mathbb{P}\{\xi_H \in A\}| \leq C \frac{H^{13/4}}{N^{1/2}}.$$  \hfill (S13)

To end this subsection, we briefly comment on the literature of multivariate permutational BEBs and make a comparison between the existing results and Theorem S2. Bolthausen and Gotze (1993) proved a multivariate permutational BEB under some conditions, but their bound did not specify explicit dependence on the dimension ($H$ in our notation). Chatterjee and Meckes (2007) proposed methods based on exchangeable pairs for multivariate normal approximation and applied it to permutational distributions. However, their methods only allows to establish the following result:

$$\sup_{g \in C^2(\mathbb{R}^H)} |\mathbb{E}\{g(\Gamma)\} - \mathbb{E}\{g(\xi_H)\}| \leq C \frac{H^3}{N^{1/2}}.$$  \hfill (S14)

where $C^2(\mathbb{R}^H)$ represents the collection of second-order continuously differentiable functions on $\mathbb{R}^H$. While the rate over $H$ is slightly better than (S13), the function class $C^2(\mathbb{R}^H)$ cannot cover the indicator functions. Răic (2015) conjectured the following result:

$$\sup_{A \in \mathcal{A}} |\mathbb{P}\{\Gamma \in A\} - \mathbb{P}\{\xi_H \in A\}| \leq C \frac{H^{1/4}}{N} \sum_{i \in [N]} \sum_{j \in [N]} \left( \sum_{h \in [H]} M_h(i,j)^2 \right)^{3/2}.$$  \hfill (S14)

When $B_N = O(N^{-1/2})$, (S14) has order $O(H^{7/4} N^{-1/2})$. However, Răic (2015) did not provide any
proof for (S14). Wang and Li (2022) proved a BEB for binary treatment randomized experiment using the coupling method, with the dependence on \( N \) is slower than \( N^{-1/2} \). The dependence on \( H \) may be further improved but it is beyond the scope of the current work.

B. Proofs of the results in Appendix A

In this section, we prove the results in Appendix A. Section B.1 presents several lemmas that are essential to the proofs. The main proofs start from Section B.4.

B.1. Lemmas

Lemma S8 below gives the conditional moments of the exchangeable pair \((\Gamma, \Gamma')\) constructed in (S2) and (S11).

Lemma S8 (Lemma 8 in Chatterjee and Meckes (2007)). Construct an exchangeable pair \((\Gamma, \Gamma')\) based on (S2) and (S11).

(i) We restate Lemma S7:

\[
E\{\Gamma' - \Gamma \mid \pi\} = -\frac{2}{N-1}\Gamma.
\]

(ii) For the \(h\)-th coordinate \((\Gamma_h, \Gamma_h')\), we have

\[
E\{(\Gamma_h - \Gamma_h')^2 \mid \pi\} = \frac{2(N+1)}{N(N-1)} \sum_{i=1}^{N} M_h(i, \pi(i))^2 + \frac{2}{N} + \frac{2}{N(N-1)} \Gamma_h^2 + \frac{2}{N(N-1)} \sum_{i \neq j} M_h(i, \pi(j)) M_h(j, \pi(i)).
\]

(iii) For the \(h\)-th coordinate \((\Gamma_h, \Gamma_h')\) and \(l\)-th coordinate \((\Gamma_l, \Gamma_l')\), we have

\[
E\{(\Gamma_h - \Gamma_h')(\Gamma_l - \Gamma_l') \mid \pi\} = \frac{2(N+1)}{N(N-1)} \sum_{i=1}^{N} M_h(i, \pi(i)) M_l(i, \pi(i)) + \frac{2}{N(N-1)} \Gamma_h \Gamma_l + \frac{2}{N(N-1)} \sum_{i \neq j} M_h(i, \pi(j)) M_l(j, \pi(i)).
\]

Lemma S9 below bounds the variances of linear permutational statistics.

Lemma S9. We have the following variance bounds for \( N \) large enough.

(i) \( \text{Var}\left\{ \sum_{h=1}^{H} X_h \right\} \leq H \sum_{h=1}^{H} \text{Var}\{X_i\}. \)
(ii) If \(|M_0(i, j)| \leq B_N\), then
\[
\text{Var} \left\{ \sum_{i=1}^{N} M_0(i, \pi(i)) \right\} = (N - 1)^{-1} \sum_{i=1}^{N} \sum_{j=1}^{N} \left\{ M_0(i, \pi(i)) - N^{-1}M_0(i, +) - N^{-1}M_0(+, j) + N^{-2}M_0(+, +) \right\}^2 \\
\leq 32NB_N^2. \tag{S15}
\]

(iii) Suppose \(M_1 = (a_{ij})\) and \(M_2 = (b_{ij})\) have zero column and row sums. If \(|a_{ij}| \leq B_N, |b_{ij}| \leq B'_N\), then
\[
\text{Var} \left\{ \sum_{i\neq j} a_{i\pi(i)}b_{j\pi(j)} \right\} \leq 54N^2B_N^2B_N'^2.
\]

(iv) Suppose \(M_1 = (a_{ij})\) and \(M_2 = (b_{ij})\) have zero column and row sums. If \(|a_{ij}| \leq B_N, |b_{ij}| \leq B'_N\), then
\[
\text{Var} \left\{ \sum_{i\neq j} a_{i\pi(j)}b_{j\pi(i)} \right\} \leq 54N^2B_N^2B_N'^2.
\]

(v) Suppose \(M_1 = (a_{ij}), M_2 = (b_{ij}), M_3 = (c_{ij})\) all have zero column and row sums. If \(|a_{ij}| \leq B_N, |b_{ij}| \leq B'_N, |c_{ij}| \leq B''_N\), then
\[
\text{Var} \left\{ \sum_{i\neq j} a_{i\pi(i)}b_{j\pi(j)}c_{i\pi(j)} \right\} \leq 15N^3B_N^2B_N'^2B_N''^2.
\]

(vi) Suppose \(M_1 = (a_{ij}), M_2 = (b_{ij}), M_3 = (c_{ij})\) all have zero column and row sums. If \(|a_{ij}| \leq B_N, |b_{ij}| \leq B'_N, |c_{ij}| \leq B''_N\), then
\[
\text{Var} \left\{ \sum_{i\neq j} a_{i\pi(i)}b_{j\pi(i)}c_{i\pi(j)} \right\} \leq 15N^3B_N^2B_N'^2B_N''^2.
\]

Proof of Lemma S9. (i) This is a standard result by the Cauchy-Schwarz inequality.

(ii) This is due to the variance formula of linear permutational statistics. See Lemma S1.

(iii) We calculate
\[
\mathbb{E} \left\{ \sum_{i\neq j} a_{i\pi(i)}b_{j\pi(j)} \right\}^2
\]
\[
E \left\{ \sum_{i,k} \sum_{j,l \neq k} a_{i\pi(i)} b_{j\pi(j)} a_{k\pi(k)} b_{l\pi(l)} \right\} \\
= \frac{1}{N(N-1)} \sum_{i,j,m \neq n} \left\{ a_{im}^2 b_{jn}^2 + a_{in} b_{jn} a_{jm} b_{jm} \right\} \\
+ \frac{1}{N(N-1)(N-2)} \sum_{i,j,k} \sum_{m,n \neq o} \left\{ a_{im} b_{jn} b_{ko} + a_{im} a_{jn} b_{ko}^2 + a_{im} b_{im} a_{jn} b_{ko} + a_{im} b_{jn} a_{ko} b_{ko} \right\} \\
+ \frac{1}{N(N-1)(N-2)(N-3)} \sum_{i,j,k,l} \sum_{m,n,o \neq p} \left\{ a_{im} b_{jn} a_{ko} b_{lp} \right\} \\
= I + II + III.
\]

For I, we have

\[
N(N-1)I \leq N^2(N-1)^2 \cdot 2B_N^2 B_N'^2 = 2N^2(N-1)^2 B_N^2 B_N'^2.
\]  \hspace{1cm} (S16)

For II, using the property of zero column and row sums, we have

\[
N(N-1)(N-2)II \leq 16N^2(N-1)^2 B_N^2 B_N'^2.
\]  \hspace{1cm} (S17)

To see why (S17) is true, consider the first part of the summation:

\[
\left| \sum_{i,j,k} \sum_{m,n \neq o} a_{im}^2 b_{jn} b_{ko} \right| \\
= \left| \sum_{i,j,k} \sum_{m,n \neq o} a_{im}^2 b_{jn} (-b_{km} - b_{kn}) \right| \\
= \left| \sum_{i,j} \sum_{m,n \neq o} a_{im}^2 b_{jn} (b_{im} + b_{jm} + b_{jn}) \right| \\
\leq 4N^2(N-1)^2 B_N^2 B_N'^2.
\]

Similar results hold for the other parts of the summation. Adding terms together, we obtain (S17).

For III, use the zero column and row sums property again, we have

\[
N(N-1)(N-2)(N-3)III \leq 36N^2(N-1)^2 B_N^2 B_N'^2.
\]  \hspace{1cm} (S18)
Summing up (S16)–(S18) to obtain

\[
\text{Var} \left\{ \sum_{i \neq j} a_{i \pi(i)} b_{j \pi(j)} \right\} \leq 54N^2B_N^2B'_N^2.
\]

(iv) We calculate

\[
\mathbb{E} \left\{ \sum_{i \neq j} a_{i \pi(j)} b_{j \pi(i)} \right\}^2 = \mathbb{E} \left\{ \sum_{i, k, j \neq i, l \neq k} a_{i \pi(j)} b_{j \pi(i)} a_{k \pi(l)} b_{l \pi(k)} \right\}
\]

\[
= \frac{1}{N(N-1)} \sum_{i \neq j, m \neq n} \left\{ a_{im}^2 b_{jn}^2 + a_{im} b_{im} a_{jn} b_{jn} \right\}
\]

\[
+ \frac{1}{N(N-1)(N-2)} \sum_{i \neq j, k \neq l, m \neq n \neq o} \left\{ a_{im} b_{jm} a_{io} b_{ko} b_{kn} \right\}
\]

\[
+ \frac{1}{N(N-1)(N-2)(N-3)} \sum_{i \neq j, k \neq l, m \neq n \neq o \neq p} \left\{ a_{im} b_{jm} b_{km} c_{kn} \right\}
\]

\[
= I + II + III.
\]

The rest of the analysis is nearly identical to part (iii). We omit the details.

(v) We calculate

\[
\mathbb{E} \left\{ \sum_{i \neq j} a_{i \pi(i)} b_{j \pi(j)} c_{i \pi(j)} \right\}^2 = \mathbb{E} \left\{ \sum_{i, j, k \neq i, l \neq k} a_{i \pi(j)} b_{j \pi(i)} c_{i \pi(j)} a_{k \pi(l)} b_{l \pi(k)} c_{k \pi(l)} \right\}
\]

\[
= \frac{1}{N(N-1)} \sum_{i \neq j, m \neq n} \left\{ a_{im}^2 b_{jn}^2 c_{in}^2 + a_{im} b_{jm} c_{in} a_{jn} b_{im} c_{jm} \right\}
\]

\[
+ \frac{1}{N(N-1)(N-2)} \sum_{i \neq j, k \neq l, m \neq n \neq o} \left\{ a_{im}^2 b_{jm} c_{in} a_{ko} b_{km} c_{kn} \right\}
\]

\[
+ \frac{1}{N(N-1)(N-2)(N-3)} \sum_{i \neq j, k \neq l, m \neq n \neq o \neq p} a_{im} b_{jm} c_{in} a_{ko} b_{lp} c_{kp}
\]

\[
= I + II + III.
\]
For I, using the triangle inequality, we have

\[ N(N - 1)I \leq 2N^2(N - 1)^2 B_N^2 B_N'^2 B_N''. \quad \text{(S19)} \]

For II, using the triangle inequality, we have

\[ N(N - 1)(N - 2)II \leq 4N^2(N - 1)^2(N - 2)^2 B_N^2 B_N'^2 B_N''. \quad \text{(S20)} \]

For III, expanding along the indices \( l \) and \( o \), we have

\[ N(N - 1)(N - 2)(N - 3)III \leq 9N^6 B_N^2 B_N'^2 B_N''. \quad \text{(S21)} \]

Sum up (S19)–(S21) to get the final result.

(vi) We calculate

\[
\mathbb{E}\left\{ \sum_{i \neq j}^{N} a_{i\pi(i)}b_{j\pi(j)}c_{i\pi(j)} \right\}^2 \\
= \mathbb{E}\left\{ \sum_{i \neq j} \sum_{k \neq l} a_{i\pi(i)}b_{j\pi(j)}c_{i\pi(k)}b_{l\pi(l)}c_{k\pi(l)} \right\} \\
= \frac{1}{N(N - 1)} \sum_{i \neq j} \sum_{m \neq n} \left\{ a_{im}^2 b_{jm}^2 c_{in}^2 + a_{im} b_{jm} c_{in} a_{jn} c_{jm} \right\} \\
+ \frac{1}{N(N - 1)(N - 2)} \sum_{i \neq j \neq k} \sum_{m \neq n \neq o} \left\{ a_{im}^2 b_{jm} c_{in} b_{km} c_{io} + a_{im} b_{jm} c_{in} a_{ko} c_{io} c_{km} \right. \\
\quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad + a_{im} b_{jm} c_{in} a_{jn} c_{jo} c_{kn} + a_{im} b_{jm} c_{in} a_{ko} b_{jo} c_{kp} \right\} \\
= I + II + III.
\]

For I, using the triangle inequality, we have

\[ N(N - 1)I \leq 2N^2(N - 1)^2 B_N^2 B_N'^2 B_N''. \quad \text{(S22)} \]

For II, using the triangle inequality, we have

\[ N(N - 1)(N - 2)II \leq 4N^2(N - 1)^2(N - 2)^2 B_N^2 B_N'^2 B_N''. \quad \text{(S23)} \]
For III, expanding along the indices \( l \) and \( p \), we have

\[
N(N-1)(N-2)(N-3)\III \leq 9N^6B_N^2B_N'^2B_N''^2. 
\] (S24)

Sum up (S22)–(S24) to get the final result.

\[
\square
\]

B.2. Proof of Lemma S1

The proof follows from combining the permutational distribution of \( P \) with matrix algebra.

Proof of Lemma S1. Proof of (S4). Use the fact that each column of \( P \) follows a uniform distribution over the canonical bases.

Proof of (S5). Use the fact that \( P(·, i)P(·, j)^\top \) is uniformly distributed over all the \( N(N-1) \) off-diagonal positions.

Proof of (S6). (S6) follows from Lemma S1(i) and the linearity of \( \text{Tr}(·) \).

Proof of (S7). For (S7), we have

\[
\mathbb{E}\{\Gamma_h\Gamma_l\} = \mathbb{E}\left\{ \left( \sum_{i=1}^N M_h(i, ·)P(·, i) \right) \left( \sum_{i=1}^N M_l(i, ·)P(·, i) \right) \right\}
\]

\[
= \mathbb{E}\left\{ \sum_{i=1}^N M_h(i, ·)P(·, i) \sum_{i=1}^N M_l(i, ·)P(·, i) \right\}
\]

\[
= \mathbb{E}\left\{ \sum_{i=1}^N \sum_{j=1}^N M_h(i, ·)P(·, i)P(·, j)^\top M_l(j, ·)^\top \right\}
\]

\[
= \frac{1}{N} \sum_{i=1}^N M_h(i, ·)M_l(i, ·)^\top + \frac{1}{N(N-1)} \sum_{i \neq j}^N M_h(i, ·)(1_{N \times N} - I_N)M_l(j, ·)^\top
\]

\[
= \frac{1}{N-1} \sum_{i=1}^N M_h(i, ·)M_l(i, ·)^\top + \frac{1}{N(N-1)} \sum_{i \neq j}^N M_h(i, ·)1_{N \times N}M_l(j, ·)^\top
\]

\[
- \frac{1}{N(N-1)} \left\{ \sum_{i=1}^N M_h(i, ·) \right\} \left\{ \sum_{i=1}^N M_l(i, ·)^\top \right\}
\]

\[
= \frac{1}{N-1} \langle M_h, M_l \rangle + \frac{1}{N(N-1)} \sum_{i \neq j}^N M_h(i, +)M_l(j, +) - \frac{1}{N(N-1)} \sum_{k=1}^N M_h(+, k)M_l(+, k)
\]

\[
= \frac{1}{N-1} \langle M_h, M_l \rangle + \frac{1}{N(N-1)} \sum_{i=1}^N M_h(i, +)M_l(j, +)
\]

\[
- \frac{1}{N(N-1)} \sum_{k=1}^N M_h(+, k)M_l(+, k) - \frac{1}{N(N-1)} \sum_{k=1}^N M_h(k, +)M_l(k, +)
\]

\[
= \frac{1}{N-1} \langle M_h, M_l \rangle + \frac{1}{N(N-1)} M_h(+, +)M_l(+, +)
\]
\[- \frac{1}{N(N - 1)} \sum_{k=1}^{N} M_h(+, k) M_l(+, k) - \frac{1}{N(N - 1)} \sum_{k=1}^{N} M_h(k, +) M_l(k, +). \]

**B.3. Proof of Lemma S2**

**Proof of Lemma S2.** (i) By definition,

\[
\Gamma_h - \mathbb{E}\{\Gamma_h\} = \sum_{i=1}^{N} M_h(i, \pi(i)) - N^{-1} \sum_{i=1}^{N} \sum_{j=1}^{N} M_h(i, j) \\
= \sum_{i=1}^{N} V_{hh}^{-1/2} \left\{ M_h(i, \pi(i)) - N^{-1} M_h(i, +) - N^{-1} M_h(+, \pi(i)) + N^{-2} M_h(+, +) \right\}.
\]

Now introduce a new matrix \( M'_h \) with entries

\[
M'_h(i, j) = M_h(i, j) - N^{-1} M_h(i, +) - N^{-1} M_h(+, j) + N^{-2} M_h(+, +). \tag{S25}
\]

Let \( \tilde{V} = V^{-1/2} \) and let \( \tilde{\Gamma} = \tilde{V} (\Gamma - \mathbb{E}\{\Gamma\}) \) with \( \text{Var}\{\tilde{\Gamma}\} = I_H, \mathbb{E}\{\tilde{\Gamma}\} = 0. \) Define \( M''_h = \sum_{l=1}^{H} \tilde{V}_{hl} M'_l. \)

Because \( M'_h \)'s have zero row and column sums, we can verify that \( M''_h \)'s also satisfy:

\[
M''_h(i, +) = 0, \quad M''_h(+, j) = 0, \quad \forall \ i, j \in [N].
\]

Besides,

\[
\tilde{\Gamma}_h = \sum_{l=1}^{H} \tilde{V}_{hl}(\text{Tr}(M'_l P) - \mathbb{E}\{\text{Tr}(M'_l P)\}) = \text{Tr}(M''_h P).
\]

Hence, combining Lemma S1, we have

\[
\mathbb{E}\{\tilde{\Gamma}_h \tilde{\Gamma}_l\} = \frac{1}{N - 1} \langle M''_h, M''_l \rangle + \frac{1}{N(N - 1)} M''_h(+, +) M''_l(+, +) \\
- \frac{1}{N(N - 1)} \sum_{k=1}^{N} M''_h(+, k) M''_l(+, k) - \frac{1}{N(N - 1)} \sum_{k=1}^{N} M''_h(k, +) M''_l(k, +) \tag{S26}
\]

\[
= \frac{1}{N - 1} \langle M''_h, M''_l \rangle. \tag{S27}
\]

Recall

\[
\mathbb{E}\{\tilde{\Gamma}_h \tilde{\Gamma}_l\} = \begin{cases} 1, & h = l; \\ 0, & h \neq l. \end{cases} \tag{S28}
\]
Combining (S26) and (S28), we conclude

\[
\frac{1}{N-1} \langle M''_h, M''_l \rangle = \begin{cases} 
1, & h = l; \\
0, & h \neq l. 
\end{cases}
\]

Therefore, Condition S1 holds for \( M''_h \)'s.

(ii) For \( i, j \in [N] \), define the vectors

\[
c' = [M'_1(i,j), \ldots, M'_H(i,j)]^\top \in \mathbb{R}^H 
\]

and

\[
c'' = [M''_1(i,j), \ldots, M''_H(i,j)]^\top \in \mathbb{R}^H. 
\]

We have

\[
\max_{h=1,\ldots,H} |M''_h(i,j)| \leq \|c''\|_2 \leq \theta_{\min}(V)^{-1/2} \|c'\|_2 \leq \theta_{\min}(V)^{-1/2} \sqrt{H} \max_{h=1,\ldots,H} |M'_h(i,j)|. 
\]

\[\square\]

B.4. Proof of Theorem S1

Proving Theorem S1 reduces to checking the conditions of Lemma S3.

Proof of Theorem S1. We have

\[
b^\top \Gamma = \sum_{h=1}^H b_h \text{Tr} (M_h P) = \text{Tr} \left( \sum_{h=1}^H b_h M_h \right) P. 
\]

Define

\[
M' = \sum_{h=1}^H b_h M_h. 
\]

We can verify that the row sums and column sums of \( M' \) are all zero. Also, using Condition S1,

\[
\langle M', M' \rangle = \sum_{h=1, l=1}^H b_h b_l \langle M_h, M_l \rangle = (N-1) \sum_{h=1}^H b_h^2 = N-1. 
\]

(S29)

Applying Lemma S3, there exists an absolute constant \( C > 0 \), such that

\[
\sup_{t \in \mathbb{R}} |\mathbb{P}\{b^\top T \leq t\} - \Phi(t)| \leq \frac{C}{N} \sum_{i,j} |M'(i,j)|^3 \leq \frac{C(N-1)}{N} \max_{i,j\in[N]} |M'(i,j)| \leq C \max_{i,j\in[N]} |M'(i,j)|. 
\]

\[\square\]
B.5. Proof of Theorem S2

Proof of Theorem S2. We will apply Lemma S6. The key step is to figure out the orders of $B_1, B_2, B_3$ in Lemma S6. One can upper bound $\text{Var} \{ \mathbb{E}(\cdot | \Gamma) \}$ by $\text{Var} \{ \mathbb{E}(\cdot | F) \}$ if $\sigma(\Gamma) \subset F$. This is a standard trick in Stein’s method and will be used without further mentioning.

Now we compute the quantities involved in Lemma S6. Recall we use the random transposition $\tau = (IJ)$ to construct exchangeable pairs. The $h$-th coordinate of $D = \Gamma' - \Gamma$ equals

$$D_h = M_h(I, \pi(I)) + M_h(J, \pi(J)) - M_h(I, \pi(J)) - M_h(J, \pi(I)).$$

Hence

$$|D_h| \leq 4B_N, \quad |G_h| \leq (N - 1)B_N, \quad \|D\|_2 \leq 4\sqrt{HB_N}, \quad \|G\|_2 \leq (N - 1)\sqrt{HB_N}.$$

To apply Lemma S6, we need to bound the following quantities:

(i) $\mathbb{E}\{\|D\|_2^2 | \pi\}$ and $\mathbb{E}\{\|D\|_2^2\}$.

(ii) $B_1 = \sqrt{\text{Var} \{ \mathbb{E}(\|D\|_2^2 | \Gamma) \}}$ and $B_2 = \sqrt{\sum_{k,l=1}^{H} \text{Var} \{ \mathbb{E}(G_hD_l | \Gamma) \}}$.

(iii) $B_3 = \sqrt{\sum_{k,l,m=1}^{H} \text{Var} \{ \mathbb{E}(G_hD_lD_m | \Gamma) \}}$.

(i) **Bound $\mathbb{E}\{\|D\|_2^2 | \pi\}$ and $\mathbb{E}\{\|D\|_2^2\}$.**

By Lemma S8,

$$\mathbb{E}\{\|D\|_2^2 | \pi\} = \sum_{h=1}^{H} \mathbb{E}\{D_h^2 | \pi\} = \sum_{h=1}^{H} \mathbb{E}\{(\Gamma_h - \Gamma'_h)^2 | \pi\}$$

$$= \frac{2(N + 1)}{N(N - 1)} \sum_{h=1}^{H} \sum_{i=1}^{N} M_h(i, \pi(i))^2 + \frac{2H}{N} + \frac{2}{N(N - 1)} \sum_{h=1}^{H} \Gamma_h^2$$

$$+ \frac{2}{N(N - 1)} \sum_{h=1}^{H} \sum_{i \neq j} M_h(i, \pi(j))M_h(j, \pi(i))$$

$$\leq \frac{2(N + 1)HB_N^2}{N - 1} + \frac{2H}{N} + \frac{2HNB_N^2}{(N - 1)} + 2HB_N^2 \leq 12HB_N^2 + \frac{2H}{N}.$$

This implies

$$\mathbb{E}\{\|D\|_2^2\} = \mathbb{E}_\pi \mathbb{E}\{\|D\|_2^2 | \pi\} \leq 12HB_N^2 + \frac{2H}{N}.$$

(ii) **Bound $B_1$ and $B_2$.**

We prove the following result: there exists a universal constant $C > 0$, such that

$$B_1 \leq CHN^{-1/2}B_N^2, \quad B_2 \leq CHN^{1/2}B_N^2.$$
By Lemma S8,

\[
\mathbb{E}\{D_h^2 \mid \pi\} = \frac{2(N + 1)}{N(N - 1)} \sum_{i=1}^{N} M_h(i, \pi(i))^2 + \frac{2}{N} + \frac{2}{N(N - 1)} \Gamma_h^2
\]

\begin{align*}
&+ \frac{2}{N(N - 1)} \sum_{i \neq j} M_h(i, \pi(j)) M_h(j, \pi(i)) \\
&= \frac{2(N + 2)}{N(N - 1)} \sum_{i=1}^{N} M_h(i, \pi(i))^2 + \frac{2}{N(N - 1)} \sum_{i \neq j} M_h(i, \pi(j)) M_h(i, \pi(j)) \\
&+ \frac{2}{N(N - 1)} \sum_{i \neq j} M_h(i, \pi(j)) M_h(j, \pi(i)) + \frac{2}{N} \\
&= I + II + III + \frac{2}{N}.
\end{align*}

For \( h \neq l \),

\[
\mathbb{E}\{D_h D_l \mid \pi\} = \frac{2(N + 1)}{N(N - 1)} \sum_{i=1}^{N} M_h(i, \pi(i)) M_l(i, \pi(i)) + \frac{2}{N(N - 1)} \Gamma_h \Gamma_l
\]

\begin{align*}
&+ \frac{2}{N(N - 1)} \sum_{i \neq j} M_h(i, \pi(j)) M_l(j, \pi(i)) \\
&= \frac{2(N + 2)}{N(N - 1)} \sum_{i=1}^{N} M_h(i, \pi(i)) M_l(i, \pi(i)) + \frac{2}{N(N - 1)} \sum_{i \neq j} M_h(i, \pi(j)) M_l(i, \pi(j)) \\
&+ \frac{2}{N(N - 1)} \sum_{i \neq j} M_h(i, \pi(j)) M_l(j, \pi(i)) \\
&= IV + V + VI.
\end{align*}

For \( B_1 \), using Lemma S9(ii)–(iv), we have

\[
\text{Var} \{I\} \leq \frac{4(N + 2)^2}{N^2(N - 1)^2} \cdot 32 N B_N^4 \leq \frac{256 B_N^4}{N},
\]

\[
\text{Var} \{II\} \leq \frac{4}{N^2(N - 1)^2} \cdot 54 N^2 B_N^4 \leq \frac{216 B_N^4}{N},
\]

\[
\text{Var} \{III\} \leq \frac{4}{N^2(N - 1)^2} \cdot 54 N^2 B_N^4 \leq \frac{256 B_N^4}{N}.
\]

Now apply Lemma S9(i) to obtain

\[
B_1^2 = \text{Var} \{\mathbb{E}(\|D\|_2^2 \mid \Gamma)\} = \text{Var} \left\{ \mathbb{E} \left( \sum_{h=1}^{H} D_h^2 \mid \Gamma \right) \right\} \leq H \sum_{h=1}^{H} \text{Var} \{\mathbb{E}(D_h^2 \mid \Gamma)\} \leq CH^2 N^{-1} B_N^4.
\]
Similarly, for $B_2$, we have

\[
B_2^2 = \sum_{h,l=1}^{H} \text{Var} \{ \mathbb{E}(G_hD_l | \Gamma) \} = \left( \frac{N-1}{4} \right)^2 \sum_{k,l=1}^{H} \text{Var} \{ \mathbb{E}(D_hD_l | \Gamma) \} \leq CH^2NB_N^3.
\]

(iii) **Bound** $B_3$.

We prove the following result: there exists a universal constant $C > 0$, such that

\[
B_3 \leq CH^{3/2}N^{1/2}B_N^3.
\]

For simplicity, we write $a_{ij} = M_h(i,j)$, $b_{ij} = M_l(i,j)$ and $c_{ij} = M_m(i,j)$. Recall $G_h = (N - 1)D_h/4$. We have

\[
\mathbb{E}\{D_hD_lD_m | \pi\} = \mathbb{E}\{(a_{I\pi(I)} + a_{J\pi(J)} - a_{I\pi(J)} - a_{J\pi(I)})
\cdot (b_{I\pi(I)} + b_{J\pi(J)} - b_{I\pi(J)} - b_{J\pi(I)})
\cdot (c_{I\pi(I)} + c_{J\pi(J)} - c_{I\pi(J)} - c_{J\pi(I)}) | \pi\}.
\]  

The expansion of (S30) has $4^3 = 64$ terms, which can be characterized by the following categories of $a_{i\pi(i)}b_{i\pi(i)}c_{i\pi(i)}$:

- $a_{I\pi(I)}b_{I\pi(I)}c_{I\pi(I)}$. There are 2 terms in total. We have

\[
\mathbb{E}\{a_{I\pi(I)}b_{I\pi(I)}c_{I\pi(I)} | \pi\} = \frac{1}{N} \sum_{i=1}^{N} a_{i\pi(i)}b_{i\pi(i)}c_{i\pi(i)}.
\]

Because $|a_{i\pi(i)}b_{i\pi(i)}c_{i\pi(i)}| \leq B_N^3$, by (S15), we have

\[
\text{Var} \{ \mathbb{E}\{a_{I\pi(I)}b_{I\pi(I)}c_{I\pi(I)} | \pi\} \} \leq \frac{32NB_N^6}{N^2} = \frac{32B_N^6}{N}.
\]

- $a_{I\pi(J)}b_{I\pi(J)}c_{I\pi(J)}$. There are 2 terms in total. We have

\[
\mathbb{E}\{a_{I\pi(J)}b_{I\pi(J)}c_{I\pi(J)} | \pi\} = \frac{1}{N(N-1)} \sum_{i\neq j}^{N} a_{i\pi(j)}b_{i\pi(j)}c_{i\pi(j)}
\]

\[
= \frac{1}{N(N-1)} \sum_{j=1}^{N} \sum_{i\neq j} a_{i\pi(j)}b_{i\pi(j)}c_{i\pi(j)}.
\]

(S31) can be viewed as univariate linear permutation statistics coming from a population matrix filled with entries that are identical on each row:

\[
d_{kl} = \sum_{m\neq l} a_{ml}b_{ml}c_{ml}.
\]
Because $|d_{kl}| \leq (N - 1)B_N^3$, by Lemma S9 (ii), we have

$$\text{Var} \left\{ \mathbb{E}\{a_{I\pi(I)}b_{I\pi(I)}c_{I\pi(I)} | \pi \} \right\} \leq \frac{16N \cdot \{(N - 1)B_N^3\}^2}{N^2(N - 1)^2} \leq \frac{32B_N^6}{N}.$$

- $a_{I\pi(I)}b_{I\pi(I)}c_{J\pi(I)}$. There are 6 terms in total. We have

$$\mathbb{E}\{a_{I\pi(I)}b_{I\pi(I)}c_{J\pi(I)} | \pi \} = \frac{1}{N(N - 1)} \sum_{i \neq j}^N a_{\pi(i)}b_{\pi(i)}c_{j\pi(i)}$$

$$= \frac{1}{N(N - 1)} \sum_{i = 1}^N \left\{ \sum_{j \neq i} a_{\pi(i)}b_{\pi(i)}c_{j\pi(i)} \right\}$$

$$= \frac{1}{N(N - 1)} \sum_{i = 1}^N \left\{ -a_{\pi(i)}b_{\pi(i)}c_{\pi(i)} \right\}$$

(since the column sums of $c_{ij}$ are all zero).

Apply Lemma S9 (ii) to obtain

$$\text{Var} \left\{ \mathbb{E}\{a_{I\pi(I)}b_{I\pi(I)}c_{J\pi(I)} | \pi \} \right\} \leq \frac{16NB_N^6}{N^2(N - 1)^2} \leq \frac{32B_N^6}{N^3}.$$

- $a_{I\pi(I)}b_{I\pi(I)}c_{J\pi(I)}$. There are 6 terms in total. This part is similar to the last one:

$$\text{Var} \left\{ \mathbb{E}\{a_{I\pi(I)}b_{I\pi(I)}c_{J\pi(I)} | \pi \} \right\} \leq \frac{16NB_N^6}{N^2(N - 1)^2} \leq \frac{32B_N^6}{N^3}.$$

- $a_{I\pi(I)}b_{J\pi(I)}c_{J\pi(I)}$. There are 6 terms in total. We have

$$\mathbb{E}\{a_{I\pi(I)}b_{J\pi(I)}c_{J\pi(I)} | \pi \} = \frac{1}{N(N - 1)} \sum_{i \neq j}^N a_{\pi(i)}b_{\pi(i)}c_{j\pi(i)}$$

$$= \frac{1}{N(N - 1)} \sum_{i = 1}^N \left\{ \sum_{j \neq i} a_{\pi(i)}b_{\pi(i)}c_{j\pi(i)} \right\}.$$

(S32) can be viewed as a univariate linear permutation statistics from a population matrix with entries

$$d_{kl} = a_{kl} \sum_{m \neq k} b_{ml}c_{ml}.$$ 

Because $|d_{kl}| \leq (N - 1)B_N^3$, we have

$$\text{Var} \left\{ \mathbb{E}\{a_{I\pi(I)}b_{I\pi(I)}c_{I\pi(I)} | \pi \} \right\} \leq \frac{16N \cdot \{(N - 1)B_N^3\}^2}{N^2(N - 1)^2} \leq \frac{16B_N^6}{N}.$$
• $a_{I\pi(i)}b_{I\pi(J)}c_{I\pi(J)}$. There are 6 terms in total. We can check (by using $\pi^{-1}$) that this term is similar to the last one:

$$\text{Var} \left\{ \mathbb{E}\{a_{I\pi(i)}b_{I\pi(J)}c_{I\pi(J)} \mid \pi \} \right\} \leq \frac{16N \cdot \{(N - 1)B_N^3\}^2}{N^2(N - 1)^2} \leq \frac{16B_N^6}{N}.$$ 

• $a_{I\pi(i)}b_{I\pi(J)}c_{J\pi(J)}$. There are 6 terms in total. Let $(d_{kl}) = (a_{kl}b_{kl})$ and $d^*_{kl} = d_{kl} - d_l - d_k + d$. be the centered version with $|d^*_{kl}| \leq 4B_N^2$. We have

$$\mathbb{E}\{a_{I\pi(i)}b_{I\pi(J)}c_{J\pi(J)} \mid \pi \} = \frac{1}{N(N - 1)} \sum_{i \neq j} a_{i\pi(i)}b_{i\pi(i)}c_{j\pi(j)}$$

$$= \frac{1}{N(N - 1)} \left\{ \sum_{i \neq j} d^*_{i\pi(i)}c_{j\pi(j)} + \sum_{i \neq j} (d_{i\pi(i)} - d_{..})c_{j\pi(j)} + \sum_{i \neq j} d_{j\pi(j)} \right\}$$

$$= I + II + III.$$

For I, by Lemma S9 (iii), we know

$$\text{Var}\{I\} \leq \frac{54N^2 \cdot (4B_N^2)^2 \cdot (B_N^2)}{N^2(N - 1)^2} \leq \frac{864B_N^6}{N^2(N - 1)^2}.$$ 

For II, by re-indexing $h = \pi(i), l = \pi(j)$, we have

$$II = \frac{1}{N(N - 1)} \sum_{l=1}^{N} \sum_{k \neq l} (d_{k} - d_{..})c_{\pi^{-1}(l)i}.$$ 

Let $e_{kl} = \sum_{m \neq l}(d_{k} - d_{..})c_{ml}$. By Lemma S9 (ii) and the fact that $|\sum_{k \neq i}(d_{k} - d_{..})c_{mi}| \leq 2(N - 1)B_N^3$, we have

$$\text{Var}\{II\} \leq \frac{32N\{(N - 1)B_N^3\}^2}{N^2(N - 1)^2} \leq \frac{128B_N^6}{N}.$$ 

For III, the analysis is similar to II:

$$\text{Var}\{III\} \leq \frac{32N\{(N - 1)B_N^3\}^2}{N^2(N - 1)^2} \leq \frac{32B_N^6}{N}.$$ 

Since $\text{Var}\{I\}$ is of lower order compared with that of II and III, we have

$$\text{Var}\{\mathbb{E}\{a_{I\pi(i)}b_{I\pi(J)}c_{J\pi(J)} \mid \pi \}\} \leq \frac{600B_N^6}{N}.$$ 

• $a_{I\pi(J)}b_{I\pi(i)}c_{J\pi(i)}$. There are 6 terms in total. The analysis for this part is similar to the last part. The only difference is that, we need to apply Lemma S9 (iv) instead of (iii) to bound the variance for a term that looks like the I in the previous part. But the upper bound in
(iii) and (iv) are the same. Hence

\[
\text{Var} \left\{ \mathbb{E} \{ a_{I\pi(I)} b_{J\pi(J)} c_{J\pi(I)} \mid \pi \} \right\} \leq \frac{600 B_N^6}{N}.
\]

- \( a_{I\pi(I)} b_{J\pi(J)} c_{J\pi(I)} \). There are 12 terms in total. We have

\[
\mathbb{E} \{ a_{I\pi(I)} b_{J\pi(J)} c_{J\pi(I)} \mid \pi \} = \frac{1}{N(N - 1)} \sum_{i \neq j}^N a_{i\pi(i)} b_{j\pi(j)} c_{i\pi(j)}.
\]

By Lemma S9 (v), we have

\[
\text{Var} \left\{ \mathbb{E} \{ a_{I\pi(I)} b_{J\pi(J)} c_{J\pi(I)} \mid \pi \} \right\} \leq \frac{15N^3 B_N^6}{N^2(N - 1)^2} \leq \frac{30B_N^6}{N}.
\]

- \( a_{I\pi(I)} b_{J\pi(I)} c_{J\pi(I)} \). There are 12 terms in total. We have

\[
\mathbb{E} \{ a_{I\pi(I)} b_{J\pi(I)} c_{J\pi(I)} \mid \pi \} = \frac{1}{N(N - 1)} \sum_{i \neq j}^N a_{i\pi(i)} b_{j\pi(i)} c_{i\pi(j)}.
\]

By Lemma S9 (vi), we have

\[
\text{Var} \left\{ \mathbb{E} \{ a_{I\pi(I)} b_{J\pi(I)} c_{J\pi(I)} \mid \pi \} \right\} \leq \frac{15N^3 B_N^6}{N^2(N - 1)^2} \leq \frac{30B_N^6}{N}.
\]

Now summing up the bullet points above, we have

\[
\text{Var} \left\{ \mathbb{E} \{ D_h D_l D_m \mid \pi \} \right\} \leq \frac{CB_N^6}{N},
\]

for some absolute constant \( C > 0 \).

(iv) Summarize (i) (ii) (iii) above.

As a brief review, we have proved the following results: when \( N \) is large,

1. \( \| G \|_2 \leq \alpha = C(N - 1) H^{1/2} B_N, \| D \|_2 \leq \beta = CH^{1/2} B_N \).
2. \( \mathbb{E} \{ \| D \|_2^2 \} \leq C(HB_N^2 + HN^{-1}) \).
3. \( B_1 = \sqrt{\text{Var} \left\{ \mathbb{E} \{ \| D \|_2^2 \mid \Gamma \} \right\}} \leq CHN^{-1/2} B_N^2 \).
4. \( B_2 = \sqrt{\sum_{k,l=1}^H \text{Var} \left\{ \mathbb{E} \{ G_h D_l \mid \Gamma \} \right\}} \leq CHN^{1/2} B_N^2 \).
5. \( B_3 = \sqrt{\sum_{k,l,m=1}^H \text{Var} \left\{ \mathbb{E} \{ G_h D_l D_m \mid \Gamma \} \right\}} \leq CH^{3/2} N^{1/2} B_N^3 \).
Using Lemma S6 with (1) - (5), we have

\[
\sup_{A \in \mathcal{A}} |P\{\Gamma \in A\} - P\{\xi_H \in A\}|
\leq C (H^{1/4} \alpha \mathbb{E}\|D\|_2^2 + H^{1/4} \beta + H^{7/8} \alpha^{1/2} B_1^{1/2} + H^{3/8} B_2 + H^{1/8} B_3^{1/2})
\leq CH^{13/4} N B_N (B_2^2 + N^{-1}) + CH^{3/4} B_N + CH^{13/8} N^{1/4} B_N^{3/2}
+ CH^{11/8} N^{1/2} B_N^2 + CH^{7/8} N^{1/4} B_N^{3/2}.
\]

\[
\square
\]

C. Additional results for randomization-based causal inference

Appendix C presents some additional results for randomization-based causal inference. Section C.1 presents general BEBs for quadratic forms, which are derived based on the results in Appendix A. Section C.2 establishes some bound on the high order moments of the sample averages. Section C.3 and C.4 provide more delicate tail bounds for linear combination of sample variances. Section C.5 extends the BEBs to vector potential outcomes.

C.1. BEBs for quadratic forms

In Section 2, we proved the BEBs for linear projections of multivariate permutational statistics in randomized experiments. In this subsection, we study a more general type of distance:

\[
d_{\mathcal{A}}(\tilde{\gamma}, \xi_H) = \sup_{A \in \mathcal{A}} |P\{\tilde{\gamma} \in A\} - P\{\xi_H \in A\}|, \tag{S33}
\]

where \(\mathcal{A}\) is the collection of all Borel convex sets, \(\tilde{\gamma}\) is defined as (S43), and \(\xi_H\) is a random vector in \(\mathbb{R}^H\) with standard multivariate Normal distribution. \(\mathcal{A}\) can cover many specific convex class. For example, the set of ellipsoids defined as follows are a subset of of \(\mathcal{A}\):

\[
\mathcal{A}_2(\lambda, t) = \left\{ \gamma \in \mathbb{R}^H : \sum_{h=1}^H \lambda_h \gamma_h^2 \leq t \right\}, \quad \lambda_h > 0, \ t > 0. \tag{S34}
\]

(S34) is useful for deriving BEBs for quadratic forms of \(\tilde{\gamma}\).

Recall \(\tilde{\gamma}\) from (6). We study the asymptotic distribution of the following random variable:

\[
T = \tilde{\gamma}^\top W \tilde{\gamma},
\]

where \(W\) is a given positive definite matrix in \(\mathbb{R}^{H \times H}\). We also write \(T_0\) as the counterpart with \(\tilde{\gamma}\) replaced by Normal vectors \(\xi_H\):

\[
T_0 = \xi_H^\top W \xi_H, \quad \xi_H \sim \mathcal{N}(0, I_H). \tag{S35}
\]
For the problems in the main paper, we need to deal with the class of ellipsoids (S34), which are convex. Applying Theorem S2, we obtain the following result:

**Theorem S3** (Permutational BEBs for quadratic forms). We have

\[
\sup_{t \in \mathbb{R}} |\mathbb{P}(T \leq t) - \mathbb{P}(T_0 \leq t)| \leq C(H^{13/4}NB_N(B_N^2 + N^{-1}) + H^{3/4}B_N + H^{13/8}N^{1/4}B_N^{3/2} + H^{11/8}N^{1/2}B_N^2),
\]

where

\[
B_N = \varrho_{\min}(V^\gamma)^{-1/2} \sqrt{H} \max_{h \in [H]} \max_{i \in [N], q \in [Q]} |f_{qh}N_q^{-1}(Y_i(q) - \overline{Y}(q))|.
\]

When \(B_N \leq CH^{1/2}N^{-1/2}\), we have

\[
\sup_{t \in \mathbb{R}} |\mathbb{P}(T \leq t) - \mathbb{P}(T_0 \leq t)| \leq \frac{CH^{19/4}}{N^{1/2}}.
\]

**Remark S1.** The proof for Theorem S3 is an application of the bound over convex sets in Theorem S2. In general, the bound (S37) might not be sharp for quadratic forms. While the BEB achieved the rate \(N^{-1/2}\) which is analogous to the i.i.d. scenario, the rate in \(H\) might not be optimal. However, we do not pursue the best possible bound here. In many cases, (S37) suffices for establishing asymptotics. For example, in factorial experiments, if we focus on lower order effects, \(H\) is approximately the order of \(\log(N)\). Therefore, we can justify the asymptotic Normality as \(N \to \infty\) using (S37).

We discuss how to bound \(B_N\) to obtain a usable result from (S37). The following lemma covers nearly uniform designs and non-uniform designs:

**Lemma S10.** Assume Conditions 1 and 2.

(i) For nearly uniform design with either replicated or unreplicated arms, there exists a constant \(C = C(c, c', \zeta, \nu)\) that only depends on the constants in Definition 2 and Condition 2, such that

\[
\sup_{t \in \mathbb{R}} |\mathbb{P}(T \leq t) - \mathbb{P}(T_0 \leq t)| \leq C \frac{\max_{q \in [Q]} M_N(q)^3}{\{\min_{q \in [Q]} S(q, q)\}^{3/2}} \cdot \frac{H^{19/4}}{N^{1/2}}.
\]

Moreover, under Condition 4, we have

\[
B_N \leq 2^{1/2}C^{-1}N^{-1/2} \cdot \left(\frac{H}{QN_0}\right)^{1/2}
\]
and the BEB (S39) holds.

(ii) For non-uniform design, assume (14). There exists some constant $C = C(c, c', \underline{c}, \overline{c})$ that only depends on the constants in Definition 3 and Condition 2, such that

$$\sup_{t \in \mathbb{R}} |\mathbb{P}(T \leq t) - \mathbb{P}(T_0 \leq t)| \leq C \frac{\max_{q \in [Q]} M_N(q)^3}{\{n^{-1} \min_{q \in \mathbb{Q}_n} S(q, q)\}^{3/2}} \frac{H^{19/4}}{N^{1/2}}.$$ 

Moreover, under Condition 4 and $N = O(Q)$, we have

$$B_N \leq \frac{2vcH^{1/2}}{(c' \sqrt{\frac{1}{N}} S)^{1/2} Q^{1/2}}$$

and the BEB (S39) holds.

We have a thorough understanding of the distribution of $T_0$. By eigenvalue decomposition,

$$T_0 \sim \sum_{h=1}^{H} \rho_h \bar{\xi}_{0, h}^2 \lesssim \rho_1 \chi^2(H),$$

where $\rho_1 \geq \cdots \geq \rho_H$ are eigenvalues of $W$ and $\bar{\xi}_{0, 1}, \ldots, \bar{\xi}_{0, H}$ are i.i.d. $\mathcal{N}(0, 1)$. Therefore, $T_0$ is stochastically dominated by $\chi^2(H)$. When $H$ is fixed, the asymptotic distribution of $T$ follows immediately. When $H$ diverges, we need to further use the asymptotic distribution for sum of independent random variables based on the Lindeberg–Lévy CLT and classical BEBs. Corollary S1 below summarizes the results.

**Corollary S1** (Limiting distribution of the quadratic form). Let $N \to \infty$. Assume the upper bound in (S37) vanishes:

$$CH^{13/4} NB_N(B_N^2 + N^{-1}) + CH^{3/4} B_N + CH^{13/8} N^{1/4} E_N^{3/2} + CH^{11/8} N^{1/2} B_N^2 \to 0.$$ 

1. If $H$ is fixed, then $T \sim T_0$.

2. If $H$ diverges, then

$$\frac{T - \text{Tr}(W)}{\sqrt{2 \text{Tr}(W^2)}} \sim \mathcal{N}(0, 1).$$

**C.2. High order moments of $\hat{Y}$**

In this subsection, we presents some delicate characterizations of the high order moments of the sample average $\hat{Y}$, which are crucial for the proofs of our main results and might be of independent interest for other problems.

**Lemma S11** (High order moments of $\hat{Y}$). Assume complete randomization and Condition 3.
\(\hat{Y}_q - Y(q)\) \(\hat{Y}_q - Y(q')\) \(\hat{Y}_q - Y(q')\)

Lemma S12 (High order moments under unreplicated designs). Assume the potential outcomes are centered: \(Y(q) = 0\) for all \(q \in [Q]\). Assume complete randomization and Condition 3. For the unreplicated design in Definition 3, there exists a universal constant \(C > 0\), such that

(i) \(\mathbb{E}\{(\hat{Y}_q - Y(q))^2\} \leq \frac{C \Delta^2}{N_q}\);

(ii) \(\mathbb{E}\{(\hat{Y}_q - Y(q))^4\} \leq \frac{C \Delta^4}{N_q}\);

(iii) \(\text{Cov}\{(\hat{Y}_q - Y(q))^2, (\hat{Y}_{q'} - Y(q'))^2\} \leq \frac{C(N_q + N_{q'}) \Delta^4}{N_q N_{q'} (N-1)}\).

We assume the potential outcomes are centered in Lemma S12 to simplify the formulas. Without this assumption, all results in Lemma S12 hold if we subtract the means of the potential outcomes from the corresponding observed outcomes.

C.3. Tail probability of variance estimation for nearly uniform design

For an arbitrary set of indices \(Q \subseteq [Q]\), define

\[
\hat{v} = \sum_{q \in Q} w_q N_q^{-1} \hat{S}(q, q)
\]

if \(N_q \geq 2\) for all \(q \in Q\). Lemma S13 below gives the tail probability of \(\hat{v}\).

Lemma S13 (Tail probability of variance estimation). Consider the nearly uniform design satisfying Definition 2. Assume Condition 3 and \(\min_{q \in [Q]} N_q \geq 2\). Assume \((w_q)_{q \in [Q]}\) is a sequence of bounded real number:

\[
\max_{q \in [Q]} |w_q| \leq \overline{w}.
\]

Then there exists a universal constant \(C > 0\), such that

\[
\mathbb{P}\{|\hat{v} - \mathbb{E}\{\hat{v}\}| \geq t\} \leq \frac{C \epsilon^2 \overline{w}^2 |Q| N_0^{-3} \Delta^4}{t^2}.
\]
C.4. Tail probability of variance estimation for unreplicated arms

Recall the notation in Section 3.2. Define

\[ \hat{v} = \sum_{\langle g \rangle \in G} \sum_{q \in \langle g \rangle} w_q \left( Y_q - \hat{Y}_{\langle g \rangle} \right)^2. \] (S40)

Lemma S14 below gives the tail probability of \( \hat{v} \).

**Lemma S14** (Analysis of \( \hat{v} \) under unreplicated arms). Assume Conditions 3 and 6. Assume \((w_q)_{q \in Q_u}\) is a sequence of bounded real number:

\[ \max_{q \in Q_u} |w_q| \leq \overline{w}. \]

Then there exists a universal constant \( C > 0 \), such that

\[ P \{|\hat{v} - E\{\hat{v}\}| \geq t\} \leq \frac{C\overline{w}^2(\Delta^4 + \Delta^2\zeta^2)N}{t^2}. \]

C.5. Extension to vector potential outcomes

In some settings, we are interested in vector potential outcomes. Li and Ding (2017) proved some CLTs for vector outcomes. For binary treatments, Wang and Li (2022) proved some BEBs based on the coupling method. However, the general theory for BEB is still incomplete.

Let \( \{Y_i(q) \in \mathbb{R}^p : i \in [N], q \in [Q]\} \) be a collection of potential outcomes. Let \( F_1, \ldots, F_Q \) be \( Q \) coefficient matrices in \( \mathbb{R}^{H \times p} \). Define \( \gamma = \sum_{q=1}^{Q} F_q \bar{Y}(q) \), and the moment estimator is \( \hat{\gamma} = \sum_{q=1}^{Q} F_q \hat{Y}_q \). Li and Ding (2017) calculated the mean and covariance of \( \hat{\gamma} \):

\[ \mathbb{E}\{\hat{\gamma}\} = \sum_{q=1}^{Q} F_q \bar{Y}(q), \quad \text{Var}(\hat{\gamma}) = \sum_{q=1}^{Q} N^{-1} F_q S(q, q) F_q^\top - N^{-1} S_F := V_{\hat{\gamma}}, \]

where

\[ S(q, q') = (N - 1)^{-1} \sum_{i=1}^{N} (Y_i(q) - \bar{Y}(q))(Y_i(q') - \bar{Y}(q'))^\top, \quad q, q' \in [Q], \]

\[ S_F = (N - 1)^{-1} \sum_{i=1}^{N} (\gamma_i - \bar{\gamma})(\gamma_i - \bar{\gamma})^\top, \quad \gamma_i = \sum_{q=1}^{Q} F_q Y_i(q), \quad \bar{\gamma} = N^{-1} \sum_{i=1}^{N} \gamma_i. \]

Define

\[ \hat{Y}_i(q) = Y_i(q) - \bar{Y}(q) \text{ for all } q \in [Q]. \]

Theorem S4 below gives BEBs for projections of the standardized \( \hat{\gamma} \).
**Theorem S4** (BEB for projections of the standardized $\hat{\gamma}$). Let

$$\tilde{\gamma} = \{V_{\hat{\gamma}}\}^{-1/2}(\hat{\gamma} - E\{\hat{\gamma}\}).$$

Assume complete randomization. (i) There exists a universal constant $C > 0$, such that for any $b \in \mathbb{R}^H$ with $\|b\|_2 = 1$, we have

$$\left| \mathbb{P}\{b^T \tilde{\gamma} \leq t\} - \Phi(t) \right| \leq C \max_{i \in [N], q \in [Q]} \left| b^T V_{\tilde{\gamma}}^{-1/2} N_q^{-1} F_q \hat{Y}_i(q) \right|.$$  

(ii) If there exists $\sigma_F \geq 1$, such that

$$\sum_{q=1}^{Q} N_q^{-1} F_q S(q,q) F_q^\top \preceq \sigma_F^2 V_{\tilde{\gamma}},$$

then

$$\sup_{b \in \mathbb{R}^H, \|b\|_2 = 1} \mathbb{P}\{b^T \tilde{\gamma} \leq t\} - \Phi(t) \leq C \max_{i \in [N], q \in [Q]} \min \left\{ 2\sigma_F \sqrt{N_q^{-1} Y_i(q)^\top S(q,q)^{-1} Y_i(q)}, \frac{\|F_q\|_{2,1} N_q^{-1} \|Y_i(q)\|_\infty}{\sqrt{\min\{V_{\tilde{\gamma}}\}}} \right\}. \tag{S42}$$

Theorem S4 extends Theorem 1 to vector potential outcomes. If $p = 1$, Theorem S4 recovers Theorem 1. The novel part of the extension is to decide the appropriate vector and matrix norms in the upper bound for the vector potential outcomes $\hat{Y}_i(q)$'s and the coefficient matrices $F_q$'s. The proof provides more insights into the choices. Moreover, we can derive many corollaries from Theorem S4 as in the main paper. To avoid repetitions, we omit the details.

### D. Proofs of the results in the main paper and Appendix C

#### D.1. Proof of Theorem 1

The proof of Theorem 1 is based on Theorem S1. There are two key steps: (i) formulate $\tilde{\gamma}$ as a linear permutational statistic that satisfies the conditions of Theorem S1; (ii) find explicit bounds for the BEB in Theorem S1.

**Proof of Theorem 1.** Recall

$$\tilde{\gamma} = (V_{\hat{\gamma}})^{-1/2}(\hat{\gamma} - \gamma) = \text{Var} \left\{ F^\top \hat{Y} \right\}^{-1/2} (F^\top \hat{Y} - E\{F^\top \hat{Y}\}). \tag{S43}$$

**Step 1: Reformulate $\tilde{\gamma}$ as a multivariate linear permutational statistic.**

We show that, there exist population matrices $M''_1, \ldots, M''_H$ that satisfy Condition S1, such that

$$\tilde{\gamma} = (\text{Tr} (M''_h P))_{h=1}^H.$$
1. Construction of $M'_h$'s. Define

$$
\tilde{Y}_i(q) = Y_i(q) - \Upsilon(q), \quad \tilde{\tau}_hi = N^{-1} \sum_{q'=1}^{Q} f_{q'h} \tilde{Y}_i(q').
$$

(S44)

For each $i, j$, define

$$
M'_h(i,j) = N_q^{-1} f_{qh} \tilde{Y}_i(q) - \tilde{\tau}_hi, \quad \sum_{q'=0}^{q-1} N_q + 1 \leq j \leq \sum_{q'=0}^{q} N_q
$$

such that $M'_h$ is the centered version of

$$
M_h = \begin{pmatrix}
Z = 1 & \cdots & Z = q & \cdots & Z = Q \\
1 & f_{1h}N_1^{-1}Y_1(1) \cdot 1_{N_1}^\top & \cdots & f_{qh}N_q^{-1}Y_q(1) \cdot 1_{N_q}^\top & \cdots & f_{Qh}N_Q^{-1}Y_Q(1) \cdot 1_{N_Q}^\top \\
2 & f_{1h}N_1^{-1}Y_1(2) \cdot 1_{N_1}^\top & \cdots & f_{qh}N_q^{-1}Y_q(2) \cdot 1_{N_q}^\top & \cdots & f_{Qh}N_Q^{-1}Y_Q(2) \cdot 1_{N_Q}^\top \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
N & f_{1h}N_1^{-1}Y_N(1) \cdot 1_{N_1}^\top & \cdots & f_{qh}N_q^{-1}Y_q(N) \cdot 1_{N_q}^\top & \cdots & f_{Qh}N_Q^{-1}Y_Q(N) \cdot 1_{N_Q}^\top
\end{pmatrix}
$$

(S45)

Observe that

$$
\hat{\gamma} - \gamma = (\operatorname{Tr}(M'_1P), \ldots, \operatorname{Tr}(M'_HP))^\top = \begin{pmatrix}
\{\operatorname{vec}(M'_1)\}^\top \\
\vdots \\
\{\operatorname{vec}(M'_H)\}^\top
\end{pmatrix} \vec(P).
$$

(S46)

Construct $M''_h$'s as follows:

$$
\begin{pmatrix}
\{\operatorname{vec}(M''_1)\}^\top \\
\vdots \\
\{\operatorname{vec}(M''_H)\}^\top
\end{pmatrix} = V^{-1/2} \begin{pmatrix}
\{\operatorname{vec}(M'_1)\}^\top \\
\vdots \\
\{\operatorname{vec}(M'_H)\}^\top
\end{pmatrix}.
$$

(S47)

Combining (S47) and (S46), we can show $\tilde{\gamma} = (\operatorname{Tr}(M''_1P), \ldots, \operatorname{Tr}(M''_HP))^\top$. The next step is to show $M''_h$'s satisfy Condition S1.

2. Verify Condition S1. To verify that $M''_h$’s have zero row and column sums, we notice that summation of $j$-th column (or row) corresponds to a linear mapping from $\mathbb{R}^{N\times N}$ to $\mathbb{R}$ that can be defined by the trace inner product:

$$
\sum_{i=1}^{N} M''_h(i,j) = \operatorname{Tr}(M''_h T_j) \text{ with } T_j = (0, \ldots, 1_{N_{\text{column } j}}, \ldots, 0).
$$
Given that $M'_h$'s are row and column centered, we can use (S47) to show that
\[
\begin{pmatrix}
\{\text{vec}(M'_1)\}^\top \\
\vdots \\
\{\text{vec}(M'_H)\}^\top
\end{pmatrix}
\vec(T_j) = V_\tilde{\gamma}^{-1/2}
\begin{pmatrix}
\{\text{vec}(M'_1)\}^\top \\
\vdots \\
\{\text{vec}(M'_H)\}^\top
\end{pmatrix}
\vec(T_j) = 0.
\]

To show $M''_h$'s are standardized and mutually orthogonal, we notice
\[
\text{Var}\{\tilde{\gamma}\} = I_H.
\] (S48)

Now using Lemma S1(ii), we have
\[
\text{Var}\{\tilde{\gamma}\} = \left(\frac{1}{N-1}\langle M''_h, M''_l\rangle\right)_{h,l\in[H]}.
\] (S49)

Comparing (S48) and (S49), we obtain the desired conclusion.

**Step 2: Apply Theorem S1 by finding explicit bounds for the BEB.**

Apply Theorem S1 to obtain that: for any $b \in \mathbb{R}^H$ with $\|b\|_2 = 1$, we have
\[
\sup_{t \in \mathbb{R}} |\mathbb{P}\{b^\top \tilde{\gamma} \leq t\} - \Phi(t)| \leq C \max_{i,j \in [N]} \sum_{h=1}^H b_h M''_h(i,j) \bigg|.
\] (S50)

Each column of the matrix (S45) corresponds to a treatment group $q$. For ease of presentation, it is convenient to highlight this connection with notation $q_j$, meaning the $j$-th column is constructed based on potential outcomes from treatment level $q_j$.

Based on (S47), we have
\[
\sum_{h=1}^H b_h M''_h(i,j) = b^\top V_\tilde{\gamma}^{-1/2}
\begin{pmatrix}
N_{q_j}^{-1} f_{q_j 1} \tilde{Y}_i(q_j) - \hat{\tau}_{1i} \\
\vdots \\
N_{q_j}^{-1} f_{q_j H} \tilde{Y}_i(q_j) - \hat{\tau}_{Hi}
\end{pmatrix}
\]
\[
= b^\top V_\tilde{\gamma}^{-1/2}
\begin{pmatrix}
N_{q_j}^{-1} f_{q_j 1} \tilde{Y}_i(q_j) \\
\vdots \\
N_{q_j}^{-1} f_{q_j H} \tilde{Y}_i(q_j)
\end{pmatrix} - b^\top V_\tilde{\gamma}^{-1/2}
\begin{pmatrix}
\hat{\tau}_{1i} \\
\vdots \\
\hat{\tau}_{Hi}
\end{pmatrix}
\]
\] (S51) (S52)

From the definition (S44), term II is the average of term I over $j \in [N]$. Therefore, if we can bound term I for all $i, j$, then we can also bound term II by the triangle inequality. We now use two ways to bound term I.

**First Bound for term I:** For $b \in \mathbb{R}^H$ with $\|b\|_2 = 1$, construct $b_0 = V_\tilde{\gamma}^{-1/2} b / \|V_\tilde{\gamma}^{-1/2} b\|_2 \in \mathbb{R}^H$.
with \( \|b_0\|_2 = 1 \). We can verify that

\[
b = \frac{V_{\gamma}^{1/2}b_0}{\sqrt{b_0^\top V_{\gamma}b_0}}.
\]

We have

\[
|b^\top V_{\gamma}^{-1/2} \begin{pmatrix} N_{q_j}^{-1} f_{q_j} \hat{Y}_i(q_j) \\ \vdots \\ N_{q_j}^{-1} f_{q_j,r} \hat{Y}_i(q_j) \end{pmatrix}| = |b^\top V_{\gamma}^{-1/2} \begin{pmatrix} f_{q_j1} \\ \vdots \\ f_{q_j H} \end{pmatrix} \cdot N_{q_j}^{-1} \hat{Y}_i(q_j)|
\]

\[
= |b_0^\top \begin{pmatrix} f_{q_j1} \\ \vdots \\ f_{q_j H} \end{pmatrix} \frac{N_{q_j}^{-1} \hat{Y}_i(q_j)}{\sqrt{b_0^\top V_{\gamma}b_0}}|
\]

\[
= |F(q_j, \cdot)b_0| \cdot \frac{N_{q_j}^{-1} \hat{Y}_i(q_j)}{\sqrt{b_0^\top V_{\gamma}b_0}}.
\]

To get a uniform bound, we need to bound \( |F(q_j, \cdot)b_0| \) and \( b_0^\top V_{\gamma}b_0 \). We can show

\[
|F(q_j, \cdot)b_0| \leq \|F(q_j, \cdot)\|_2, \quad b_0^\top V_{\gamma}b_0 \geq \varrho_{\min}\{V_{\gamma}\}.
\]

Hence,

\[
|F(q_j, \cdot)b_0| \cdot \frac{N_{q_j}^{-1} \hat{Y}_i(q_j)}{\sqrt{b_0^\top V_{\gamma}b_0}} \leq \frac{\|F(q_j, \cdot)\|_2 \cdot N_{q_j}^{-1} |Y_i(q_j) - \bar{Y}(q_j)|}{\sqrt{\varrho_{\min}\{V_{\gamma}\}}}.
\] (S53)

**Second bound for term I:** We have

\[
|b^\top V_{\gamma}^{-1/2} \begin{pmatrix} N_{q_j}^{-1} f_{q_j} \hat{Y}_i(q_j) \\ \vdots \\ N_{q_j}^{-1} f_{q_j,r} \hat{Y}_i(q_j) \end{pmatrix}| \leq |b^\top V_{\gamma}^{-1/2} \begin{pmatrix} f_{q_j1} \\ \vdots \\ f_{q_j H} \end{pmatrix} \cdot \sqrt{N_{q_j}^{-1} S(q_j, q_j)} \cdot \frac{N_{q_j}^{-1} \hat{Y}_i(q_j)}{\sqrt{N_{q_j}^{-1} S(q_j, q_j)}}|
\]

\[
\leq |b^\top V_{\gamma}^{-1/2} \begin{pmatrix} f_{q_j1} \\ \vdots \\ f_{q_j H} \end{pmatrix} \cdot \sqrt{N_{q_j}^{-1} S(q_j, q_j)}| \cdot \frac{N_{q_j}^{-1} \hat{Y}_i(q_j)}{\sqrt{N_{q_j}^{-1} S(q_j, q_j)}}
\]

\[
\leq \left|b^\top V_{\gamma}^{-1/2} F^\top \text{Diag}\{N_q^{-1} S(q, q)\}^{1/2}\right|_{\infty} \cdot \frac{N_{q_j}^{-1} \hat{Y}_i(q_j)}{\sqrt{N_{q_j}^{-1} S(q_j, q_j)}}.
\] (S54)

The infinity norm is upper bounded by the \( \ell_2 \) norm:

\[
\left\|b^\top V_{\gamma}^{-1/2} F^\top \text{Diag}\{N_q^{-1} S(q, q)\}^{1/2}\right\|_{\infty}
\]

S30
\[
\leq \left\| b^\top V^{-1/2}_\gamma F^\top \text{Diag} \left\{ N_q^{-1} S(q, q) \right\}^{1/2} \right\|_2 \\
= \sqrt{b^\top V^{-1/2}_\gamma F^\top \text{Diag} \left\{ N_q^{-1} S(q, q) \right\} F V^{-1/2}_\gamma b} \\
\leq \sqrt{b^\top V^{-1/2}_\gamma (\sigma^2 F V^{-1/2}_\gamma) V^{-1/2}_\gamma b} \quad \text{(by Condition 1)} \\
\leq \sigma_F. \quad \text{(S55)}
\]

Combining (S54) and (S55), we have

\[
\left| \sum_{h=1}^H b_h M''_h(i, j) \right| \leq 2\sigma_F \left| \frac{\hat{Y}(q_j)}{\sqrt{N_q S(q_j, q_j)}} \right|. \quad \text{(S56)}
\]

Combining (S53) and (S56), we have

\[
\left| \sum_{h=1}^H b_h M''_h(i, j) \right| \leq 2 \min \left\{ \sigma_F \left| \frac{Y_i(q_j) - \bar{Y}(q_j)}{\sqrt{N_q S(q_j, q_j)}} \right|, \frac{\|F(q_j, \cdot)\|_2 \cdot N_q^{-1}|Y_i(q_j) - \bar{Y}(q_j)|}{\sqrt{\rho_{\min}(V^*_Y)}} \right\}. \quad \text{(S57)}
\]

Now we can take maximum over \(i, j \in [N]\) in (S57) and use (S50) to conclude the proof. \(\square\)

D.2. Proof of Theorem 2

The proof is an application of Lemma S10 (i).

D.3. Proof of Lemma 1

Proof of Lemma 1. (i) Suppose the individual causal effects are constant. Then

\[ F^\top \text{Diag} \left\{ N_q^{-1} S(q, q) \right\} F = V^*_Y. \]

(ii) Suppose the condition number of the correlation matrix corresponding to \(V^*_Y\) is upper bounded by \(\sigma^2\). Then

\[ Q = \sum_{q=1}^Q \rho_q(V^*_Y) \leq Q \cdot \rho_{\max}(V^*_Y) \leq \sigma^2 Q \cdot \rho_{\min}(V^*_Y), \]

which implies \(\rho_{\min}(V^*_Y) \geq \sigma^{-2}\). Let \(D = \text{Diag} \left\{ (N_q^{-1} - N^{-1}) S(q, q) \right\} \). Then

\[
V^*_Y = F^\top V^*_Y F \\
= F^\top D^{1/2} V^*_Y D^{1/2} F \\
\geq F^\top D^{1/2} (\sigma^{-2} I_Q) D^{1/2} F \\
\geq \sigma^{-2} F^\top \text{Diag} \left\{ (N_q^{-1} - N^{-1}) S(q, q) \right\} F \\
\geq c \sigma^{-2} F^\top \text{Diag} \left\{ N_q^{-1} S(q, q) \right\} F
\]
(using \( N_q \leq (1 - c)N \)).

\[ \text{D.4. Proof of Corollary 1} \]

**Proof of Corollary 1.** It suffices to further control term II of the upper bound in (8):

\[
\| F(q, \cdot) \|_2 \cdot N_q^{-1} | Y_i(q) - \bar{Y}(q) | \cdot \sqrt{q_{\min} \{ \text{Var} \{ F^\top \hat{Y} \} \}}
\]

By definition of 2-norm, \( \| F(q, \cdot) \|_2 \leq \sqrt{H} \| F \|_\infty \). By Definition 2, \( N_q^{-1} \leq c^{-1} N_0^{-1} \). Under Condition 1, \( q_{\min} \{ \text{Var} \{ F^\top \hat{Y} \} \} \geq \sigma - \frac{2}{F} \rho_{\min} \{ F^\top \text{Diag} \{ N_q^{-1} S(q, q) \} F \} \geq \sigma - \frac{2}{F} \rho_{\min} \{ F^\top \text{Diag} \{ N_q^{-1} S(q, q) \} \} \min \{ N_q^{-1} S(q, q) \} \geq \sigma - \frac{2}{F} \min \{ N_q^{-1} S(q, q) \} \}
\]

Now (12) is obtained by using (10) and plugging in these results.

\[ \text{D.5. Proof of Corollary 2} \]

The key idea is to find explicit bounds on the BEB given by Theorem 1 for non-uniform designs. We partition the arms into \( Q_s \cup Q_l \), and apply different parts in the general BEB in (9) to these two groups respectively.

**Proof of Corollary 2.** Recall the bound (9) in Theorem 1. The two parts in the upper bound shall be applied to different categories of arms from Definition 3. Because each \( N_q \) is large for \( q \in Q_l \), we keep the first part of (8) for \( Q_l \):

\[
\max_{i \in [N], q \in Q_l} \sigma_F \left| \frac{Y_i(q) - \bar{Y}(q)}{\sqrt{N_q S(q, q)}} \right|.
\]

For the small groups in \( Q_s \), we apply the second part of (8). First, we have \( N_q^{-1} \leq 1 \). Besides, under Condition 1,

\[
\rho_{\min} \left( \text{Var} \{ F^\top \hat{Y} \} \right) \geq \sigma_F^{-2} \rho_{\min} \{ F^\top \text{Diag} \{ N_q^{-1} S(q, q) \} \} \min \{ N_q^{-1} S(q, q) \} \rho_{\min} \{ F^\top F \} \geq \sigma_F^{-2} \min \{ N_q^{-1} S(q, q) \} \rho_{\min} \{ F^\top F \}
\]
\[ \geq \sigma_F^2 \pi^{-1} \min_{q \in Q_s} \{S(q, q)\} \varrho_{\min} \{F_s^T F_s\}. \]  

(S59)

Hence for \( q \in Q_s \), we keep the second part of (8) and use (S59) to obtain upper bound:

\[ \frac{\epsilon^{-1} \pi^{-1} \sigma_F \|F(q, \cdot)\|_2 \cdot |Y(q) - \bar{Y}(q)|}{(\pi^{-1} \min_{q \in Q_s} \{S(q, q)\} \varrho_{\min} \{F_s^T F_s\})^{1/2}}. \]

Under Condition 2, we have

\[ \|F(q, \cdot)\|_2 \leq cQ^{-1} \sqrt{H} \]

and

\[ \varrho_{\min} \{F_s^T F_s\} = \varrho_{\min} \{F^T F - F^T F_L\} \]
\[ \geq \varrho_{\min} \{F^T F\} - \varrho_{\max} \{F^T F_L\} \]
\[ \geq c' Q^{-1} - c^2 H |Q_L| Q^{-2} \]

because \( \varrho_{\max} \{F^T F_L\} \leq \text{Tr} \left( F^T F_L \right) = c^2 H |Q_L| Q^{-2} \). Hence,

\[ \frac{\|F(q, \cdot)\|_2}{(\varrho_{\min} \{F_s^T F_s\})^{1/2}} \leq \sqrt{\frac{c^2 H}{c' Q - c^2 H |Q_L|}}. \]  

(S60)

Because we assumed \( Q \geq 2(c^2/c')H|Q_L| \), (S60) implies

\[ \frac{\|F(q, \cdot)\|_2}{(\varrho_{\min} \{F_s^T F_s\})^{1/2}} \leq \sqrt{\frac{2c^2 H}{c' Q}}. \]  

(S61)

Putting (S58), (S59) and (S61) into (8) concludes the proof.

D.6. Proof of Theorem 3

Proof of Theorem 3.  (i) It is well known.

(ii) For the stochastic order in \( L_{\infty} \) norm, we shall apply Lemma S13 with \( Q = [Q] \). We have

\[ \hat{V}_{\delta}(h, h') = \sum_{q \in Q} F(h, q)F(h', q)N_q^{-1} \hat{S}(q, q) \]
\[ = \sum_{q \in Q} w_q N_q^{-1} \hat{S}(q, q), \]

where

\[ w_q = F(h, q)F(h', q), \quad |w_q| \leq \|F\|_\infty^2. \]
Applying Lemma S13, we have
\[
P\{|\hat{v} - \mathbb{E}\{\hat{v}\}| \geq t\} \leq \frac{Ct\varepsilon^{-4} \|F\|_{\infty}^4 QN_{0}^{-3}\Delta^4}{t^2} := \odot_1,
\]
which implies
\[
\forall h, h' \in [H], \quad P\left\{|\hat{V}_\gamma(h, h') - \mathbb{E}\{\hat{V}_\gamma(h, h')\}| > t\right\} \leq \odot_1.
\]
Taking union bound over \(h, h' \in [H]\), we have
\[
P\left\{\max_{h, h' \in [H]} |\hat{V}_\gamma(h, h') - \mathbb{E}\{\hat{V}_\gamma(h, h')\}| > t\right\} \leq \odot_1 \cdot H^2.
\]
Therefore,
\[
\|\hat{V}_\gamma - \mathbb{E}\{\hat{V}_\gamma\}\|_{\infty}^2 = \mathcal{O}_P(\odot_1 \cdot H^2).
\]

(iii) It follows from (S1).

\[\square\]

D.7. Proof of Theorem 4

Proof of Theorem 4. We prove the “fixed \(H\)” and “diverging \(H\)” scenarios separately. In each scenario, we apply BEBs to obtain CLTs with the true variances, and then apply the variance estimation results to justify the statistical properties after plugging in the variance estimators.

(i) Consider fixed \(H\). By Corollary 1, under Conditions 1, 2 and 4, the property of joint asymptotic Normality holds:
\[
V_{\gamma}^{-1/2}(\hat{\gamma} - \gamma) \sim \mathcal{N}(0, I_H).
\]
The continuous mapping theorem implies
\[
(\hat{\gamma} - \gamma)^\top V_{\gamma}^{-1} (\hat{\gamma} - \gamma) \sim \chi^2_H,
\]
\[
(\hat{\gamma} - \gamma)^\top \mathbb{E}\{\hat{V}_\gamma\}^{-1} (\hat{\gamma} - \gamma) = (\hat{\gamma} - \gamma)^\top V_{\gamma}^{-1/2} W_N V_{\gamma}^{-1/2} (\hat{\gamma} - \gamma) \sim \mathcal{L}.
\]
Because \(\mathbb{E}\{\hat{V}_\gamma\} \succeq V_\gamma\), we have \(I_H \succeq W_\infty\) and \(\mathcal{L} \lesssim \chi^2(H)\).

For variance estimation, under Conditions 1, 2, 3 and 4, the stochastic order in Theorem 3 implies \(N\hat{V}_\gamma - N\mathbb{E}\{\hat{V}_\gamma\} = \mathcal{O}_p(1)\). Hence \(N^{-1}\hat{V}_\gamma^{-1} - N^{-1}\mathbb{E}\{\hat{V}_\gamma\}^{-1} = \mathcal{O}_p(1)\). Moreover,
\[
\|\hat{\gamma} - \gamma\|_2^2 = \mathcal{O}_p(\|V_\gamma\|_{op}) = \mathcal{O}_p(\|F^\top \text{Diag} \{N_q^{-1}S(q, q)\} F\|_{op}) = \mathcal{O}_p(\Delta^2 N_0^{-1}\|F^\top F\|_{op}).
\]
Using
\[ \|F^T F\|_{\text{op}} \leq \text{Tr} \left( F^T F \right) \leq c^2 Q^{-2} \cdot (QH) \leq c^2 Q^{-1} H, \]
we can derive
\[ N \|\hat{\gamma} - \gamma\|^2 = O_p(H). \]

Therefore,
\[ (\hat{\gamma} - \gamma)^T \hat{V}_{\hat{\gamma}}^{-1} (\hat{\gamma} - \gamma) = (\hat{\gamma} - \gamma)^T \mathbb{E} \left\{ \hat{V}_{\hat{\gamma}} \right\}^{-1} (\hat{\gamma} - \gamma) \]
\[ + (\hat{\gamma} - \gamma)^T \left( \hat{V}_{\hat{\gamma}}^{-1} - \mathbb{E} \left\{ \hat{V}_{\hat{\gamma}} \right\}^{-1} \right) (\hat{\gamma} - \gamma), \]
where (S63) has the order
\[ (\hat{\gamma} - \gamma)^T \left( \hat{V}_{\hat{\gamma}}^{-1} - \mathbb{E} \left\{ \hat{V}_{\hat{\gamma}} \right\}^{-1} \right) (\hat{\gamma} - \gamma) = O_p(H) \cdot o_p(1) = o_p(1). \]

Now using Slutsky’s theorem, we prove the results.

(ii) Consider diverging \( H \). We use a quadratic form CLT stated in Corollary S1. By Corollary S1, under Conditions 1, 2 and 4, when \( H^{19/4} N^{-1/2} \to 0 \), with \( W_N = V_{\hat{\gamma}}^{1/2} \mathbb{E} \left\{ \hat{V}_{\hat{\gamma}} \right\}^{-1/2} V_{\hat{\gamma}}^{1/2} \), we have
\[ \frac{(\hat{\gamma} - \gamma)^T \mathbb{E} \left\{ \hat{V}_{\hat{\gamma}} \right\}^{-1} (\hat{\gamma} - \gamma) - \text{Tr} \left( W_N^2 \right)}{\sqrt{2 \text{Tr} \left( W_N \right)}} \sim N(0, 1). \quad \text{(S64)} \]
Because \( \mathbb{E} \{ \hat{V}_{\hat{\gamma}} \} \succeq V_{\hat{\gamma}} \), we have
\[ \text{Tr} \left( W_N \right) \leq H, \quad \text{Tr} \left( W_N^2 \right) \leq H. \quad \text{(S65)} \]

Now we consider the difference induced by plugging in the variance estimator:
\[ |(\hat{\gamma} - \gamma)^T (\hat{V}_{\hat{\gamma}}^{-1} - \mathbb{E} \{ \hat{V}_{\hat{\gamma}} \}^{-1}) \hat{\gamma} - \gamma)| \]
\[ \leq |(\hat{\gamma} - \gamma)^T V_{\hat{\gamma}}^{-1} (\hat{\gamma} - \gamma)| \cdot \| V_{\hat{\gamma}} \|_{\text{op}} \cdot \| \hat{V}_{\hat{\gamma}}^{-1} - \mathbb{E} \{ \hat{V}_{\hat{\gamma}} \}^{-1} \|_{\text{op}}. \]

Use the matrix identity
\[ \hat{V}_{\hat{\gamma}}^{-1} - \mathbb{E} \{ \hat{V}_{\hat{\gamma}} \}^{-1} = -\hat{V}_{\hat{\gamma}}^{-1} (\hat{V}_{\hat{\gamma}} - \mathbb{E} \{ \hat{V}_{\hat{\gamma}} \}) \mathbb{E} \{ \hat{V}_{\hat{\gamma}} \}^{-1}, \]
we can verify that

\[ \| \tilde{V}^{-1}_\gamma - \mathbb{E}\{\tilde{V}_\gamma\}^{-1} \|_{\text{op}} = \| \tilde{V}^{-1}_\gamma (\tilde{V}_\gamma - \mathbb{E}\{\tilde{V}_\gamma\}) \mathbb{E}\{\tilde{V}_\gamma\}^{-1} \|_{\text{op}} \leq \| \tilde{V}^{-1}_\gamma \|_{\text{op}} \| \tilde{V}_\gamma - \mathbb{E}\{\tilde{V}_\gamma\} \|_{\text{op}} \| \mathbb{E}\{\tilde{V}_\gamma\}^{-1} \|_{\text{op}}. \]

Theorem 3 ensures

\[ N \| \tilde{V}_\gamma - \mathbb{E}\{\tilde{V}_\gamma\} \|_{\text{op}} = O_F(H^2 N^{-1/2}), \quad \| \mathbb{E}\{\tilde{V}_\gamma\}^{-1} \|_{\text{op}} = O(1), \quad \| \tilde{V}_\gamma^{-1} \|_{\text{op}} = O_F(N), \quad \| V_\gamma \|_{\text{op}} = O_F(N^{-1}). \]

Corollary S1 ensures

\[ (\hat{\gamma} - \gamma)^\top V^{-1}_\gamma (\hat{\gamma} - \gamma) = O_F(H). \]

Under Condition 1, we have

\[
\begin{align*}
\text{Tr} \left( W^2_N \right) &= \text{Tr} \left( V^{1/2}_\gamma \mathbb{E}\{\tilde{V}_\gamma\}^{-1} V^{1/2}_\gamma \mathbb{E}\{\tilde{V}_\gamma\}^{-1} V^{1/2}_\gamma \right) \\
&\geq \sigma_F^{-2} \text{Tr} \left( V^{1/2}_\gamma \mathbb{E}\{\tilde{V}_\gamma\}^{-1} V^{1/2}_\gamma \right) \\
&= \sigma_F^{-2} \text{Tr} \left( \mathbb{E}\{\tilde{V}_\gamma\}^{-1} V^{1/2}_\gamma \right) \\
&\geq \sigma_F^{-4} \text{Tr}(I_H) = \sigma_F^{-4} H.
\end{align*}
\]

Using these results, we obtain

\[
\begin{align*}
\frac{|(\hat{\gamma} - \gamma)^\top (\tilde{V}_\gamma^{-1} - \mathbb{E}\{\tilde{V}_\gamma\}^{-1}) (\hat{\gamma} - \gamma)|}{\sqrt{2 \text{Tr} \left( W^2_N \right)}} = O_F(H^{5/2} N^{-1/2}), \tag{S66}
\end{align*}
\]

which converges to 0 if \( H^{19/4} N^{-1/2} \to 0 \). Combine (S64) and (S66) to establish the desired CLT.

To prove the validity of the confidence set, we notice that

\[
\begin{align*}
&\mathbb{P} \left\{ (\hat{\gamma} - \gamma)^\top \tilde{V}_\gamma^{-1} (\hat{\gamma} - \gamma) \geq q_\alpha \right\} \\
\leq &\mathbb{P} \left\{ (\hat{\gamma} - \gamma)^\top \mathbb{E}\{\tilde{V}_\gamma\}^{-1} (\hat{\gamma} - \gamma) + |(\hat{\gamma} - \gamma)^\top (\tilde{V}_\gamma^{-1} - \mathbb{E}\{\tilde{V}_\gamma\}^{-1}) (\hat{\gamma} - \gamma)| \geq q_\alpha \right\} \\
\leq &\mathbb{P} \left\{ (\hat{\gamma} - \gamma)^\top \mathbb{E}\{\tilde{V}_\gamma\}^{-1} (\hat{\gamma} - \gamma) \geq q_\alpha - cH^4 N^{-1/2} \right\} \\
&+ \mathbb{P} \left\{ |(\hat{\gamma} - \gamma)^\top (\tilde{V}_\gamma^{-1} - \mathbb{E}\{\tilde{V}_\gamma\}^{-1}) (\hat{\gamma} - \gamma)| \geq cH^4 N^{-1/2} \right\}. \tag{S67}
\end{align*}
\]

Using (S65) and (S66), (S68) converges to zero if \( H^{19/4} N^{-1/2} \to 0 \).
For (S67), using Lemma S10 (i),

\[
\left| \mathbb{P}\left\{ (\hat{\gamma} - \gamma)^\top \mathbb{E}\{\hat{V}_{\hat{\gamma}}\}^{-1}(\hat{\gamma} - \gamma) \geq q_\alpha - cH^4N^{-1/2} \right\} - \mathbb{P}\left\{ \xi^\top_H W_N \xi_H \geq q_\alpha - cH^4N^{-1/2} \right\} \right| = o(1).
\]

(S69)

Now because \( W_N \preceq I_H \),

\[
\mathbb{P}\left\{ \xi^\top_H W_N \xi_H \geq q_\alpha - cH^4N^{-1/2} \right\} \leq \mathbb{P}\left\{ \xi^\top_H \xi_H \geq q_\alpha - cH^4N^{-1/2} \right\}.
\]

(S70)

Moreover,

\[
\sup_{t \in \mathbb{R}} \left| \mathbb{P}\left\{ \frac{\xi^\top_H \xi_H - H}{\sqrt{2H}} \leq t \right\} - \Phi(t) \right| = o(1) \text{ as } H \to \infty.
\]

(S71)

Hence,

\[
\left| \mathbb{P}\left\{ \frac{\xi^\top_H \xi_H - H}{\sqrt{2H}} \geq \frac{q_\alpha - H - cH^4N^{-1/2}}{\sqrt{2H}} \right\} - \mathbb{P}\left\{ \frac{\xi^\top_H \xi_H - H}{\sqrt{2H}} \geq \frac{q_\alpha - H}{\sqrt{2H}} \right\} \right|
\]

\[
= |\Phi\left( \frac{q_\alpha - H - cH^4N^{-1/2}}{\sqrt{2H}} \right) - \Phi\left( \frac{q_\alpha - H}{\sqrt{2H}} \right)| + o(1) \leq \frac{1}{\sqrt{2\pi}} H^{7/2}N^{-1/2} + o(1) = o(1).
\]

(S72)

Combining (S69)–(S72), we conclude that, if \( H^{19/4}N^{-1/2} \to 0 \), then

\[
\lim_{H,N \to \infty} \mathbb{P}\left\{ (\hat{\gamma} - \gamma)^\top \mathbb{E}\{\hat{V}_{\hat{\gamma}}\}^{-1}(\hat{\gamma} - \gamma) \geq q_\alpha - cH^4N^{-1/2} \right\} \leq \alpha.
\]

(S73)

From (S67) and (S68), we conclude the asymptotic validity of the Wald-type inference.

\[\square\]

D.8. Proof of Theorem 5

The proof is an application of Lemma S10 (i).

D.9. Proof of Lemma 2 and Theorem 6

Lemma 2 is a special case of Theorem 6(i). We first give a proof for Theorem 6, then add some discussions on improving variance estimation under more assumptions.

Proof of Theorem 6. (i) We first compute the expectation of (20):

\[
\mathbb{E}\{(Y_q - \hat{Y}_{(g)})^2\}
\]

\[
= \mathbb{E}\{(Y_q - \bar{Y}(g) + \bar{Y}(g) - \bar{Y}_{(g)} - \hat{Y}_{(g)})^2\}
\]

S37
We can upper bound $\Theta_{1}(S_74)$ reflects the within group variation for arm $q$. $(S_{75})$ reflects the pooled variation for the arms except $q$ in group $\langle g \rangle$. $(S_{76})$ captures the correlation between arm $q$ and the rest in $\langle g \rangle$. $(S_{77})$ represents the between group variation.

For $(S_{75})$, we have

$$
\begin{align*}
|\langle g \rangle|^{-2} & \mathbb{E} \left[ \left\{ \sum_{q' \in (g), q' \neq q} (Y_{q'} - \bar{Y}(q')) \right\}^2 \right] \\
= & |\langle g \rangle|^{-2} \mathbb{E} \left[ \left\{ \sum_{q' \in (g), q' \neq q} (Y_{q'} - \bar{Y}(q')) \right\}^2 \right] \\
- & 2(1 - |\langle g \rangle|^{-1}) |\langle g \rangle|^{-1} \sum_{q' \in (g), q' \neq q} \mathbb{E}\{ (Y_q - \bar{Y}(q)) (Y_{q'} - \bar{Y}(q')) \} \\
+ & \mathbb{E}\{ (\bar{Y}(q) - \bar{Y}(q)) \} \\
= & (1 - |\langle g \rangle|^{-1})^2 (1 - N^{-1}) S(q, q) \\
+ & |\langle g \rangle|^{-2} \mathbb{E} \left[ \left\{ \sum_{q' \in (g), q' \neq q} (Y_{q'} - \bar{Y}(q')) \right\}^2 \right] \\
- & 2(1 - |\langle g \rangle|^{-1}) |\langle g \rangle|^{-1} N^{-1} \sum_{q' \in (g), q' \neq q} S(q, q') \\
+ & (\bar{Y}(q) - \bar{Y}(q))^2. \\
\end{align*}
$$

$(S_{74})$ reflects the within group variation for arm $q$. $(S_{75})$ reflects the pooled variation for the arms except $q$ in group $\langle g \rangle$. $(S_{76})$ captures the correlation between arm $q$ and the rest in $\langle g \rangle$. $(S_{77})$ represents the between group variation.

For $(S_{75})$, we have

$$
\begin{align*}
|\langle g \rangle|^{-2} & \mathbb{E} \left[ \left\{ \sum_{q' \in (g), q' \neq q} (Y_{q'} - \bar{Y}(q')) \right\}^2 \right] \\
= & |\langle g \rangle|^{-2} 1^T \mathbf{Diag} \left\{ S(q', q') \right\}_{q' \in (g), q' \neq q} - N^{-1} (S(q', q''))_{q', q'' \in (g) \setminus \{q\}} |1 \\
= & |\langle g \rangle|^{-2} (1 - N^{-1} \rho_{(g)}) \sum_{q' \in (g), q' \neq q} S(q', q') + N^{-1} \mu_{(g)}^{-1} \Theta_1(q, q), \\
\end{align*}
$$

where

$$
\Theta_1(q, q) = \mu_{(g)} |\langle g \rangle|^{-2} 1^T \{ \rho_{(g)} \mathbf{Diag} \{ S(q', q') \}_{q' \in (g), q' \neq q} - (S(q', q''))_{q', q'' \in (g) \setminus \{q\}} \} 1 \geq 0.
$$

We can upper bound $\Theta_1(q, q)$ as follows:

$$
\begin{align*}
\Theta_1(q, q) & \leq \mu_{(g)} |\langle g \rangle|^{-2} 1^T \{ \rho_{(g)} \mathbf{Diag} \{ S(q', q') \}_{q' \in (g), q' \neq q} \} 1 \\
& = \mu_{(g)} \cdot \frac{\rho_{(g)}}{|\langle g \rangle|} \cdot |\langle g \rangle|^{-1} \sum_{q' \in (g), q' \neq q} S(q', q') \\
& \leq \mu_{(g)} |\langle g \rangle|^{-1} \sum_{q' \in (g)} S(q', q') \leq \mu_{(g)} \max_{q' \in (g)} S(q', q'). \\
\end{align*}
$$

S38
For (S76), we have
\[
2(1 - |\langle g \rangle|^{-1})|\langle g \rangle|^{-1}N^{-1} \sum_{q' \in \langle g \rangle : q' \neq q} S(q, q') \leq 2(1 - |\langle g \rangle|^{-1})|\langle g \rangle|^{-1}N^{-1} \sum_{q' \in \langle g \rangle : q' \neq q} \sqrt{S(q, q)S(q', q')} \quad \text{(by the Cauchy-Schwarz inequality)}
\]
\[
\leq (1 - |\langle g \rangle|^{-1})|\langle g \rangle|^{-1}N^{-1} \sum_{q' \in \langle g \rangle : q' \neq q} \frac{S(q, q) + S(q', q')}{2} \leq (1 - |\langle g \rangle|^{-1})|\langle g \rangle|^{-1}N^{-1} \sum_{q' \in \langle g \rangle : q' \neq q} S(q', q')
\]
\[
= (1 - |\langle g \rangle|^{-1})^2N^{-1}S(q, q) + (1 - |\langle g \rangle|^{-1})|\langle g \rangle|^{-1}N^{-1} \sum_{q' \in \langle g \rangle : q' \neq q} S(q', q'). \tag{S80}
\]

Define
\[
\Theta_2(q, q) = \mu_{(g)} (1 - |\langle g \rangle|^{-1})|\langle g \rangle|^{-1} \sum_{q' \in \langle g \rangle : q' \neq q} \{ S(q, q) + S(q', q') - 2S(q, q') \} \geq 0. \tag{S81}
\]

We can upper bound \( \Theta_2(q, q) \) by
\[
\Theta_2(q, q) \leq 4\mu_{(g)} \max_{q' \in \langle g \rangle} S(q', q').
\]

Now using (22) and (S80), we have
\[
\mathbb{E}\{\widehat{V}_F(q, q)\} = \mu_{(g)} (1 - |\langle g \rangle|^{-1})^2(1 - 2N^{-1})S(q, q) + \mu_{(g)}\mathbb{E}\{(\overline{V}(q) - \overline{Y}_{(g)})^2\}
\]
\[
+ \mu_{(g)}|\langle g \rangle|^{-2}N^{-1}\{N - \varrho_{(g)} - (|\langle g \rangle| - 1)\} \sum_{q' \in \langle g \rangle : q' \neq q} S(q', q')
\]
\[
+N^{-1}\Theta(q, q),
\]

where
\[
\Theta(q, q) = \Theta_1(q, q) + \Theta_2(q, q), \quad 0 \leq \Theta(q, q) \leq 5\mu_{(g)} \max_{q' \in \langle g \rangle} S(q', q').
\]

Using \( \mu_{(g)} = (1 - |\langle g \rangle|^{-1})^{-2}(1 - 2N^{-1})^{-1} \) and Condition 5, we obtain that
\[
\mathbb{E}\{\widehat{V}_F(q, q)\} \geq S(q, q) + \mu_{(g)}(\overline{V}(q) - \overline{Y}_{(g)})^2 \geq S(q, q).
\]

(ii) We can show that
\[
\widehat{V}_{\gamma}(h, h') = \sum_{q \in \mathcal{Q}} F(h, q)F(h', q)\widehat{V}_F(q, q)
\]

S39
$$= \sum_{(g) \in \mathcal{G}} \sum_{q \in (g)} w_q \left( Y_q - \bar{Y}_{(g)} \right)^2$$

where

$$w_q = \mu(q) F(h, q) F(h', q'),$$ if \( q \in (g) \)

satisfies

$$|w_q| \leq (\max_{g \in \mathcal{G}} \mu(g)) \|F\|_\infty^2 := \bar{w}.$$

Applying Lemma S14, we have

$$\mathbb{P}\left\{ \left| \hat{\tilde{V}}_{\tilde{\gamma}}(h, h') - \mathbb{E}\{\hat{\tilde{V}}_{\tilde{\gamma}}(h, h')\} \right| \geq t \right\} \leq \frac{Cm^2 \Delta^2 (\Delta^2 + \zeta^2) N}{t^2} = \frac{C(\max_{g \in \mathcal{G}} \mu(g))^2 \|F\|_\infty^4 \Delta^2 (\Delta^2 + \zeta^2) N}{t^2} := \diamondsuit_2.$$

Taking union bound over \( h, h' \in [H] \), we obtain

$$\mathbb{P}\left\{ \|\hat{\tilde{V}}_{\tilde{\gamma}} - \mathbb{E}\{\hat{\tilde{V}}_{\tilde{\gamma}}\}\|_\infty \geq t \right\} \leq \frac{\diamondsuit_2 \cdot H^2}{t^2}.$$

(iii) It follows from (S1). \( \square \)

**More discussions on the conservativeness of \( \hat{\tilde{V}}_{\tilde{\gamma}} \).** Theorem 6(i) shows

$$\mathbb{E}\{\hat{\tilde{V}}_{\tilde{\gamma}}\} = \bar{V} + \Omega + \text{Diag}\{\mu(g)(\bar{Y}(q) - \bar{Y}_{(g)})^2\}_{q \in \mathcal{Q}_v} + N^{-1}(\Theta + S).$$

Following Lemma 2, we commented that the conservativeness can be reduced under different assumptions:

- If we assume homogeneity in means within subgroups, i.e.,

  $$\bar{Y}(q) = \bar{Y}_{(g)}, \text{ for all } q \in (g), \quad (S82)$$

  then the term

  $$\text{Diag}\{\mu(g)(\bar{Y}(q) - \bar{Y}_{(g)})^2\}_{q \in \mathcal{Q}_v}$$

  vanishes.

- If we assume homoskedasticity across treatment arms within the same subgroup, i.e.,

  $$S(q, q) = S(q', q'), \text{ for all } q, q' \in (g), \quad (S83)$$

S40
then \( \Omega \) has diagonals:

\[
\Omega(q, q) = \mu_{(g)}(|g| - 1)|g|^{-2} \left( 1 - \frac{\varrho(g)}{N} - \frac{|g| - 1}{N} \right) S(q, q),
\]

which can also contribute to \( S(q, q) \) and suggest that we can use a smaller correction factor \( \mu'_{(g)} \) to reduce the conservativeness:

\[
\mu'_{(g)} = (1 - |g|^{-1})^{-1}\{(1 - |g|^{-1})(1 - 2N^{-1}) + |g|^{-1}(1 - (2|g| - 1)/N)\}^{-1} \leq \mu_{(g)}.
\]

When \( |g| \) is large (say of the same order as \( N \)), \( \mu'_{(g)} \) is close to \( \mu_{(g)} \) because \( |g|^{-1}(1 - (2|g| - 1)/N) \) is small. When \( |g| \) is small, say for pairing, \( |g| = 2 \),

\[
\mu'_{(g)} \leq 2(1 - 3N^{-1})^{-1}, \quad \mu_{(g)} = 4(1 - 2N^{-1})^{-1}.
\]

Hence \( \mu'_{(g)} \) induces much less conservativeness than \( \mu_{(g)} \) under stronger assumptions.

- If we assume the strong null hypothesis within subgroups, i.e.,

\[
Y_i(q) = Y_i(q'), \text{ for all } i \in [N] \text{ and } q, q' \in \langle g \rangle,
\]

then both (S82) and (S83) are satisfied. Then

\[
\text{Diag} \left\{ \mu_{(g)}(\bar{Y}(q) - \bar{Y}_{(g)})^2 \right\}_{q \in Q_0} = 0,
\]

\[
\Theta = 0 \text{ (by the definitions of } \Theta_1 \text{ in (S79) and } \Theta_2 \text{ in (S81)).}
\]

Applying the correction factor \( \mu'_{(g)} \), we can show

\[
\mathbb{E}\{\hat{V}_Y(q, q)\} = S(q, q).
\]

**D.10. Proof of Theorem 7**

Based on Corollary 1 and Theorem 6, the proof can be done similarly as Theorem 4. We omit the details here.

**D.11. Proof of Theorem 8**

The proof is an application of Lemma S10 (ii).
D.12. Proof of Theorem 9

Proof of Theorem 9. (i) Combining the decomposition (29) and the results from Theorems 3 and 6, we have

\[
E\left\{\hat{V}_{\gamma}\right\} = E\left\{F_u^T \hat{V}_{\gamma,u} F_u + F_r^T \hat{V}_{\gamma,r} F_r + F_l^T \hat{V}_{\gamma,l} F_l\right\} \\
\geq F_u^T \text{Diag}\{S(q,q)\}_{q \in Q_u} F_u + F_u^T \Omega F_u + F_u^T \text{Diag}\{\mu_{(g)}(\gamma(q) - \gamma_g)^2\}_{q \in Q_u} F_u \\
+ F_r^T \text{Diag}\{N_q^{-1}S(q,q)\}_{q \in Q_r} F_r + F_l^T \text{Diag}\{N_q^{-1}S(q,q)\}_{q \in Q_l} F_l.
\]

Therefore, \( E\{\hat{V}_{\gamma}\} \geq F_u^T \hat{V}_{\gamma} F \geq V_{\gamma} \).

(ii) Decompose \( \hat{V}_{\gamma}(h,h') \) into three terms:

\[
\hat{V}_{\gamma}(h,h') = \sum_{q \in Q} F(k,q)F(k',q)\hat{V}_{\gamma}(q,q) \\
= \sum_{(g) \in (g)} \sum_{q \in (g)} F_u(k,q)F_u(k',q)\mu_{(g)}(Y_q - \gamma_g)^2 \\
+ \sum_{q \in Q_S} F_r(k,q)F_r(k',q)N_q^{-1}\hat{S}(q,q) \\
+ \sum_{q \in Q_L} F_l(k,q)F_l(k',q)N_q^{-1}\hat{S}(q,q),
\]

Applying Lemma S14, we have

\[
P\left\{|\hat{v}_1 - E\{\hat{v}_1\}| \geq t\right\} \leq \frac{C(\max_{g \in [G]} \mu_{(g)})^2\|F_u\|_\infty^4 \Delta^2 (\Delta^2 + \zeta^2)|Q_u|}{t^2} := \oplus_4.
\]

Applying Lemma S13 with \( Q = Q_r, \tau = \pi, \zeta = 1, N_0 = 1, \) we have

\[
P\left\{|\hat{v}_\Pi - E\{\hat{v}_\Pi\}| \geq t\right\} \leq \frac{C\pi\|F_r\|_\infty^4 |Q_r|\Delta^4}{t^2} := \oplus_5.
\]

Applying Lemma S13 with \( Q = Q_l, \) we have

\[
P\left\{|\hat{v}_{\Pi} - E\{\hat{v}_{\Pi}\}| \geq t\right\} \leq \frac{C\pi\|F_l\|_\infty^4 |Q_l|N_0^{-3}\Delta^4}{t^2} := \oplus_6.
\]

Therefore,

\[
P\left\{|\hat{V}_{\gamma}(h,h') - E\{\hat{V}_{\gamma}(h,h')\}| \geq t\right\}
\]
\[
\begin{align*}
&\leq P \{ |\hat{v}_1 - E\{\hat{v}_1\}| \geq t/3 \} \cup \{ |\hat{v}_II - E\{\hat{v}_II\}| \geq t/3 \} \cup \{ |\hat{v}_III - E\{\hat{v}_III\}| \geq t/3 \} \\
&\leq 9(\oplus_4 + \oplus_5 + \oplus_6).
\end{align*}
\]

Taking union bound over \( h, h' \in [H] \), we have
\[
P \left\{ \|\hat{V}_I - E\{\hat{V}_I\}\|_\infty \geq t \right\} \leq 9H^2(\oplus_4 + \oplus_5 + \oplus_6).
\]

(iii) It follows from (S1).

D.13. Proof of Theorem 10

Based on Corollary 2 and Theorem 9, the proof is similar to Theorem 4. We omit the details here.

D.14. Proof of Theorem S3

*Proof of Theorem S3.* For a given matrix \( W \), let \( B_t(x; W) = \{ y \in \mathbb{R}^H : (y - x)^\top W(y - x) \leq t \} \), which is convex. By Theorem S2,
\[
\sup_{t \in \mathbb{R}} |P(T \leq t) - P(T_0 \leq t)| = \sup_{t \in \mathbb{R}} |P\{\tilde{\gamma} \in B_t(0; W)\} - P\{\xi_H \in B_t(0; W)\}| \\
\leq \sup_{A \in A} |P\{\tilde{\gamma} \in A\} - P\{\xi_H \in A\}| \\
\leq CH^{13/4}NB_N(B_N^2 + N^{-1}) + CH^{3/4}B_N + CH^{13/8}N^{1/4}B_N^{3/2} \\
+ CH^{11/8}N^{1/2}B_N^2 + CH^{7/8}N^{1/4}B_N^{3/2},
\]
where \( B_N = \max_{h \in [H]} \max_{i,j \in [N]} |M''_h(i,j)| \). Here \( M''_h(i,j) \) is the standardized population matrix given by Lemma S2. Now applying (S8) in Lemma S2, we can further upper bound \( B_N \):
\[
B_N \leq \varrho_{\min}(V_\gamma)^{-1/2} \sqrt{H} \max_{h \in [H]} \max_{i,q \in [N]} |f_{qh}N_q^{-1}(Y_i(q) - \bar{Y}(q))|, \quad (S85)
\]

D.15. Proof of Lemma S10

*Proof of Lemma S10.* We derive upper bounds on \( B_N \) by bounding the quantities \( \varrho_{\min}(V_\gamma) \) and \( \max_{i,q \in [N]} |f_{qh}N_q^{-1}(Y_i(q) - \bar{Y}(q))| \). When bounds on \( B_N \) are obtained, the BEB for \( W \) is a direct application of Theorem S3.

(i) Under Conditions 1, 2 and 4, we have
\[
\varrho_{\min}(V_\gamma) \geq \varrho_{\min}(F^\top F) \cdot \min_{q \in [Q]} N_q^{-1}S(q, q),
\]
\[
\max_{i,q \in [N]} |f_{qh}N_q^{-1}(Y_i(q) - \overline{Y}(q))| \leq 2\|F\|_{\infty} \cdot \varepsilon^{-1}N_0^{-1} \max_{i \in [N], q \in [Q]} |Y_i(q) - \overline{Y}(q)|.
\]

Now use Condition 2 and the upper bound for \(B_N\) (S85) to obtain
\[
B_N \leq \frac{2c^{1/2}N_q^{-1}\max_{i \in [N], q \in [Q]} |Y_i(q) - \overline{Y}(q)|}{(c'\min_{q \in [Q]} S(q, q))^{1/2}} \cdot \left(\frac{H}{QN_0}\right)^{1/2}.
\]

Then we can apply Theorem S3 to derive the BEB.

If we further assume Condition 4, then \(B_N = O(H^{1/2}N^{-1/2})\). Then (S39) in Theorem S3 holds.

(ii) In non-uniform designs, we first give a lower bound on \(q_{\min}(V_\gamma)\):
\[
q_{\min}(V_\gamma) \geq q_{\min}(F_s^TF_s) \cdot (\overline{n}^{-1} \min_{q \in Q_s} S(q, q)). \tag{S86}
\]

Use Condition 2 to obtain
\[
q_{\min}\{F_s^TF_s\} = q_{\min}\{F^TF - F_L^TF_L\}
\geq q_{\min}\{F^TF\} - q_{\max}\{F_L^TF_L\}
\geq c'Q^{-1} - c^2H|Q_L|Q^{-2}
\geq (c'/2)Q^{-1}
\]
(because \(q_{\max}\{F_L^TF_L\} \leq \text{Tr}(F_L^TF_L) = c^2H|Q_L|Q^{-2}\)).

Then we bound the maximum part of \(B_N\) in (S38) by considering arms in \(Q_s\) and \(Q_L\) separately. For \(q \in Q_s\), because \(N_q \geq 1\), under Condition 2 we have
\[
\max_{h \in [H], i \in [N], q \in Q_s} |f_{qh}N_q^{-1}(Y_i(q) - \overline{Y}(q))| \leq 2cQ^{-1} \max_{i \in [N], q \in Q_s} |Y_i(q) - \overline{Y}(q)|. \tag{S87}
\]

For \(q \in Q_L\), we have
\[
\max_{h \in [H], i \in [N], q \in Q_L} |f_{qh}N_q^{-1}(Y_i(q) - \overline{Y}(q))| \leq 2c\varepsilon^{-1}Q^{-1}N_0^{-1} \max_{i \in [N], q \in Q_L} |Y_i(q) - \overline{Y}(q)|. \tag{S88}
\]

Now plugging (S86)–(S88) into (S38), we have
\[
B_N \leq \frac{2cH^{1/2} \max_{i \in [N], q \in [Q]} |Y_i(q) - \overline{Y}(q)|}{(c'\max_{q \in Q_s} S(q, q))^{1/2}} \cdot \max \left\{\frac{1}{Q}, \frac{1}{c'\varepsilon QN_0}\right\}
\leq \frac{2c \max_{i \in [N], q \in Q_s} |Y_i(q) - \overline{Y}(q)| H^{1/2}}{(c'\min_{q \in Q} S(q, q))^{1/2} Q^{1/2}}.
\]

S44
Now we can apply Theorem S3 to derive the BEB. If we further assume Condition 4 and \( N = O(Q) \), then \( B_N = O(H^{1/2} N^{-1/2}) \). Then (S39) in Theorem S3 holds.

**D.16. Proof of Corollary S1**

_Proof of Corollary S1._ No matter \( H \) is increasing or not, by the conditions and Theorem S3, we know that as \( N \to \infty \),

\[
\sup_{t \in \mathbb{R}} |\mathbb{P}(T \leq t) - \mathbb{P}(T_0 \leq t)| = o(1).
\]

(i) When \( H \) is fixed, the proof is done.

(ii) When \( H \) is increasing to infinity, by the classical Lindeberg CLT, we have for a standard Normal variable \( Z \),

\[
\sup_{t \in \mathbb{R}} |\mathbb{P}\{T_0 \leq t\} - \mathbb{P}\left\{ \sqrt{\text{Var}\{T_0\}} Z + \mathbb{E}(T_0) \leq t \right\}| = o(1).
\]

Using the expectation and variance calculation for \( T_0 \) in (S64), we conclude the second part.

**D.17. Proof of Lemma S11**

_Proof of Lemma S11._ Without loss of generality, we assume the potential outcomes are centered: \( \bar{Y}(q) = 0 \) for all \( q \in [Q] \).

(i) The first part follows from the variance formula of \( \hat{Y}_q \).

(ii) Now we bound the fourth moment of \( \hat{Y}_q \):

\[
\mathbb{E}\left\{ \hat{Y}_q^4 \right\} = \frac{1}{N q^4} \mathbb{E}\left\{ \sum_{i=1}^{N} Y_i(q)^4 \mathbb{1}\{Z_i = q\} \right\} \tag{II.2-1}
\]

\[
+ \frac{4}{N q^4} \mathbb{E}\left\{ \sum_{i \neq j}^{N} Y_i(q)^3 Y_j(q) \mathbb{1}\{Z_i = Z_j = q\} \right\} \tag{II.2-2}
\]

\[
+ \frac{3}{N q^4} \mathbb{E}\left\{ \sum_{i \neq j}^{N} Y_i(q)^2 Y_j(q)^2 \mathbb{1}\{Z_i = Z_j = q\} \right\} \tag{II.2-3}
\]
\[
\begin{align*}
\text{II.2-1} &= \frac{1}{N_q^3} \sum_{i=1}^{N} Y_i(q)^4, \\
\text{II.2-2} &= \frac{4}{N_q^4} \mathbb{E} \left\{ \sum_{i \neq j}^{N} Y_i(q)^3 Y_j(q) 1 \{Z_i = Z_j = q\} \right\} \\
&= \frac{4(N_q - 1)}{N_q^3 N(N - 1)} \sum_{i \neq j}^{N} Y_i(q)^3 Y_j(q) \\
&= -\frac{4(N_q - 1)}{N_q^3 N(N - 1)} \sum_{i \neq j}^{N} Y_i(q)^4, \\
\text{II.2-3} &= \frac{3(N_q - 1)}{N_q^3 N(N - 1)} \sum_{i \neq j}^{N} Y_i(q)^2 Y_j(q)^2, \\
\text{II.2-4} &= \frac{3(N_q - 1)(N_q - 2)}{N_q^3 N(N - 1)(N - 2)} \sum_{i \neq j \neq k}^{N} Y_i(q)Y_j(q)Y_k(q)^2 \\
&= \frac{3(N_q - 1)(N_q - 2)}{N_q^3 N(N - 1)(N - 2)} \sum_{j \neq k}^{N} (Y_j(q) + Y_k(q)) Y_j(q)Y_k(q)^2 \\
&= -\frac{3(N_q - 1)(N_q - 2)}{N_q^3 N(N - 1)(N - 2)} \sum_{j \neq k}^{N} Y_j(q)^2 Y_k(q)^2 + \frac{3(N_q - 1)(N_q - 2)}{N_q^3 N(N - 1)(N - 2)} \sum_{k}^{N} Y_k(q)^4, \\
\text{II.2-5} &= \frac{N_q(N_q - 1)(N_q - 2)(N_q - 3)}{N_q^4 N(N - 1)(N - 2)(N - 3)} \sum_{i \neq j \neq k \neq l}^{N} Y_i(q)Y_j(q)Y_k(q)Y_l(q) \\
&= -\frac{3N_q(N_q - 1)(N_q - 2)(N_q - 3)}{N_q^4 N(N - 1)(N - 2)(N - 3)} \sum_{i \neq j \neq k}^{N} Y_i(q)Y_j(q)Y_k(q)^2 \\
&= \frac{3N_q(N_q - 1)(N_q - 2)(N_q - 3)}{N_q^4 N(N - 1)(N - 2)(N - 3)} \sum_{j \neq k}^{N} Y_j(q)^2 Y_k(q)^2 \\
&= -\frac{3N_q(N_q - 1)(N_q - 2)(N_q - 3)}{N_q^4 N(N - 1)(N - 2)(N - 3)} \sum_{k}^{N} Y_k(q)^4.
\end{align*}
\]
Now bound these terms:

\[ |\text{II.2-1}| \leq \frac{\Delta^4}{N_q^3}, \quad |\text{II.2-2}| \leq \frac{4\Delta^4}{N_q^2 N}, \]

\[ |\text{II.2-3}| \leq \frac{6\Delta^4}{N_q^2 N^2} \left( \text{using} \sum_{i \neq j} Y_i(q)^2 Y_j(q)^2 \leq \sum_i Y_i(q)^2 \sum_j Y_j(q)^2 \right), \]

\[ |\text{II.2-4}| \leq \frac{6\Delta^4}{N_q(N-2)} + \frac{3\Delta^4}{N_q(N-1)(N-2)}, \]

\[ |\text{II.2-5}| \leq \frac{6\Delta^4}{(N-2)(N-3)} + \frac{3\Delta^4}{(N-1)(N-2)(N-3)}. \]

Choose \( N \) large enough to obtain

\[ \mathbb{E} \left\{ \hat{Y}_q^4 \right\} \leq \frac{C\Delta^4}{N_q^2}. \]

(iii) Then we compute the covariance terms:

\[
\mathbb{E} \left\{ \hat{Y}_q^2 \hat{Y}_{q'}^2 \right\} - \mathbb{E} \left\{ \hat{Y}_q^2 \right\} \mathbb{E} \left\{ \hat{Y}_{q'}^2 \right\} = \\
\underbrace{\frac{1}{N_q^2 N_q'} \sum_{i \neq k} Y_i(q)^2 Y_k(q')^2 \frac{N_q N_q'}{N(N-1)}}_{\text{II.2-1}} + \\
\underbrace{\frac{1}{N_q^2 N_q'} \sum_{i \neq j \neq k} Y_i(q) Y_j(q) Y_k(q')^2 \frac{N_q(N_q-1)N_q'}{N(N-1)(N-2)}}_{\text{II.2-2}} + \\
\underbrace{\frac{1}{N_q^2 N_q'} \sum_{i \neq j \neq k} Y_i(q)^2 Y_k(q') Y_j(q') \frac{N_q N_q(N_q'-1)}{N(N-1)(N-2)}}_{\text{II.2-3}} + \\
\underbrace{\frac{1}{N_q^2 N_q'} \sum_{i \neq j \neq k} Y_i(q) Y_j(q) Y_k(q') Y_i(q') \frac{N_q(N_q-1)N_q'(N_q'-1)}{N(N-1)(N-2)(N-3)}}_{\text{II.2-4}} - \\
\underbrace{\left\{ \frac{1}{N_q} - \frac{1}{N} \right\} S(q,q) \cdot \left\{ \frac{1}{N_q'} - \frac{1}{N} \right\} S(q',q')}_{\text{II.2-5}}.
\]

For II.2-1 and II.2-5:

\[
\left| \frac{1}{N_q^2 N_q'} \sum_{i \neq k} Y_i(q)^2 Y_k(q')^2 \frac{N_q N_q'}{N(N-1)} - \frac{1}{(N-1)^2} \left( \frac{N - N_q}{N_q N} \right) \left( \frac{N - N_q'}{N_q' N} \right) \left\{ \sum_{i=1}^N Y_i(q)^2 \right\} \left\{ \sum_{k=1}^N Y_i(q')^2 \right\} \right|
\]
For II.2-2:

\[ \left| \sum_{i \neq j \neq k} Y_i(q) Y_j(q) Y_k(q') \right| \leq \frac{1}{N_q N_q' N(N-1)(N-2)} \sum_{i \neq k} Y_i(q) \{ Y_i(q) + Y_k(q) \} Y_k(q') \frac{N_q(N_q-1)N_q'}{N(N-1)(N-2)} \]

\[ \leq \frac{N_q - 1}{N_q N_q' N(N-1)(N-2)} \sum_{i \neq k} \left\{ \frac{1}{2} Y_i(q)^4 + \frac{1}{2} Y_k(q')^4 + \frac{1}{4} Y_i(q)^4 + \frac{1}{4} Y_k(q)^4 + \frac{1}{2} Y_k(q')^4 \right\} \]

\[ \leq \frac{N_q - 1}{N_q N_q' N(N-1)(N-2)} \{ N(N-1) \cdot 2\Delta^4 \} \leq \frac{2(N_q + N_q') \Delta^4}{N_q N_q' (N-2)}. \]

II.2-3 is similar to II.2-2:

\[ \left| \sum_{i \neq j \neq k} Y_i(q)^2 Y_j(q') Y_k(q') \right| \leq \frac{2(N_q + N_q') \Delta^4}{N_q N_q' (N-2)}. \]

For II.2-4:

\[ \left| \sum_{i \neq j \neq k \neq l} Y_i(q) Y_j(q) Y_k(q') Y_l(q') \right| \leq \frac{1}{N_q N_q' N(N-1)(N-2)(N-3)} \sum_{i \neq j \neq k \neq l} Y_i(q) \{ Y_i(q) + Y_j(q) + Y_k(q') + Y_l(q') \} \frac{N_q(N_q - 1)N_q'(N_q' - 1)}{N(N-1)(N-2)(N-3)} \]

\[ \leq \frac{(N_q - 1)(N_q' - 1)}{N_q N_q' N(N-1)(N-2)(N-3)} \cdot 6N(N-1) \Delta^4 \text{ (reduce terms like II.2-2)} \]

\[ \leq \frac{3(N_q - 1)(N_q' - 1) \Delta^4}{N_q N_q' (N-2)(N-3)}. \]

Summarizing II.2-1 to II.2-5,

\[ \left| \text{Cov} \left\{ \bar{Y}_q^2, \bar{Y}_q^3 \right\} \right| \leq \frac{C(N_q + N_q') \Delta^4}{N_q N_q' N}. \] (S89)
D.18. Proof of Lemma S12

Proof of Lemma S12. Part (i) and Part (ii) can be shown by constructing new potential outcomes \( \{Y_i(q)^2\} \) and apply the variance formula for the sample average. Thus we omit the proof.

For Part (iii), we have

\[
|\text{Cov} \{ Y_{q_1}^2, Y_{q_1} Y_{q_2} \}| = |E \{ Y_{q_1} Y_{q_2} \} - E \{ Y_{q_1}^2 \} E \{ Y_{q_1} Y_{q_2} \} |
\]
\[
= \left| \frac{1}{(N)^2} \sum_{i \neq j} Y_i(q_1)^3 Y_j(q_2) + (1 - N^{-1}) S_Y(q_1, q_1) \cdot N^{-1} S(q_1, q_2) \right| \leq \frac{C \Delta^4}{N}.
\]

For Part (iv), we have

\[
|\text{Cov} \{ Y_{q_1}^2, Y_{q_2} Y_{q_3} \}| = |E \{ (Y_{q_1}^2 - E \{ Y_{q_1}^2 \}) Y_{q_2} Y_{q_3}^2 \} |
\]
\[
= \left| E \left\{ \sum_{i \neq j \neq k} \{ Y_i(q_1)^2 - N^{-1} \sum_{i \in [N]} Y_i(q_1)^2 \} Y_j(q_2) Y_k(q_3) \right\} 1 \{ Z_i = q_1, Z_j = q_2, Z_k = q_3 \} \right|
\]
\[
= \left| \frac{1}{(N)^3} \sum_{i \neq j \neq k} \{ Y_i(q_1)^2 - N^{-1} \sum_{i \in [N]} Y_i(q_1)^2 \} Y_j(q_2) Y_k(q_3) \right|
\]
\[
= \left| - \frac{1}{(N)^3} \sum_{j \neq k} \{ Y_j(q_1)^2 + Y_k(q_1)^2 - 2N^{-1} \sum_{i \in [N]} Y_i(q_1)^2 \} Y_j(q_2) Y_k(q_3) \right| \leq \frac{C \Delta^4}{N}.
\]

For Part (v), we have

\[
|\text{Cov} \{ Y_{q_1} Y_{q_2}, Y_{q_3} Y_{q_1} \} |
\]
\[
= \left| \frac{1}{(N)^4} \sum_{i \neq j \neq k \neq l} \left\{ Y_i(q_1) Y_j(q_2) - \frac{1}{(N)^2} \sum_{i \neq j} Y_i(q_1) Y_j(q_2) \right\} Y_k(q_3) Y_l(q_4) \right|
\]
\[
= \left| - \frac{1}{(N)^4} \sum_{i \neq j \neq k} \left\{ Y_i(q_1) Y_j(q_2) - \frac{1}{N(N-1)} \sum_{i \neq j} Y_i(q_1) Y_j(q_2) \right\} Y_k(q_3) (Y_i(q_4) + Y_j(q_4) + Y_k(q_4)) \right|.
\]

Further we have

\[
\left| \frac{1}{(N)^4} \sum_{i \neq j \neq k} \left\{ Y_i(q_1) Y_j(q_2) - \frac{1}{(N)^2} \sum_{i \neq j} Y_i(q_1) Y_j(q_2) \right\} Y_k(q_3) Y_l(q_4) \right|
\]
\[
= \left| - \frac{1}{(N)^4} \sum_{i \neq j} \left\{ Y_i(q_1) Y_j(q_2) - \frac{1}{(N)^2} \sum_{i \neq j} Y_i(q_1) Y_j(q_2) \right\} (Y_i(q_3) + Y_j(q_3)) Y_l(q_4) \right| \leq \frac{C \Delta^4}{N^2}.
\]
Similar for the summation
\[
\left| \frac{1}{(N)^4} \sum_{i \neq j \neq k} \left\{ Y_i(q_1)Y_j(q_2) - \frac{1}{(N)^2} \sum_{i \neq j} Y_i(q_1)Y_j(q_2) \right\} Y_k(q_3)Y_j(q_4) \right| \leq C\Delta^4 \frac{N^2}{N^2}.
\]

Last, it remains to bound
\[
\left| \frac{1}{(N)^4} \sum_{i \neq j \neq k} \left\{ Y_i(q_1)Y_j(q_2) - \frac{1}{(N)^2} \sum_{i \neq j} Y_i(q_1)Y_j(q_2) \right\} Y_k(q_3)^2 \right|
= \left| \frac{1}{(N)^4} \sum_{j \neq k} \left\{ -(Y_j(q_1) + Y_k(q_1))Y_j(q_2) + \frac{N-2}{(N)^2} \sum_i Y_i(q_1)^2 \right\} Y_k(q_3)^2 \right|
\leq C\Delta^4 \frac{N^2}{N^2}.
\]

Hence we conclude the proof by combining the above parts. \( \square \)

D.19. Proof of Lemma S13

**Proof of Lemma S13.** The proof is based on Chebyshev’s inequality and bounding the variance of
\[
\sum_{q \in \mathcal{Q}} w_q N_q^{-1} \hat{S}(q, q) = \sum_{q \in \mathcal{Q}} w_q N_q^{-1} (N_q - 1)^{-1} \sum_{q_i=q} (Y_i - \overline{Y}(q))^2 \tag{II.1}
- \sum_{q \in \mathcal{Q}} w_q (N_q - 1)^{-1} \left( \hat{Y}(q) - \overline{Y}(q) \right)^2 \tag{II.2}.
\]

The above decomposition ensures that we can assume \( Y_i(q)’s \) are centered without loss of generality. For II.1, we have
\[
\text{Var} \{\text{II.1}\} \leq \sum_{q \in \mathcal{Q}} w_q^2 (N_q - 1)^{-1} N_q^{-2} S_{Y^2}(q, q) \leq 4\varepsilon^{-3} \overline{w}^2 |\mathcal{Q}| N_0^{-3} \Delta^4. \tag{S90}
\]

For II.2, we have
\[
\text{Var} \{\text{II.2}\} \leq \sum_{q \in \mathcal{Q}} w_q^2 (N_q - 1)^{-2} \text{Var} \left\{ \hat{Y}_q^2 \right\} \\
+ \sum_{q \neq q' \in \mathcal{Q}} w_q w_{q'} (N_q - 1)(N_{q'} - 1) \text{Cov} \left\{ \hat{Y}_q^2, \hat{Y}_{q'}^2 \right\} \\
\leq \sum_{q \in \mathcal{Q}} w_q^2 (N_q - 1)^{-2} \mathbb{E} \left\{ \hat{S}_q^4 \right\} \\
+ \sum_{q \neq q' \in \mathcal{Q}} w_q w_{q'} (N_q - 1)(N_{q'} - 1) \text{Cov} \left\{ \hat{Y}_q^2, \hat{Y}_{q'}^2 \right\}
\]
\[
\begin{align*}
&\leq \sum_{q \in Q} w_q^2 (N_q - 1)^{-2} (C \Delta^4 N_q^{-2}) \\
&+ \sum_{q \neq q' \in Q} w_q w_{q'} (N_q - 1)^{-1} (N_{q'} - 1)^{-1} \frac{C(N_q + N_{q'}) \Delta^4}{N_q N_{q'} N} \\
&(\text{By Lemma S11}).
\end{align*}
\]

For (S91), we have
\[
\sum_{q \in Q} w_q^2 (N_q - 1)^{-2} (C \Delta^4 N_q^{-2}) \leq C \varepsilon^{-4} w^2 |Q| N_0^{-4} \Delta^4. \tag{S93}
\]

For (S92), we have
\[
\left| \sum_{q \neq q' \in Q} w_q w_{q'} (N_q - 1)^{-1} (N_{q'} - 1)^{-1} \frac{C(N_q + N_{q'}) \Delta^4}{N_q N_{q'} N} \right| \\
\leq \sum_{q \neq q' \in Q} \bar{w}^2 \cdot 4(\varepsilon N_0)^{-4} \cdot \frac{C \varepsilon N_0 \Delta^4}{\varepsilon Q N_0} \\
\leq \bar{w}^2 \cdot 4(\varepsilon N_0)^{-4} \cdot \frac{C \varepsilon |Q|^2 \Delta^4}{\varepsilon Q} \\
\leq C \varepsilon^{-4} \bar{w}^2 |Q| N_0^{-4} \Delta^4 \\
\leq C \varepsilon^{-4} \bar{w}^2 |Q| N_0^{-3} \Delta^4, \tag{S94}
\]

where in the last inequality (S94), we use the fact that as the lower bound for the size of the arms, \(\varepsilon N_0\) is in general greater than some absolute constant (in many cases just use 1).

Combining (S90)–(S94), we have
\[
\text{Var} \left\{ \sum_{q \in Q} w_q N_q^{-1} \tilde{S}(q, q) \right\} \leq C \varepsilon^{-4} \bar{w}^2 |Q| N_0^{-3} \Delta^4.
\]

We apply Chebyshev’s inequality to conclude the proof.

\(\square\)

**D.20. Proof of Lemma S14**

*Proof of Lemma S14.* The proof is based on Chebyshev’s inequality and bounding the variance of \(\hat{v}\).

For any \(\langle g \rangle\), we have
\[
\sum_{q \in \langle g \rangle} w_q \left( Y_q - \hat{Y}_{\langle g \rangle} \right)^2 = \sum_{q \in \langle g \rangle} w_q \left( Y_q - \overline{Y}(q) + \overline{Y}(q) - \overline{Y}(q) + \overline{Y}(q) - \hat{Y}_{\langle g \rangle} \right)^2
\]
sample averages and apply Lemma S12. Take (S99) for example. We can treat \( Y \) will not make contribution to the variance. Similar derivation holds for (S100) and (S101).

\[
\begin{align*}
\text{Term I} & = \sum_{q \in (g)} w_q (Y_q - \overline{Y}(q))^2 + \sum_{q \in (g)} w_q (\overline{Y}(q) - \overline{Y}_{(g)})^2 + \sum_{q \in (g)} w_q (\overline{Y}(g) - \overline{Y}_{(g)})^2 \\
\text{Term II} & = + 2 \sum_{q \in (g)} w_q \{(Y_q - \overline{Y}(q))(\overline{Y}(q) - \overline{Y}_{(g)})\} \\
\text{Term IV} & = + 2 (\overline{Y}(g) - \overline{Y}_{(g)}) \sum_{q \in (g)} w_q \{(Y_q - \overline{Y}(q))\} \\
\text{Term V} & = + 2 (\overline{Y}(g) - \overline{Y}_{(g)}) \sum_{q \in (g)} w_q \{(\overline{Y}(q) - \overline{Y}_{(g)})\} \\
\text{Term VI} & = + 2 (\overline{Y}(g) - \overline{Y}_{(g)}) \sum_{q \in (g)} w_q \{(\overline{Y}(q) - \overline{Y}_{(g)})\}
\end{align*}
\]

(S95)

There are six terms in (S95) to (S98). We deal with them separately.

**Bound summations involving Term I, IV and VI.** We first show upper bounds for the variance of Term I, IV and VI (summed over \( g \in [G] \)):

\[
\begin{align*}
\text{Var} \left\{ \sum_{q \in G} \sum_{q \in (g)} w_q (Y_q - \overline{Y}(q))^2 \right\} & \leq C \sum_{q \in [Q]} w_q^2 \Delta^4, \quad (S99) \\
\text{Var} \left\{ \sum_{g \in [G]} \sum_{q \in (g)} w_q \{(Y_q - \overline{Y}(q))(\overline{Y}(q) - \overline{Y}_{(g)})\} \right\} & \leq C \sum_{q \in [Q]} w_q^2 \Delta^2 \zeta^2, \quad (S100) \\
\text{Var} \left\{ \sum_{g \in [G]} (\overline{Y}(g) - \overline{Y}_{(g)}) \sum_{q \in (g)} w_q \{(\overline{Y}(q) - \overline{Y}_{(g)})\} \right\} & \leq C \sum_{q \in [Q]} w_q^2 \Delta^2 \zeta^2. \quad (S101)
\end{align*}
\]

The key idea for proving (S99)–(S101) is to treat the summations as linear combinations of sample averages and apply Lemma S12. Take (S99) for example. We can treat \( Y_q'(q) = (Y_i(q) - \overline{Y}(g))^2 \) as pseudo potential outcomes and obtain:

\[
\begin{align*}
\text{Var} \left\{ \sum_{q \in G} \sum_{q \in (g)} w_q (Y_q - \overline{Y}(q))^2 \right\} & \leq \sum_{g \in \mathcal{G}} \sum_{q \in (g)} w_q^2 S_{Y_i'(q)} \leq C \sum_{q \in [Q]} w_q^2 \Delta^4.
\end{align*}
\]

(S102)

Similar derivation holds for (S100) and (S101).

**Bound summations involving Term II.** Term II is a non-random quantity. Therefore, it will not make contribution to the variance.

**Bound summations involving Terms III.** Now we bound

\[
\text{Var} \left\{ \sum_{g \in [G]} |(g)| \overline{m}_{(g)} (\overline{Y}_{(g)} - \overline{Y}_{(g)})^2 \right\}, \text{ (where } \overline{m}_{(g)} = |(g)|^{-1} \sum_{q \in (g)} w_q). \quad (S102)
\]

S52
Using (S104), we have

\[ \begin{align*}
(S102) = & \sum_{g \in [G]} |\langle g \rangle|^2 \mathbb{w}^2_{(g)} \text{Var} \left\{ (\hat{Y}_{(g)} - \bar{Y}_{(g)})^2 \right\} \\
& + \sum_{g \neq g' \in [G]} |\langle g \rangle||\langle g' \rangle| \mathbb{w}^2_{(g)} \mathbb{w}^2_{(g')} \text{Cov} \left\{ (\hat{Y}_{(g)} - \bar{Y}_{(g)})^2, (\hat{Y}_{(g')} - \bar{Y}_{(g')})^2 \right\}.
\end{align*} \]

For Term III.1, we can show

\[ \begin{align*}
\sum_{g \in [G]} |\langle g \rangle|^2 \mathbb{w}^2_{(g)} \text{Var} \left\{ (\hat{Y}_{(g)} - \bar{Y}_{(g)})^2 \right\} \\
& = \sum_{g \in [G]} |\langle g \rangle|^2 \mathbb{w}^2_{(g)} \text{Cov} \left\{ (\hat{Y}_{(g)} - \bar{Y}_{(g)})^2, (\hat{Y}_{(g)} - \bar{Y}_{(g)})^2 \right\} \\
& = \sum_{g \in [G]} |\langle g \rangle|^2 \mathbb{w}^2_{(g)} |\langle g \rangle|^{-4} \left\{ \sum_{q \in [g]} \text{Var} \left\{ (Y_q - \bar{Y}(g))^2 \right\} + \sum_{q_1 \neq q_2 \in [\langle g \rangle]} \text{Cov} \left\{ (Y_{q_1} - \bar{Y}(q_1))^2, (Y_{q_1} - \bar{Y}(q_1))(Y_{q_2} - \bar{Y}(q_2)) \right\} \\
& + \sum_{q_1 \neq q_2 \neq q_3 \in [\langle g \rangle]} \text{Cov} \left\{ (Y_{q_1} - \bar{Y}(q_1))(Y_{q_2} - \bar{Y}(q_2)), (Y_{q_3} - \bar{Y}(q_3))(Y_{q_4} - \bar{Y}(q_4)) \right\} \right\} \\
& \leq \sum_{g \in [G]} |\langle g \rangle|^{-2} \mathbb{w}^2_{(g)} \left\{ C||\langle g \rangle||^4 + C||\langle g \rangle||^2 \Delta^4 / N + C||\langle g \rangle||^4 \Delta^4 / N + C||\langle g \rangle||^4 \Delta^4 / N^2 \right\} \\
& \leq C \sum_{g \in [G]} \mathbb{w}^2_{(g)} \Delta^4 \leq C \mathbb{w}^2 \Delta^4 \leq C \mathbb{w}^2 \Delta^4 N_u. \quad \text{(S103)}
\end{align*} \]

To bound Term III.2, we first obtain the following bound using Lemma S12:

\[ \left| \text{Cov} \left\{ (\hat{Y}_{(g)} - \bar{Y}_{(g)})^2, (\hat{Y}_{(g')} - \bar{Y}_{(g')})^2 \right\} \right| \leq \frac{C \Delta^4(||\langle g \rangle|| + ||\langle g' \rangle||)}{|\langle g \rangle||\langle g' \rangle| N}, \forall g \neq g' \in [G]. \quad \text{(S104)} \]

The derivation is similar to what we did when handling Term III.1, thus we omit the details here. Using (S104), we have

\[ \begin{align*}
\left| \sum_{g \neq g' \in [G]} |\langle g \rangle||\langle g' \rangle| \mathbb{w}^2_{(g)} \mathbb{w}^2_{(g')} \text{Cov} \left\{ (\hat{Y}_{(g)} - \bar{Y}_{(g)})^2, (\hat{Y}_{(g')} - \bar{Y}_{(g')})^2 \right\} \right| \leq \frac{C N^2 \mathbb{w}^2 \Delta^4}{N} \leq C \mathbb{w}^2 \Delta^4 N_u. \quad \text{(S105)}
\end{align*} \]
Combine (S103) and (S105) to obtain

\[(S102) \leq Cw^2\Delta^4N_U.\]  

Bound summations involving Term V. Now we bound

\[
\text{Var} \left\{ \sum_{g \in [G]} (\bar{Y}_{(g)} - \hat{Y}_{(g)}) \sum_{q \in (g)} w_q \{ (Y_q - \bar{Y}(q)) \} \right\}.
\]  

We can show

\[(S107) = \sum_{g \in [G]} \text{Var} \left\{ (\bar{Y}_{(g)} - \hat{Y}_{(g)}) \sum_{q \in (g)} w_q (Y_q - \bar{Y}(q)) \right\} + \sum_{g \neq g \in [G]} \text{Cov} \left\{ (\bar{Y}_{(g)} - \hat{Y}_{(g)}) \sum_{q \in (g)} w_q (Y_q - \bar{Y}(q)), (\bar{Y}_{(g')'} - \hat{Y}_{(g')'}) \sum_{q \in (g')'} w_q (Y_q - \bar{Y}(q)) \right\}.
\]

The analysis is very similar to (S102). We omit the proof and directly state the conclusion:

\[
\sum_{g \in [G]} \text{Var} \left\{ (\bar{Y}_{(g)} - \hat{Y}_{(g)}) \sum_{q \in (g)} w_q (Y_q - \bar{Y}(q)) \right\} \leq Cw^2\Delta^4G \leq Cw^2\Delta^4N_U,
\]

\[
\sum_{g \neq g \in [G]} \text{Cov} \left\{ (\bar{Y}_{(g)} - \hat{Y}_{(g)}) \sum_{q \in (g)} w_q (Y_q - \bar{Y}(q)), (\bar{Y}_{(g')'} - \hat{Y}_{(g')'}) \sum_{q \in (g')'} w_q (Y_q - \bar{Y}(q)) \right\} \leq Cw^2\Delta^4N_U,
\]

\[(S107) \leq Cw^2\Delta^4N_U.\]  

Summarize results. Combining (S99), (S100), (S101), (S106) and (S108), for the unreplicated design, we have

\[
\text{Var} \{ \hat{v} \} \leq Cw^2(\Delta^4 + \Delta^2\zeta^2)N_U.
\]

Now the tail bound can be obtained by Chebyshev’s inequality. \[\square\]

D.21. Proof of Theorem S4

Proof of Theorem S4. The proof extends that of Theorem 1. The main difference is that we need to carefully choose the norms and get more delicate bounds. By Lemma S2, there are population matrices $M''_n, \ldots, M''_H$ that satisfy Condition S1 and $\bar{\gamma} = (\text{Tr} (M''_h P))_{h=1}^H$. We apply Theorem S1 to obtain that for any $b \in \mathbb{R}^H$ with $\|b\|_2 = 1$,

\[
\sup_{t \in \mathbb{R}} |\mathbb{P}\{ b^T \bar{\gamma} \leq t \} - \Phi(t) | \leq C \max_{i,j \in [N]} \left| \sum_{h=1}^H b_h M''_h(i,j) \right|.
\]
Here following the proof of Lemma S2, \( M'_h \) is obtained through the following definition of \( M'_h \).

Define

\[
\bar{Y}_i(q) = Y_i(q) - \bar{Y}(q), \quad \gamma_i = N^{-1} \sum_{q'=1}^{Q} F_{q'} \bar{Y}_i(q').
\]  

(S109)

For each \( i, j \in [N] \), define

\[
M'_h(i, j) = N_q^{-1} F_q(h, \cdot) \bar{Y}_i(q) - \gamma_i, \quad \sum_{q'=0}^{q-1} N_q + 1 \leq j \leq \sum_{q'=0}^{q} N_q.
\]  

(S110)

indicates a natural mapping from column \( j \) to a particular treatment level \( q_j \). Then

\[
\begin{aligned}
&b^\top \left( \{\text{vec}(M''_1)\}^\top \right) = b^\top V_{\tilde{\gamma}}^{-1/2} \left( \{\text{vec}(M'_1)\}^\top \right) \\
&\quad \vdots \\
&\quad \{\text{vec}(M''_H)\}^\top \\
&= b^\top V_{\tilde{\gamma}}^{-1/2} \left( \begin{array}{c}
N_q^{-1} F_{q_j}(1, \cdot) \bar{Y}_i(q_j) - \gamma_{1i} \\
\vdots \\
N_q^{-1} F_{q_j}(H, \cdot) \bar{Y}_i(q_j) - \gamma_{Hi}
\end{array} \right) - b^\top V_{\tilde{\gamma}}^{-1/2} \left( \begin{array}{c}
\gamma_{1i} \\
\vdots \\
\gamma_{Hi}
\end{array} \right) \\
&= \left( b^\top V_{\tilde{\gamma}}^{-1/2} N_q^{-1} F_{q_j} \bar{Y}_i(q_j) \right) - \left( b^\top V_{\tilde{\gamma}}^{-1/2} \gamma_i \right) \\
&= \left( b^\top V_{\tilde{\gamma}}^{-1/2} N_q^{-1} F_{q_j} \bar{Y}_i(q_j) \right) - \left( b^\top V_{\tilde{\gamma}}^{-1/2} \gamma_i \right). \tag{term I} \\
\end{aligned}
\]

From (S109), term II is the average of term I over \( j \in [N] \). Therefore, we can bound term I for all \( i, q \) and use triangle inequality to obtain a bound for term II.

**First bound for term I.** For \( b \in \mathbb{R}^H \) with \( \|b\|_2 = 1 \), construct \( b_0 = V_{\tilde{\gamma}}^{-1/2} b / \|V_{\tilde{\gamma}}^{-1/2} b\|_2 \in \mathbb{R}^H \) with \( \|b_0\|_2 = 1 \). We can verify that

\[
b = \frac{V_{\tilde{\gamma}}^{-1/2} b_0}{\sqrt{b_0^\top V_{\tilde{\gamma}} b_0}}.
\]

Then

\[
\left| b^\top V_{\tilde{\gamma}}^{-1/2} N_q^{-1} F_{q_j} \bar{Y}_i(q_j) \right| = \left| b_0^\top N_q^{-1} F_{q_j} \bar{Y}_i(q_j) \right| \cdot \frac{1}{\sqrt{b_0^\top V_{\tilde{\gamma}} b_0}} \leq \left\| b_0^\top F_{q_j} \right\|_1 \cdot \frac{N_q^{-1} \|\bar{Y}_i(q_j)\|_\infty}{\sqrt{b_0^\top V_{\tilde{\gamma}} b_0}}.
\]

S55
This gives the bounds that depends on the choice of $b$.
To get a uniform bound, we need to bound $\|b_0^T F_{q_j}\|_1$ and $b_0^T V_{\tilde{\gamma}} b_0$. We can show

$$\|b_0^T F_{q_j}\|_1 = \sum_{k \in [p]} |b_0^T F_{q_j}(\cdot, k)| \leq \sum_{k \in [p]} \|F_{q_j}(\cdot, k)\|_2 = \|F_{q_j}\|_{2,1}, \quad b_0^T V_{\tilde{\gamma}} b_0 \geq \theta_{\min}\{V_{\tilde{\gamma}}\}.$$  

Hence

$$\left\|b_0^T F_{q_j}\right\|_1 \cdot \frac{N_{q_j}^{-1}\|\bar{Y}_i(q_j)\|_{\infty}}{\sqrt{b_0^T V_{\tilde{\gamma}} b_0}} \leq \frac{\max_{q \in [Q]} \|F_{q_j}\|_{2,1} \cdot N_{q_j}^{-1}\|\bar{Y}_i(q_j) - \bar{Y}(q_j)\|_{\infty}}{\sqrt{\theta_{\min}\{V_{\tilde{\gamma}}\}}}.$$

(S111)

**Second bound for term I.** Revisit term I. We have

$$b^T V_{\tilde{\gamma}}^{-1/2} N_{q_j}^{-1} F_{q_j} \bar{Y}_i(q_j) = \left|b^T V_{\tilde{\gamma}}^{-1/2} F_{q_j} \{N_{q_j}^{-1} S(q_j, q_j)\}^{1/2} \{N_{q_j}^{-1} S(q_j, q_j)\}^{-1/2} \{N_{q_j}^{-1} \bar{Y}_i(q_j)\}\right| \leq \left\|b^T V_{\tilde{\gamma}}^{-1/2} F_{q_j} \{N_{q_j}^{-1} S(q_j, q_j)\}^{1/2} \cdot \{N_{q_j}^{-1} S(q_j, q_j)\}^{-1/2} \{N_{q_j}^{-1} \bar{Y}_i(q_j)\}\right\|_{2}.$$

We further bound the first term in (S112) as follows:

$$\left\|b^T V_{\tilde{\gamma}}^{-1/2} F_{q_j} \{N_{q_j}^{-1} S(q_j, q_j)\}^{1/2}\right\|_{2}^2 \leq \sum_{q=1}^{Q} \left\|b^T V_{\tilde{\gamma}}^{-1/2} F_{q} \{N_{q}^{-1} S(q, q)\}^{1/2}\right\|_{2}^2 \leq \sum_{q=1}^{Q} b^T V_{\tilde{\gamma}}^{-1/2} F_{q} \{N_{q}^{-1} S(q, q)\} F_{q} V_{\tilde{\gamma}}^{-1/2} b \leq b^T V_{\tilde{\gamma}}^{-1/2}(\sigma_F^2 V_{\tilde{\gamma}}) V_{\tilde{\gamma}}^{-1/2} b \text{ (by Condition (S41))} \leq \sigma_F^2.$$  

Combining (S112) and (S113), we have

$$\left|\sum_{h=1}^{H} b_h M''_{h}(i, j)\right|^2 \leq 4\sigma_F^2 N_{q_j}^{-1} \bar{Y}_i(q_j)^\top S(q_j, q_j)^{-1} \bar{Y}_i(q_j).$$

(S114)

Combining (S111) and (S114), we have

$$\sum_{h=1}^{H} b_h M''_{h}(i, j) \leq \min \left\{2\sigma_F \sqrt{N_{q_j}^{-1} \bar{Y}_i(q_j)^\top S(q_j, q_j)^{-1} \bar{Y}_i(q_j)}, \frac{\|F_{q_j}\|_{2,1} \cdot N_{q_j}^{-1}\|\bar{Y}_i(q_j) - \bar{Y}(q_j)\|_{\infty}}{\sqrt{\theta_{\min}\{V_{\tilde{\gamma}}\}}}, \frac{b^T V_{\tilde{\gamma}}^{-1/2} F_{q_j} \{N_{q_j}^{-1} S(q_j, q_j)\}^{1/2} \cdot \{N_{q_j}^{-1} S(q_j, q_j)\}^{-1/2} \{N_{q_j}^{-1} \bar{Y}_i(q_j)\}}{\sqrt{\theta_{\min}\{V_{\tilde{\gamma}}\}}}ight\}.$$