Optimal Rerandomization via a Criterion that Provides Insurance Against Failed Experiments

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Abstract

We present an optimized rerandomization design procedure for a non-sequential treatment-control experiment. Randomized experiments are the gold standard for finding causal effects in nature. But sometimes random assignments result in unequal partitions of the treatment and control group, visibly seen as imbalanced observed covariates, increasing estimator error. There is also imbalance on unobserved covariates which likewise increase estimator error. Rerandomization can throw away poor assignments only in the observed covariates by limiting the imbalance to a prespecified threshold. Limiting this threshold too much can increase the risk of having error due to unobserved covariates. We introduce a criterion that gauges errors due to both imbalance in the observed and the risk of imbalance in the unobserved covariates. We then use this criterion to locate the optimal rerandomization threshold based on the practitioner’s level of desired insurance. We also provide an open source R package available on CRAN named OptimalRerandExpDesigns which generates designs according to our algorithm.

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1 Introduction and Background

We consider a classic problem: a treatment-control experiment with the \( n \) subjects (individuals, participants or units) and one clearly defined outcome of interest (also called the response or endpoint) for each subject denoted \( y = [y_1, \ldots, y_n]^T \). We scope our discussion to the response being continuous and uncensored with incidence and survival being further research.

Each subject is assigned to the treatment group and a control group denoted \( T \) and \( C \) and referred to as the two arms. Here we consider the settings where all subjects along with their observed subject-specific covariates (measurements or characteristics) denoted \( x \) known beforehand and considered fixed. This non-sequential setting was studied by Fisher (1925) when assigning treatments to agricultural plots and is still of great importance today. In fact, they occur in clinical trials as “many phase I studies use ‘banks’ of healthy volunteers ... [and] ... in most cluster randomised trials, the clusters are identified before treatment is started” (Senn, 2013, page 1440). We discuss in our concluding section about how are work can extend to the widely-used sequential setting where subjects enter one-by-one and must be immediately assigned to \( T \) or \( C \).

Synonymously referred to as a randomization, an allocation or an assignment is a vector \( w = [w_1, \ldots, w_n]^T \) whose entries indicate whether the subject received \( T \) (coded as +1) or \( C \) (coded as -1) and thus this vector must be an element in \{−1, +1\}^n.

The goals of such experiments are to estimate and test a population average treatment effect (PATE) denoted \( 2\beta_T \) where (the multiplicative factor of 2 would not be present if \( w \) was coded with 0 and 1).

After the sample is provided, the only degree of control the experimenter has is to choose the entries of \( w \). This choice of division of the \( n \) subjects to the two arms we term a design, strategy, algorithm, method or procedure and denote it as the random variable \( W \sim P(w) \), a generalized multivariate Bernoulli mass function, and support \( W \), termed the allocation space. If all realizations satisfy \( w^T 1_n = 0 \), i.e. all of the assignments feature an equal number of subjects assigned to the treatment group and the control group, \( n/2 \), we term \( W \) a forced balance procedure following Rosenberger & Lachin (2016, Chapter 3.3).

The question then becomes: what is the best design strategy? This has been debated for over 100 years with loosely two main camps: those that optimize assignments and those that randomize assignments. The latter, first advocated by Fisher (1925), has prevailed, certainly in the context of causal inference and clinical trials. We show here that the design being “best” is dependent on assumptions of the response model, the degree to which observed covariates matter relative to the unobserved covariates and the fundamental assumption of where the randomness comes from. Then it depends further on choices: the choice of estimator for \( \beta_T \) and the choice of metric to gauge optimality. There is also the additional concern with how to draw inference which will be different depending on these assumptions and choices.

To build intuition about the complexity at hand, consider the following simplistic model

\[
y = \beta_T w + x + z
\]  

where \( w \) comes from a forced balance procedure and \( z \) will be explained shortly. To make
the expressions even simpler, we assume \( x \) is centered and scaled so its entries have average zero and standard deviation one.

We denote the responses coming from random variable \( Y \) but there are loosely two perspectives as to the source of this response randomness. Our work focuses on the randomization model which we defend after introducing both perspectives. To simplify our discussion in this section, we consider estimation only (not hypothesis testing).

### 1.1 Population Model Perspective

In the population model (Rosenberger & Lachin, 2016, Chapter 6.2), subjects in the treatment group are sampled at random from an infinitely-sized superpopulation and thus the responses in the treatment group are considered independent and identically distributed with density \( f_Y(y \mid \theta = \beta_T) \). Subjects in the control group are sampled analogously from a different superpopulation density \( f_Y(y \mid \theta = -\beta_T) \).

In the simple model of Equation 1, the population model can be created via the assumption that \( z \) is a random draw from \( Z \) such that \( z := y - \mathbb{E}[Y \mid x, w] \) and its entries are independent. The law of iterated expectation yields that the distribution of the \( Z_i \)'s are mean-centered. Each experiment gets one draw from \( z \) which is usually referred to as “noise” or “measurement error”. To make our expressions simpler, we also assume homoskedasticity so that each of the \( Z_i \)'s share variance denoted \( \sigma_z^2 \).

It is straightforward to demonstrate that the strategy’s mass function \( P(W) \) is ancillary to the likelihood of the responses and thus the randomization procedure can be ignored during estimation.

To investigate optimality in this perspective, we now need an estimator and a criterion. We consider for now two widely-used estimators. First is the simple differences-in-means estimator, \( \hat{\beta}_{DM}^T := \frac{1}{2}(\bar{Y}_T - \bar{Y}_C) \) where \( \bar{Y}_T \) is the random variable of the average response in the treatment group and \( \bar{Y}_C \) is the random variable of the average response in the treatment group. If the model were to be unknown, \( \hat{\beta}_{DM}^T \) would be the uniformly minimum variance unbiased estimator for the PATE (Lehmann & Casella, 1998, Example 4.7). Second is the covariate-adjusted regression estimator, \( \hat{\beta}_{LR}^T \) defined as the slope coefficient of \( w \) in an ordinary least squares fit of \( y \) using \( x \) and \( w \). If \( y \) is known to be linear in \( x \), then \( \hat{\beta}_{LR}^T \) is known to be the best linear unbiased estimator for the PATE. Since \( x \) was standardized, the intercept was omitted in this example.

Table 1 provides the expression of the estimator, its expectation, variance and mean squared error (MSE) for both the differences-in-means and linear regression estimators. The expectations are taken over the distribution of \( Z \), as this is the source of randomness in the response and thus the expressions are conditional on \( w \) and \( z \). To simplify the expressions we denote the imbalance in \( x \) as \( B_x := \bar{x}_T - \bar{x}_C \) and the imbalance in \( z \) as \( B_z := \bar{z}_T - \bar{z}_C \) where the bar notation denotes sample average and the subscript indicates arm and \( r := \frac{1}{n} \sum_{i=1}^n x_i z_i \), a covariance-like term measuring the relatedness of the observed and unobserved measurements.

\(^1\)The employment of \( \hat{\beta}_{LR}^T \) in the realistic setting where the linear model assumption is untestable and most likely wrong is a subject of a large debate (Freedman, 2008; Berk et al., 2010; Lin, 2013). In this work, we do not take sides in this debate and offer optimal designs for both estimators.
If the optimal design is selected by the MSE, then the best assignment is the one that minimizes $B_x$, the imbalance in the observed covariate. This is the main justification used to advocate against randomization and instead use deterministic optimal designs.

Here, the strategy $W$ is degenerate where $P(W = w^*) = 1$ for $w^*$, the MSE-optimal assignment. To find $w^*$ in practice is more difficult. One can formulate the procedure as a binary integer programming problem. If forced balance is required, the partitioning problem is NP hard, meaning that there does not exist a known algorithm that can find the optimal allocation in polynomial time. There are approximations that run in polynomial time that are usually close enough for practical purposes, e.g. branch and bound (Land & Doig, 1960).

Tangentially, we also observe that if the model is linear, then $\hat{\beta}^\text{LR}_T$ is more efficient than $\hat{\beta}^\text{DM}_T$ as its variance is $\approx \frac{\sigma^2}{n} + \frac{\sigma^2}{n} B_x^2$ when using two terms in a geometric series approximation versus the variance of the simple estimator $\frac{\sigma^2}{n} + B_x^2$. This will become important when we discuss our methodology in sec. 2.

Once again, those that assume the population model prefer optimal deterministic design.

### 1.2 Randomization Model Perspective

In the randomization model (Rosenberger & Lachin, 2016, Chapter 6.3) also called the “Fisher model” or “Neyman model”, the source of the randomness is in the treatment assignments $w$. “The $n$ subjects are the population of interest; they are not assumed to be randomly drawn from a superpopulation” (Lin, 2013, page 297). Table 2 provides the expression of the estimator, its expectation, variance and mean squared error (MSE) for both the differences-in-means and linear regression estimators. The expectations are taken over the distribution of $W$, as this is the source of randomness in the response and thus the expressions are conditional on $z$ and $x$.

| Finite Estimate | $\hat{\beta}^\text{DM}_T$ | $\hat{\beta}^\text{LR}_T$ |
|-----------------|-----------------|-----------------|
| Expectation     | $\beta_T + B_x + B_z$ | $\beta_T + (B_z - r B_x)(1 - B_z^2)^{-1}$ |
| Variance and MSE| $\frac{1}{n}(x + z)^\top \Sigma_W (x + z)$ | $\beta_T + O(1/\sqrt{n}) \sqrt{E(B_x^3)} + O(E(B_x^3))$ |

Table 2: Estimator properties in the randomization model.

The response model of Equation 1 under the randomization model perspective was studied by Kapelner et al. (2019) and the expressions in Table 2 can be found therein. To derive

\[2\text{And thus is only appropriate when } \frac{\sigma^2}{n} \leq 1.\]
these expressions, there was one additional assumption placed on $W$ that we will make precise in Section 2: for any assignment $w$, the assignment where the treatment group subjects are swapped for the control groups subjects, $-w$, is equally likely. Also note that for $\beta_{LR}$, no closed form expressions are available so they are approximated to the third order in a geometric series.

The $\Sigma_W$ term denotes $\text{Var}[W]$, the variance-covariance matrix of the strategy that features as ones along the diagonal and off-diagonals that gauge the covariance between subject $i$’s assignment and subject $j$’s assignment. $z_\perp$ is defined to be the component of $z$ orthogonal to $x$. It makes sense that this term is important in the error of the linear regression estimator as the linear regression can only adjust for the component of $z$ it has access to via $x$.

The most striking observation is that the optimal design strategy is not clear from the MSE expressions as they were in the population model perspective. Our response model was deliberately picked to be the most simplistic and our estimators were chosen to be the most popular. Further, if optimal design were to be defined by minimal MSE, it cannot be resolved as $z$ is unknown, a practical problem addressed this problem in Section 2.

We note that there is finite sample bias in the linear regression estimator because the regression assumed a response model that omitted the additive $z$ term. However, this bias is small as noted by Freedman (2008) and Lin (2013).

1.3 Our Assumption: the Randomization Model Perspective

The debate between the population model and randomization model is long Reichard & Gollob (see for instance 1999, pages 125-127) and there are compelling reasons for the population model as well. In this work, we employ the latter perspective following Rosenberger & Lachin (2016); Freedman (2008); Lin (2013) and others.

The population model requires the subjects to truly be sampled at random from a super-population. However, in most experiments, subjects are recruited from nonrandom sources in nonrandom locations. Experimental settings are frequently selected because of expertise, an ability to recruit subjects, and their budgetary requirements (Rosenberger & Lachin, 2016, page 99). In the context of clinical trials, Lachin (1988, page 296) states rather harshly that, “the invocation of a population model for the analysis of a clinical trial becomes a matter of faith that is based upon assumptions that are inherently untestable”.

Further, there is another reason we would like to point out. Since $y$ is deterministic under the randomization model, this implies $z$ is fixed and we believe it is realistic to believe so. Consider a clinical trial where subject gender, height and weight are assessed, the observed covariates. It is not difficult to accept that these measurement values are affixed to the subjects. However, there are many other measurements that are important for the endpoint in the study such as presence or absence of rare diseases, presence or absence of genetic SNP’s, etc. These unobserved measurements combine together to form the $z_i$’s and are just as fixed to the subjects as the observed measurements.
1.4 The Rerandomization Design

Assigning each individual to treatment by an independent fair coin flip we will term a \textit{the Bernoulli Trial} \cite{imbens2015statistical}, Chapter 4.2. In the Bernoulli Trial, all assignments are independent and thus $\Sigma_W = I_n$ where the latter notation indicates the $n \times n$ identity matrix. Any other design is termed a \textit{restricted randomization} because the permissible allocations are restricted to a subset of all possible allocations. A very weak restriction is that of forced balance. If each forced balance allocation is equally likely, we term this as the \textit{balanced completely randomized design} (BCRD) as in \cite{wu1981balanced}. Here, there is a slight, but vanishing negative covariance between the assignments and thus the off-diagonal elements of $\Sigma_W$ are all $-\frac{1}{n-1}$.

However, there is a large problem with employing bernoulli or BCRD assignments that was identified at the outset: under some unlucky random assignments there are unluckily large differences in the distribution of observed covariates between the two groups. Running the experiment under a particular unlucky assignment is destructive to both perspectives. This can be seen in our simple model of Equation 1, the estimator features an additive $B_x$ term. In the population model perspective, the MSE of $\hat{\beta}_{DM}^{T}$ suffers an additive penalty of $B_x^2$ and the MSE of $\hat{\beta}_{LR}^{T}$ suffers a multiplicative penalty of $(1 - B_x^2)^{-1}$ derived from the specific unlucky assignment (see Table 1). In the randomization model perspective, the MSE of $\hat{\beta}_{DM}^{T}$ suffers an additive penalty of $\frac{1}{n^2}E_w[B_x^2]$ and the approximate MSE of $\hat{\beta}_{LR}^{T}$ also suffers an additive penalty but it is more difficult to see as it is buried in the quartic form $E_w[B_x^2 B_z^2]$ (see Table 2). These penalties are due to the presence of many unlucky assignments in $W$.

Thus, in the randomization model, the MSE for both estimators can be diminished if these unlucky assignments are eliminated from $W$, the main reason restricted randomization has been employed for the past 100 years. An algorithm that eliminates such $w$’s can go as follows. (1) Realize a $w$ from BCRD and measure $B_x^2$ (2) If this $B_x^2$ is less than a predetermined threshold $a$, then retain $w$ and run the experiment otherwise return to step (1). Here, the variance-covariance matrix of the strategy $W$ will be dependent on both $x$ and threshold $a$.

This rerandomization procedure is not new. \cite{student1938test} wrote that after an unlucky, highly imbalanced randomization, “it would be pedantic to [run the experiment] with [an assignment] known beforehand to be likely to lead to a misleading conclusion”. His solution is for “common sense [to prevail] and chance [be] invoked a second time”. Although this rerandomization design is classic, it has been rigorously investigated only recently \cite{morgan2012rerandomization}.

However, the selection of the threshold $a$ “remains an open problem” \cite{li2018rerandomization} page 9162). This threshold is a critical quantity because it controls the degree of randomness in the design. A miniscule $a$ will demand the optimal, deterministic design; a large $a$ would allow for complete randomization. Hence, solving this problem can bridge the intellectual gap between those that deterministically design experiments via optimization and those that design experiments via randomization.

Herein, we provide an algorithm to find this threshold for both the differences-in-means estimator and the covariate adjusted estimator for a realistic response model.
2 Methodology

We assume \( p < n \) covariates measured for each subject and collect them into a row vector \( x_i := [x_{1,i}, \ldots, x_{p,i}] \). We denote \( X \) as the \( n \times p \) matrix that stacks the \( n \) vectors for each subject row-wise. Without loss of generality, we assume that each column in \( X \) is centered and scaled. We examine a general response model

\[
y = \beta^T w + X\beta + z. \tag{2}
\]

Here, \( \beta \) are the weights for each covariate as a column vector of length \( p \). And \( z \) is the fixed contribution of unobserved measurements for the subjects as in the model of Equation 1 plus the misspecification errors of the true response function \( f \) minus the linear component, i.e. \( [f(x_1) - x_1\beta \ldots f(x_n) - x_n\beta]^\top \). Because each column in \( x \) is standardized, the linear component of this model does not require the additive intercept term.

In order to simplify our expressions, we assume \( W \) has the mirror property (Assumption 2.1) whereby the treatment group and control group can be swapped without changing the probability of the assignment.

**Assumption 2.1 (Mirror Property).** For all \( w \in W \), \( P(W = w | X) = P(W = -w | X) \).

In Appendix 5.1 we show that in the randomization model the MSE of \( \hat{\beta}_T^{DM} \) is

\[
\text{MSE}_w[\hat{\beta}_T^{DM} | z, X; \beta] = \frac{1}{n^2}(X\beta + z)^\top \Sigma_W(X\beta + z) \tag{3}
\]

and in Appendix 5.3 we show that the MSE of \( \hat{\beta}_T^{LR} \) can be approximated to the third order as

\[
\text{MSE}_w[\hat{\beta}_T^{LR} | z, X; \beta] \approx \frac{1}{n^2}z^\top \left( G + \frac{2}{n}D \right) z \tag{4}
\]

where \( G := (I - P)\Sigma_W(I - P) \) where \( P := X(X^T X)^{-1}X^T \) is the standard orthogonal projection matrix onto the column space of \( X \) and \( D := \mathbb{E}_w [ww^\top Pww^\top] \), an expectation of a quartic form that cannot be simplified. Table 2 shows these expressions for the special case of \( p = 1 \) covariate. Remarkably, this expression is independent of the unknown \( \beta \) coefficients, a fact that will allow us to evaluate explicit designs in the following sections.

In theory, the optimal rerandomization strategy is to locate \( a^* \), the threshold corresponding to the minimum of Equation 3 or 4 over \( a \). As \( a \) is varied, the determining matrix of the quadratic form varies as \( \Sigma_W \) is a function of \( X \) and \( a \). However, in practice this is impossible as \( z \) (and \( \beta \) in the case of \( \hat{\beta}_T^{DM} \)) is unknown.

We now discuss three criterions that remove this dependence on the fixed set of \( z \).
2.1 Criterions of Design Optimality

2.1.1 The Minimax Design

If we assume nature to be adversarial, we can examine the MSE in the case of the supremum over the MSE, i.e. the worst possible finite vector of values $z$. The optimal minimax strategy would then be the bernoulli trial \cite[Theorem 2.1]{Kapler2019} for $\hat{\beta}_{DM}^T$ and would asymptotically be the bernoulli trial\footnote{Not even the weak restriction of the BCRD is permitted ("no free lunch" whatsoever).} for $\hat{\beta}_{LR}^T$, corresponding to $a_\ast = \infty$. This result is not only trivial but would also correspond to the situation where $z$ is aligned with one arbitrary direction in $\mathbb{R}^n$, a punitively conservative situation.

2.1.2 The Mean Unobserved Design

Can we consider the case of an “average $z$”? This would be incoherent in the randomization model where $z$ is fixed. Regardless, we consider $z$ being drawn from a continuous “faux measure” on $Z$. This measure is not necessarily believed in reality; rather, it is a useful mathematical device that yields a sensible criterion. We emphasize that the faux measure is not necessary or limiting to the inference we discuss in Section 2.3.

We assume it is mean centered in 2.2 and 2.3 and independence among the $n$ subjects’ unobserved covariates. And, only to make our expressions simpler, we assume homoskedasticity in $Z$.

**Assumption 2.2 (Faux Measure Mean Centeredness).** $\mathbb{E}[Z | X, \beta, w] = 0_n$.

**Assumption 2.3 (Faux Measure Independence).** $\mathbb{V}ar[Z | X]$ is diagonal.

**Assumption 2.4 (Faux Measure Homoskedasticity).** $\mathbb{V}ar[Z_i | X] = \sigma_z^2$ for all $i$.

In Appendix 5.2 we derive the mean criterion for $\hat{\beta}_{DM}^T$,  
\[
\mathbb{E}_z [\text{MSE}_w[\hat{\beta}_{DM}^T | z, X, \beta]] = \frac{\sigma_z^2}{n} + \frac{1}{n^2} \beta^\top X^\top \Sigma_w X \beta 
\]  (5)

and in Appendix 5.3 we derive the MSE for $\hat{\beta}_{LR}^T$ approximated to the third order as  
\[
\mathbb{E}_z [\text{MSE}_w[\hat{\beta}_{LR}^T | z, X, \beta]] \approx \frac{\sigma_z^2}{n} + \frac{\sigma^2}{n^2} \text{tr} \left[ X \Sigma_w X \perp \right] 
\]  (6)

where we denote $X \perp$ as the orthogonalized $X$ matrix with columns $x_{\perp 1}, \ldots, x_{\perp p}$.

The optimal design for $\hat{\beta}_{DM}^T$ would be the single vector $w_\ast$ that minimizes $(w^\top X \beta)^2$. Note that this assumes knowledge of $\beta$ which is unknown in practice. Thus we leave this design problem for future work. The optimal design for $\hat{\beta}_{LR}^T$ would be the single vector $w_\ast$ that minimizes $\sum_{j=1}^p (w^\top x_{\perp j})^2$ which remarkably does not depend upon $\beta$. This is similar to the optimal design under the population model setting as explained in Section 1.1.

Since there are an exponential number of $w$ vectors, the corresponding rerandomization threshold will be $a_\ast \approx 0$. Finding this vector is practically impossible as there is no
known polynomial-time algorithm. This is not a practical way of selecting a rerandomization threshold. Even if it were, there would be inferential complications with such a deterministic design that we explain in Section 2.3.

2.1.3 The Tail Unobserved Design

The supremum criterion is too conservative and the mean criterion does not incorporate the ruinous effect of vectors that can be near the supremum. Following [Kapelner et al. 2019 Section 2.2.6], we consider a tail criterion, Quantile \( z \) \( \text{MSE}_w [\hat{\beta}_T | z, X, \beta], q \) for both the estimators. This criterion gauges the average experimental error at the worst \( 1 - q \) percent of \( z \)'s. For example, a \( q = 95\% \) would be a criterion that considers the “5% worst worlds”.

As \( q \) increases, the practitioner takes out insurance on \( z \) settings that are more and more improbable. As \( q \to \infty \), the only way to insure against every event is more randomness in \( W \) (and more imbalance) as explained in Section 2.1.1. As \( q \) decreases towards the quantile corresponding to the mean, minimizing imbalance in \( W \) becomes more important at the expense of less randomization as seen in Section 2.1.2. Hence the tail provides a tradeoff between the two competing interests of optimality and randomization. We will understand the tradeoff explicitly in Section 2.2.3 but we first describe the algorithm.

2.2 Algorithms to Optimize the Tail Criterion

Our Algorithm 1 is an exhaustive search to locate a minimal MSE design for \( \hat{\beta}^{LR}_T \). An analogous algorithm to locate the minimal MSE design for \( \hat{\beta}^{DM}_T \) we leave to future work as it depends on \( \beta \), an unknown quantity. We first outline two inputs to the algorithm besides the raw data \( X \) that are required.

The algorithm takes as input a collection of assignments \( \mathbb{W}_{\text{base}} := \{ w_1, \ldots, w_S \} \) where \( S \) is large, so that \( \mathbb{W}_{\text{base}} \) loosely approximates the full space \( \mathbb{W} \). Since “rerandomization is simply a tool that allows us to draw from some predetermined set of acceptable randomizations” [Morgan & Rubin 2012 page 1267], there is no theory we know of that specifies \( \mathbb{W}_{\text{base}} \). Thus, following Morgan & Rubin [2012] and Li et al. [2018], we consider the initial set to be \( S \) draws from BCRD. In practice, this decision can limit our algorithm’s performance in certain situations that will become apparent in the simulation study in Section 3 and strategies to mitigate these limitations are discussed in Section 4.

We then sort the assignments based on imbalance in \( X \). The imbalance calculation requires the second input: a metric of imbalance, of which our algorithm is agnostic. An imbalance metric \( \mathcal{B} \) takes \( X \) and \( w \) as input and outputs a non-negative scalar. An output of zero indicates perfect balance between the treatment and control groups. One such metric is Mahalanobis distance, a collinearity adjusted squared sum of average differences in each dimension. This metric has nice properties; for instance it is an “affinely invariant scalar measure” [Morgan & Rubin 2012 page 1271]. In our notation, it can be compactly written as \( \mathcal{B}(X, w) = \frac{1}{n} w^\top P w \). We discuss other choices of metrics in Section 4.

Let \( w^{(1)} \) be the vector with the smallest imbalance in the set and \( w^{(S)} \) be the largest, i.e. \( w^{(1)} := \arg \max_{w \in \mathbb{W}_{\text{base}}} \{ \mathcal{B}(X, w) \} \). The closest vector to \( w^*_s \), the assignment that truly minimizes imbalance, in our small initial subset \( \mathbb{W}_{\text{base}} \) will be \( w^{(1)} \).
Beginning with \( W \sim \{w(1) \text{ w.p. 1}\} \), we compute \( Q \), the quantile tail criterion at \( q \) for both the estimators. In order to calculate the quantile, we require the inverse CDF function in \( z \) for Equations 3 and 4. In general the closed form of the density functions are unknown asymptotically (see e.g. Götte & Tikhomirov 2002). For both estimators, we present three procedures in the next three sections but first finish explaining the algorithm.

We then proceed to the strategy \( W \sim \{w(1) \text{ w.p. 0.5 and } w(2) \text{ w.p. 0.5}\} \) and recalculate \( Q \). We repeat this procedure until the \( S \)th iteration where \( W \sim U(W_{\text{base}}) \), the finite approximation of BCRD. Over all iterations, there is a minimum quantile \( Q_* \) corresponds to an iteration number \( s_* \leq S \), defining the approximate optimal strategy \( W_* = \{w(1), \ldots, w(s_*)\} \) and optimal threshold \( a_* \) corresponding to the imbalance \( B(X, w_{(s*)}) \).

Algorithm 1

This algorithm returns the optimal rerandomization design \( W_* \) along with the optimal threshold \( a_* \) and the value of the relative tail criterion for the minimum design \( Q'_* \).

**procedure** OptimalRerandomizationDesign(\( X, B, W_{\text{base}}, q, \text{TailMSE}, \ldots \))

\[ n \leftarrow \text{nrow}(X) \]
\[ Bs \leftarrow \{B(X, w) : w \in W_{\text{base}}\} \quad \triangleright \text{Precompute all balances} \]
\[ \{Bs_{\text{sort}}, W_{\text{base}}{\text{sort}}\} \leftarrow \text{sort_asc}(Bs, W_{\text{base}}) \quad \triangleright \text{Sort all balances from smallest to largest and use these sorted indices to sort } W_{\text{base}} \]
\[ s_f \leftarrow \text{size}(W_{\text{base}}), s_* \leftarrow \text{NULL}, Q'_* \leftarrow \infty \quad \triangleright \text{Initialize search parameters} \]

for \( s = 1 \ldots s_f \) do

\[ W_s \leftarrow W_{\text{base}}{\text{sort}}[1 : s] \quad \triangleright \text{The brackets indicate the sub-array operator} \]
\[ \Sigma_W \leftarrow \frac{1}{s} \sum_{w \in W_s} ww^\top \]
\[ Q' \leftarrow \text{TailMSE}(W_s, s, X, n, \Sigma_W, q, \ldots) \]

if \( Q' < Q'_* \) then

\[ Q'_* \leftarrow Q' \]
\[ s_* \leftarrow s \]

end if

end for

return Hash(\( W_* = W_{\text{base}}[s_* : s_f], a_* = Bs_{\text{sort}}[s_*], Q'_* = Q'_* \))

end procedure

Our exhaustive search algorithm is computationally intense but can be approximated by skip-stepping through the \( S \) iterations. Also, we conjecture that \( Q \) is convex in \( s \). Thus, we provide a binary search option in our implementation.

We now discuss three strategies to compute \( Q \) based on assumptions about the measure on \( Z \). These strategies will be different for both estimators. Algorithm 1 thus takes an argument that specifies one of three different tail computation functions found in Algorithm 2 for \( \hat{\beta}_T \).
2.2.1 Provide a Distribution Explicitly

If the distribution of $Z$ is provided explicitly, then in each iteration of Algorithm 1, the empirical quantile $q$ of the MSE of $\hat{\beta}_{LR}^T$ (Equation 4) can be approximated as the mean over many draws of $z$. As this average will be noisy, the criterion can be smoothed over $a$ by use of cubic smoothing splines (Hastie & Tibshirani, 1990, Chapter 2.2). The optimal threshold $a^*$ will be invariant to shifts or scales of the MSE and thus the $Z$ distribution can be standardized without changing the result. An analogous algorithm for the MSE of $\hat{\beta}_{DM}^T$ (Equation 3) is deferred to future work as there is an additional complication due to the dependence on the unknown $\beta$. Note that assuming independence and homoskedasticity (Assumptions 2.3 and 2.4) are unnecessary in this section.

2.2.2 Assume Normality and Use a CDF Approximation

In addition to assuming independence and homoskedasticity (Assumptions 2.3 and 2.4), we make the assumption that $Z$ is Gaussian, then the distribution of the quadratic form of the MSE of $\hat{\beta}_{LR}^T$ (Equation 4) is known explicitly. Since the optimal threshold $a^*$ will be invariant to shifts or scales of the MSE, we assume a standard Gaussian. Since the determining matrix $R$ is positive definite and symmetric, the distribution of this quadratic form is a standard result — it is a weighted sum of standard chi-squared distributions,

$$Z^T R Z \sim \sum_{i=1}^{n} \lambda_i \chi_1^2$$

where the $\lambda_i$’s are the eigenvalues of $R$. Quantiles of this distribution are unknown in closed form but can be computed by numerical integration using the characteristic function. Fast approximations have been studied since the 1930’s. Bodenham & Adams (2016) compared many approximations on accuracy and computation time and recommend the Hall-Buckley-Eagleson method (Buckley & Eagleson, 1988) which has error that is $O(n^{-1})$. This is the approximation used in our R package.

As for the MSE of $\hat{\beta}_{DM}^T$ (Equation 3), there is once again the additional complication due to the dependence on the unknown $\beta$.

2.2.3 Assume an Excess Kurtosis and Use a Double Approximation

The quantile criterion can be expressed as

$$Q := \mathbb{E}_z \left[ \text{MSE}_w[\hat{\beta}_T | z, X, \beta] \right] + c \times \text{SE}_z \left[ \text{MSE}_w[\hat{\beta}_T | z, X, \beta] \right]$$

where $q$ is one-to-one with $c$ given $\Sigma_W$. For example, if $q = 95\%$ and $\text{MSE}_w[\hat{\beta}_T | z, X, \beta]$ is normal, $c = 1.65$, the Gaussian quantile. The MSE for both estimators is conjectured to be asymptotically the form of Equation 7 which is well-approximated by the normal distribution as long as (1) there are many non-zero eigenvalues relative to $n$ and (2) these eigenvalues are fairly uniformly distributed. These assumptions will be true as long as $W$ remains fairly random i.e. this approximation will work for rerandomization thresholds that are not too
small and thus maintain randomness in $\mathcal{W}$. The simulations of Kapelner et al. (2019, Section 3) demonstrate that the Gaussian quantiles are approximately correct in many situations. This is the approximation employed in this section.

In order to derive the standard error of the MSE’s for both expressions, we need to assume 2.5 that the $Z_i$’s have a finite fourth moment and 2.6 that the third and fourth moments are independent of $X$.

**Assumption 2.5** (Faux Measure has Finite Fourth Moment). $\mathbb{E} [Z_i^4] < \infty$ for all $i$.

**Assumption 2.6** (Faux Measure has Higher Moments Independent of Observed Covariates). $\mathbb{E} [Z_i^3]$ and $\mathbb{E} [Z_i^4]$ are independent of $X$ for all $i$.

In Appendix 5.5, we derive the standard error for the MSE of the differences-in-means estimator,

$$
\text{SE}_z \left[ \text{MSE}_w [\hat{\beta}^{DM} | z, X, \beta] \right] = \frac{\sigma_z^2}{n^2} \left( n\kappa_z + 2 ||\Sigma_W||_F^2 + \frac{4}{\sigma_z^2} \beta^T X^T \Sigma_W X \beta \right)^{\frac{1}{2}}
$$

where $\kappa_z$ is the excess kurtosis in $Z$ and $||\cdot||_F$ denotes the Frobenius norm. The advantage of this method is that we can find approximately optimal rerandomizations designs for general distributions by merely specifying the excess kurtosis.

Putting Equations 5 and 9 together and recalling that the optimal threshold $a_*$ will be invariant to shifts or scales of the MSE, we can locate a tail criterion objective function that we denote $Q'$,

$$
Q'_{\beta_T^{DM}} = \frac{\beta ^T X^T \Sigma_W X \beta \sigma_z^2}{BAL_1} + c \frac{\sigma_z^2}{RAN D} \left( n\kappa_z + 2 ||\Sigma_W||_F^2 + \frac{4}{\sigma_z^2} \beta^T X^T \Sigma_W X \beta \right)^{\frac{1}{2}}
$$

where the quantities in grey are independent of the choice of design given the normal approximation. The $BAL$ terms measure observed imbalance. Over the range of possible $a_*$ values, the $BAL_1$ term ranges from $O(n)$ in the case of BCRD with down to $O(n^32^{-n})$, i.e. effectively zero, in the case of the deterministic minimal imbalance (Kallus 2018, Section 3.3). For BCRD, $BAL_2 = \frac{n}{n-1} BAL_1 = O(n)$. We have the general upper bound $BAL_2 \leq nBAL_1$. The $RAND$ term measures randomness. Over the range of possible $a_*$ values, the $RAND$ term ranges from $\approx n$ in the case of BCRD all the way to $n^2$ in the case of the deterministic minimal imbalance. The tradeoff between imbalance and randomness is now clearly seen in the tail criterion. The inequality above is proven in Appendix 5.5.

In Appendix 5.7, we derive an approximation for the standard error for the MSE in the linear regression estimator,

$$
\text{SE}_z \left[ \text{MSE}_w [\hat{\beta}^{LR} | z, X, \beta] \right] \approx \frac{\sigma_z^2}{n^2} \left( 2 ||(I - P)\Sigma_W||_F^2 + \frac{8}{n} \text{tr} [GD] + \frac{8}{n^2} \text{tr} [D^2] + \kappa_z SS \right)^{\frac{1}{2}}
$$

where $SS := \sum_{i=1}^{n} (g_{i,i} + \frac{2}{n}d_{i,i})^2$. Putting Equations 6 and 11 together and dropping additive and multiplicative constants, we find an approximate tail criterion objective function,
\[ Q'_{\beta^{LR}} \approx \text{tr} \left[ \begin{bmatrix} X^\top \Sigma_W X \end{bmatrix}_\text{BAL} \right] + c \left( 2 \| (I - P) \Sigma_W \|_F^2 \right) + 8 \frac{\text{tr} [GD]}{n} + 8 \frac{\text{tr} [D^2]}{n^2} + \kappa_z SS \right)^{\frac{1}{2}} \tag{12} \]

and once again, quantitites in grey are independent of the choice of design and the tradeoff between imbalance and randomness is clearly observed in as the quantiles of \( \hat{\beta}^{LR}_T \) errors as well. The inequalities above are proven in Appendix 5.7.

**Algorithm 2**

This algorithm provides the methods for computing the tail criterion for \( \hat{\beta}^{LR}_T \).

```plaintext
function TailDistLR(\( \mathbb{W}_s, s, X, n, \Sigma_W, q, \text{simZn, } N_Z \)) // Strategy of Section 2.2.1
  shared_lr
  Q's ← new_array(N_Z)
  for \( n_Z = 1 \ldots N_Z \) do
    z ← simZn(n)
    Q's[n_Z] = z^\top \left( G + \frac{2}{n} D \right) z
  end for
  return empirical_quantile(Q's, q)
end function

function TailNormalLR(\( \mathbb{W}_s, s, X, n, \Sigma_W, q \)) // Strategy of Section 2.2.2
  shared
  \( \lambda_s \leftarrow \text{eigen_values_of} \left( G + \frac{2}{n} D \right) \)
  return Hall_Buckley_Eagleson_Quantile_Approx(\( \lambda_s, q \))
end function

function TailMSEApproxLR(\( \mathbb{W}_s, s, X, n, \Sigma_W, q, \kappa_z \)) // Strategy of Section 2.2.3
  shared_lr
  \( X_\perp \leftarrow X \left( X^\top X \right)^{-\frac{1}{2}} \)
  \( c \leftarrow \text{normal_quantile(q)} \)
  return Equation 12 computed
end function

shared_lr{
  \( P \leftarrow X \left( X^\top X \right)^{-1} X^\top \)
  \( G \leftarrow (I - P) \Sigma_W (I - P) \)
  \( D \leftarrow \frac{1}{s} \sum_{w \in \mathbb{W}_s} w w^\top P w w^\top \)
}
```

As for the MSE of \( \hat{\beta}^{DM}_T \) (Equation 3), there is the additional complication due to the dependence on the unknown \( \beta \). Thus, we leave algorithms that minimize this MSE to future work.
2.3 Frequentist Inference in Our Designs

To run the experiment, we first realize one \( w_{\text{exp}} \) from our optimal strategy \( W \) and these treatments are administered to the subjects. Then, responses for the treatment group \( Y_{T,1}, \ldots, Y_{T,n/2} \) and for the control group \( Y_{C,1}, \ldots, Y_{C,n/2} \) are collected. Using these responses, we wish to test theories about \( \beta_T \) and produce a confidence interval for \( \beta_T \).

Under the randomization model, the only randomness is in \( w \) and thus a randomization test is most appropriate; this was Fisher’s “reasoned basis” for inference. The randomization test “can incorporate whatever rerandomization procedure was used, will preserve the significance level of the test and works for any estimator” (Morgan & Rubin, 2012, p. 1268).

This test requires a sharp null hypothesis whereby all subjects’ response will be exactly equal under both treatment and control conditions.

First, using the experimental \( w_{\text{exp}} \) we compute \( \hat{\beta}_{\text{exp}} \) for the simple estimator or the linear regression estimator depending on the choice of analysis. A null distribution can then created by using every other \( w \in \mathbb{W}_* \), the curated set of assignments thresholded by the optimal \( a_* \), and computing the same estimate (since these estimates were computed by labeling responses to treatment and control in a way unrelated to the design used in the actual experiment).

“One should analyze as one designs” (Rosenberger & Lachin, 2016, p. 105), so that replicates can only be drawn from the same restricted allocation set where \( w_{\text{exp}} \) originated.

If \( \mathbb{W}_* \) is large, the null distribution can be approximated with \( R < |\mathbb{W}_*| \) replicates where \( R \) controls the precision of the \( p \)-value. Each of the \( R \) replicates involves drawing one \( w \in \mathbb{W} \) and recomputing the estimates. Note that we cannot draw any \( w \in \{-1, +1\} \), the unrestricted set if \( W \) was a restricted randomization.

A properly-sized but \( \alpha \)-level two-sided test can be run by assessing if the experimental \( \hat{\beta}_{\text{exp}} \) falls in the retention region bounded by the \( \alpha/2 \) and the \( 1 - \alpha/2 \) quantiles of the replicate set \( \hat{\beta}_1, \ldots, \hat{\beta}_R \). By the duality of confidence intervals and hypothesis tests, one can alter the sharp null by adding (or subtracting) \( \delta \) and rerun the test. The set of values of \( \delta \) where the test rejects constitutes an approximate \( 1 - \alpha \) confidence interval for the average treatment effect. See Garthwaite (1996) for an efficient algorithm.

If the optimal threshold \( a^* \) is small, our design “must leave enough acceptable randomizations to perform a randomization test” (Morgan & Rubin, 2012, page 1268) and there may not be enough assignments of the \( S \) that satisfy this threshold. The smallest imbalance values of, i.e. the left tail of the distribution \( \{ B(X, w) : w \in \mathbb{W}_{\text{base}} \} \), will be \( O(pS^{-2/p}) \) in the case of the \( X \) being sampled from an iid Gaussian generating process and \( B \) is the Mahalanobis distance. Kallus (2018, Section 3.3) proved that the imbalance for the optimal assignment in this case is \( B(X, w_*) = O(n2^{-2n}) \). Thus, BCRD will not be able to locate vectors far into this left tail in a reasonable amount of time.

Additionally, estimating the terms in our criterion \( Q' \) of Equation 12 may suffer from smaller and smaller sets of assignments. The RAND term for instance relies on an accurate estimate of a function of the \( n \times n \) variance-covariance matrix \( \Sigma_W \) and the \( n \times n \) matrix \( D \). These matrices have an \( O(n^2) \) number of parameters and require many samples for high accuracy and a bias correction.

We now discuss a means to supplement draws from BCRD to provide many vectors with small imbalance. We consider Krieger et al. (in press, Algorithm 1), a greedy heuristic that begins with BCRD and in each iteration find the switch of treatment-control subject pair.
that is optimal until no more minimization is possible. This algorithm finds assignments that are \( O_p(p/(n^{1+2/p})) \). A nice property is that it converges quickly requiring very few switches and thus their assignments are nearly as random as BCRD. Thus, including assignments from their algorithm are unlikely to affect the RAND terms but greatly decrease the BAL terms in our criterion \( Q' \). Since the imbalance of vectors of BCRD is known, the greedy pair-switching algorithm can be used for stratified sampling for imbalance distributions upper bounded at small \( a_* \).

3 Simulations for the Linear Regression Estimator

3.1 The Three Strategies in Different Settings

We first simulate a case of \( n = 100 \) and \( p = 10 \) where the entries of \( X \) are standard normal realizations. We begin with \( \mathbb{W}_{\text{base}} \) of size \( S = 25,000 \) sampled from BCRD. The baseline imbalance are given in Fig 1. It is the job of our algorithms to threshold this distribution at \( a_* \).

![Figure 1: Imbalances in \( \mathbb{W}_{\text{base}} \).](image)

For the linear estimator, we run Algorithm 1 to find the optimal threshold for many settings and plot the 95% tail criterion over \( a \) in Figure 2.

There are many takeaways from this illustration. First, the criterion as a function of \( a \) appears long and flat from BCRD (where \( a \approx 1 \)) until relatively restricted strategies (where \( a \approx 0.1 \)) for all strategies and settings. This means the gains to MSE of the estimator due to improving imbalance a priori are small when a posteriori covariate adjustment is employed. However, it does recommend a fair degree of rerandomization however small the benefits.

The three tail strategies of Sections 2.2.1, 2.2.2 and 2.2.3 are shown in green, red and blue where the exact strategy was simulated with 1,000 standard normal draws for each \( a \) and the tail approximation used \( \kappa_z = 0 \) (paralleling the Gaussian setting). The \( a_* \)'s found by the two approximations are nearly identical meaning the gaussian tail approximation is close to the sum of scaled chi-squared approximation of Hall-Buckey-Eagleson. The \( a_* \) from the exact is a little bit larger. This can be due to the inaccuracy of the approximations and sampling variation in the exact strategy (even with smoothing attempting to attenuate it).
Figure 2: Relative tail criterion for $q = 95\%$ for many settings and strategies. In red is the normal approximation of Section 2.2.2. In blue is the tail approximation of 2.2.3 with $\kappa_z = 0$. In green is the exact strategy of Section 2.2.1 simulated with standard normal distribution and smoothed. In purple is the exact strategy simulated with a standard Laplace distribution and smoothed. In orange is the tail approximation with $\kappa_z = 3$. In black is the exact strategy simulated with a Student’s $t$ distribution with 2 degrees of freedom and smoothed. The vertical line indicates the optimal threshold $a_*$ for each strategy. For the purpose of visualizing their differences, the tail criterions were set to 1 for the full BCRD design in all three strategies. Thus, the relationships diverge from right to left as $a$ decreases.

Given the flatness of the relative tail criterion in this region, this small difference will not effect MSE performance.

We then wished to investigate how robust these approximations of the optimal rerandomization threshold are to deviations from normality. The orange line shows the exact strategy for the standard laplace distribution, a distribution similar to the normal in shape but with fatter tails and $\kappa_z = 3$ due to the exponential tail in absolute distance from the mean versus squared distance from the mean. Again, due to the flatness of the criterion in this region, the difference in $a_*$ to the red and blue lines will not make a difference in practice. To ensure the tail approximation can be adjusted for estimates of excess kurtosis, the purple line shows the tail approximation with the $\kappa_z$ argument set to 3. The $a_*$ found matches the exact simulation nearly perfectly (the purple and orange lines coincide). We then investigate a very fat-tailed measure, Student’s $t$ distribution with two degrees of freedom (in black). Even an extreme distribution such as this one does not substantially alter the threshold $a_*$. If the red and blue approximations were naively used, performance would not likely suffer as the criterion is fairly flat in this region.

### 3.2 Visualizing the Optimal MSE Tail

We now simulate response models of Equation 2 under different scenarios to demonstrate that our algorithm finds the optimal threshold for a tail quantile. We retain the same $X$ from before with $n = 100$ and $p = 10$. To draw responses, we set $\beta_T = 1$ and draw $\beta$ from $N_p(0_p, I_p)$. The entire simulation is fixed upon these values.

We then employed five design strategies: (BCRD) balanced complete randomization with
$S = 25,000$ vectors, (GOOD) The 5,000 least imbalanced vectors of the $S$, (OPT) the optimal design according to the weighted chi-squared approximation algorithm of Section 2.2.2, (DET) the deterministic design of the best vector out of the $S$ vectors and (BAD) the 5,000 most imbalanced vectors of the $S$.

For 3,000 iterations, we draw a $z$ from $\mathcal{N}_n(0_n, \sigma^2_z I_n)$ where $\sigma^2_z$ was computed so its ratio with the standard error of $X\beta$ was 3:1 thereby emulating a typical clinical case where $R^2_X \approx 25\%$. For 1,000 nested iterations, we draw a $w$ from the strategy. If the strategy is DET, we skip this nested loop as there is only one allocation $w^{(1)}$. We then compute $y$ via Equation 2 and $\hat{\beta}^{LR}_T$ from $X$, $w$ and $y$ and then we record the squared error $(\hat{\beta}^{LR}_T - \beta^T)^2$. The average over all 1,000 different $w$’s is recorded as an $\text{MSE}_w[\hat{\beta}^{LR}_T | z, X, \beta]$. Over the 3,000 draws of $z$, the MSE density is estimated. Figure 3 shows the density estimates for all five strategies. The expectation of the MSE is estimated by an average over all 3,000 draws (the vertical solid lines) and the 95% empirical quantile estimates the tail criterion (the vertical dashed lines).

Figure 3: MSE simulations for five strategies outlined in the text. In red is BCRD, pink is GOOD, OPT is green, DET is blue and BAD is black. The solid vertical lines are the average MSE and the dotted vertical lines are the empirical 95% quantiles.

There are many observations from this figure. First, as Equation 6 predicts, DET has the lowest expected MSE as shown as the solid blue line. However, note the shape of the MSE density for DET with its long right tail. The tail shape can be understand by examining the first term in the MSE expression (Equation 4) that can be written as $\frac{1}{n^2} z_\perp^T \Sigma w z_\perp$ where $z_\perp$ denotes the component of $z$ orthogonal to the column space of $X$. In the case of DET, the quadratic form becomes $(z_\perp^T w^{(1)})^2$. This implies that for $z$’s that interact poorly with the single, lowest imbalance allocation, there is a lot of error. In the case above, the 95%ile of the MSE (the dotted lines) is not even displayed for DET as its value is 2.23.

Second, the OPT design of the best 1,102 vectors of the $S = 25,000$ provides the best insurance against the 95% worst MSE (the green dotted line is the lowest of all dotted lines) for only a marginal loss in expected behavior (the green solid line is only nominally more than the solid blue line).

Third, there is a lot of leeway in finding the optimal design. The GOOD strategy of the top 5,000 assignments performs about the same as OPT. This is due to the flatness of the tail criterion among designs that neither too random or too deterministic.

Fourth, BCRD performs somewhat worse, but not terrible when compared to OPT. This
is related to the fifth observation: the BAD strategy of the worst 5,000 assignments performs only 18% worse on average than the optimal deterministic design. This is a testament to the advantage of the covariate adjusted linear estimator — the contribution of a priori imbalance is attenuated by a factor of $\frac{1}{n^2}$, a rapid rate of vanishing (Equation 6). This is another reason that the error inherent in our approximation strategies of Sections 2.2.2 and 2.2.3 are unlikely to matter in practice.

3.3 Optimal Rerandomization Threshold Dependence on $p$

We now investigate how the optimal threshold $a_*$ depends on the number of observed co-
variates $p$. We fix $n = 100$ and iteratively add more columns to $X$ varying $p \in \{1, 6, \ldots, 99\}$ where new column entries are standard normal realizations. We then recompute the optimal threshold via the weighted chi-squared approximation algorithm of Section 2.2.2.

![Graph](a)

![Graph](b)

Figure 4: Optimal threshold $a_*$ dependence on $p$. Left: $p$ vs. $a_*$ on a log-log scale. The vertical lines depict the imbalance range over all $S = 25,000$ vectors drawn from BCRD. Right: the threshold $a_*$ as the quantile over all $S = 25,000$ vectors.

Figure 4B shows the log optimal threshold increasing linearly in log $p$. Even though the $a_*$ is increasing and thus the optimal strategy appears to converge to BCRD, this can be due to the fact that the Mahalanobis $\mathcal{B}$ metric increases as $p$ increases. We examine this threshold as the quantile of all $S$ vectors conditional on $p$ in Figure 4B. This figure shows that although the threshold is increasing, the relative threshold is converging towards the deterministic design. This illustration is consonant with our intuition: as there are more observed covaraites, a priori restrictions on the randomization to decrease imbalance becomes more important to the resultant MSE. It is possible that these illustrations will be different if $S$ was increased by many orders of magnitude.

4 Discussion

We have offered an algorithm that can provide the optimal rerandomization threshold for the randomization model when inferring the average treatment effect using the simple differences-in-means estimator and the covariate-adjusted linear regression estimator. Our algorithm is much simpler and requires less choices for the practitioner when employing the linear regression estimator. The MSE of this estimator is also substantially lower in simulations
and thus we recommend it over the differences-in-means estimator. Our simulations also demonstrate that to get insurance on the 95%ile of most adversarial draws from the non-linear and unobserved component of the response function, relatively little rerandomization is needed as the thresholds are not too low when $p$ is small relative to $n$, the prevalent setting in experimental practice. This underscores the robustness of complete randomization coupled with linear adjustment as a design-estimation approach in experimentation.

There are other imbalance metrics and the choice seems arbitrary or one of convenience. Recently, [Kallus (2018) Section 2.3] proved that the optimal imbalance metric is dependent on the choice of norm for the response model. For instance, if the norm is Lipschitz, then the optimal $B$ would capture the deviation from a paire matching allocation, such as pairwise Mahalanobis distance (ibid, Theorem 4). If the norm is the sup norm, then the optimal $B$ is one that captures deviation from an incomplete blocking design (ibid, Theorem 3). If the squared norm is $\frac{1}{p} \beta^T (X^T X)^{-1} \beta$, i.e. a measure of the signal in the linear model, then the optimal $B$ is the Mahalanobis distance (ibid, Section 2.3.3). If the response function is represented by a reproducing Kernel Hilbert Space, then the optimal $B$ would be $w^T K w$ where $K$ is the $n \times n$ gram matrix, a matrix whose $i, j$ entries tally the kernel distance from $x_i$ to $x_j$ (ibid, Equation 4.2).

These kernel spaces can be infinite in dimension and thereby can model non-parametric response functions. The exponential kernel with kernel distance function $\exp(x_i^T x_j)$ can be seen as modeling all polynomials (with infinite degree) and the Gaussian kernel with kernel distance function $\exp(-||x_i - x_j||^2)$ is especially flexible (these were two examples given in ibid, Section 2.4).

Since the true model is unknown, one would want to employ an $B$ sufficiently flexible to not suffer poor performance if the model deviates from their arbitrary choice. Thus, the Gaussian kernel is recommended in practice (ibid, Section 6). Our software contains options for a wide variety of choices for $B$.

Additionally, as mentioned in Section 2.2, there is no theory we know of that specifies how $W_{base}$ should be sampled from the full space $W$. We have employed BCRD here but there may be other choices for instance those that provide more vectors with exponentially smaller imbalance. Our algorithm would proceed identically, but early simulation suggests the optimal designs can change drastically and we leave this for future research.

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**Replication**

The figures and values given in Section 3 can be duplicated by running the code in https://github.com/kapelner/CovBalAndRandExpDesign/blob/master/package testing.R. The code for our R package OptimalRerandExpDesigns can be found in the root of that repository as well.
5 Appendix

5.1 The MSE for $\hat{\beta}_T^{DM}$

This section is heavily adapted from Kapelner et al. (2019, Appendices 6.2–6.3).

We first show that the estimator is unbiased i.e. $E_w[\hat{\beta}_T^{DM} \mid z, X; \beta] = \beta_T$. Using the model given by Equation 2:

$$E_w[\hat{\beta}_T^{DM} \mid z, X; \beta] = \frac{1}{n} E_w[w^T (\beta_T w + X\beta + z) \mid z, X; \beta]$$

$$= \frac{1}{n} (E_w[\beta_T w^T w] + E_w[w^T X\beta \mid X; \beta] + E_w[w^T z \mid z])$$

$$= \frac{1}{n} (\beta_T E_w[w^T w] + E_w[w^T X\beta \mid X; \beta] + E_w[w]^T z)$$

$$= \beta_T + \frac{1}{n} (E_w[w^T X\beta \mid X; \beta] + E_w[w]^T z)$$

Since $w_i \in \{-1, +1\}$ then, $w^T w = \sum_{i=1}^n w_i^2 = n$. The assumption that $W$ is a mirror strategy (Assumption 2.1) implies that $E_w[w] = 0_n$ and

$$E_w[w^T X\beta \mid X; \beta] = \sum_{w \in W} w^T X\beta \mathbb{P}(W = w \mid X) = 0$$

(13)

since each $w$ cancels out with the summand with $-w$ with shared probability. This unbiasedness implies that the MSE equals the variance,

$$\text{Var}_w[\hat{\beta}_T \mid z, X; \beta] = E_w[\hat{\beta}_T^{DM2} \mid z, X; \beta] - \beta_T^2$$

$$= E((w^T Y/n)^2 \mid z, X; \beta) - \beta_T^2$$

$$= \frac{1}{n^2} E (w^T (\beta_T w + X\beta + z))^2 \mid z, X; \beta] - \beta_T^2$$

$$= \frac{1}{n^2} E ((\beta_T w^T w + w^T (X\beta + z))^2 \mid z, X; \beta] - \beta_T^2$$

$$= \frac{1}{n^2} E [2n\beta_T w^T (X\beta + z) + (w^T (X\beta + z))^2 \mid z, X; \beta]$$

where the last line follows from $w^T w = n$, simplification and canceling out the constant $\beta_T^2$. By the same arguments of Equation [13] $E_w[w^T (x + z) \mid z, X; \beta] = 0$ leaving us with

$$= \frac{1}{n^2} E [(w^T (X\beta + z))^2 \mid z, X; \beta]$$

$$= \frac{1}{n^2} E [(X\beta + z)^T w w^T (X\beta + z) \mid z, X; \beta]$$

$$= \frac{1}{n^2} (X\beta + z)^T \Sigma_w (X\beta + z).$$
5.2 The Expectation of the MSE for $\hat{\beta}_T^{DM}$

This section is heavily adapted from Kapelner et al. (2019, Appendix 6.4).

$$ E_z[MSE_w(\hat{\beta}_T \mid z, X; \beta)] = E_z \left[ \frac{1}{n^2} (X \beta + z) \Sigma W (X \beta + z) \mid x \right] $$

$$ = \frac{1}{n^2} E_z \left[ (X \beta)^\top \Sigma W X \beta + 2 (X \beta)^\top \Sigma W z + z^\top \Sigma W z \mid X; \beta \right] $$

$$ = \frac{1}{n^2} \beta^\top X^\top \Sigma W X \beta + \frac{2}{n^2} \beta^\top X^\top \Sigma W E_z [z \mid X] + \frac{1}{n^2} E_z [z^\top \Sigma W z] $$

Since $E_z[z \mid X] = 0_n$ (by implication of Assumption 2.2), the second term is zero. The third term is the expectation of a quadratic form. By Petersen & Pedersen (2012, Equation 318) and assuming homoskedasticity (Assumption 2.4) and the fact that since $W$ is generalized multivariate Bernoulli, this implies $\text{tr} \left[ \Sigma W \right] = n$ we arrive at

$$ E_z[MSE_w(\hat{\beta}_T \mid z, x)] = \sigma^2_n + \frac{1}{n^2} \beta^\top X^\top \Sigma W X \beta. $$

5.3 The MSE for $\hat{\beta}_T^{LR}$

We let the overall design matrix of the OLS regression be $\tilde{X} := [w \mid X]$. By standard OLS theory and Equation 2

$$ \hat{\beta}_T = \left( \tilde{X}^\top \tilde{X} \right)^{-1} \tilde{X}^\top y = \left[ \begin{array}{c|c} n & w^\top X^\top \\ \hline X w & X^\top X \end{array} \right]^{-1} \left[ \begin{array}{c} w^\top y \\ X^\top y \end{array} \right] $$

Note that the first entry of the estimator above is $\hat{\beta}_T^{LR}$, what we care about. We use formula given in Petersen & Pedersen (2012, Section 3.2.6) to provide the top row of the inverse matrix above:

$$ \hat{\beta}_T^{LR} = \left( \begin{array}{c|c} \frac{1}{n-w^\top P w} & -w^\top X (X^\top X)^{-1} \\ \hline \frac{-w^\top X (X^\top X)^{-1}}{n-w^\top P w} & N/A \end{array} \right) \left[ \begin{array}{c} w^\top y \\ X^\top y \end{array} \right] = \frac{w^\top y - w^\top P y}{n-w^\top P w} = \frac{w^\top (I-P)y}{n-w^\top P w} $$

where $P := X (X^\top X)^{-1} X^\top$, i.e. the projection matrix onto the covariates and $I$ is the $n \times n$ identity matrix. Now, replacing $y$ with the model, we find:

$$ \hat{\beta}_T^{LR} = \frac{w^\top (I-P)(\beta_T w + \beta X)}{n-w^\top P w + z} = \frac{w^\top (\beta_T w + \beta X + z) - w^\top P(\beta_T w + \beta X + z)}{n-w^\top P w} $$
\[
\begin{align*}
\text{MSE}_w[\hat{\beta}_{LR} | z] &= \mathbb{E}_w[g^2] = \mathbb{E}_w[(B_z - B'_X r')^2] \\
&= \mathbb{E}_w\left[\left(\frac{B_z - B'_X r'}{1 - B'_X B'_X}\right)^2\right] \\
&\approx \left(\frac{B_z - B'_X r'}{1 - B'_X B'_X}\right)^2 + 2 \left\| B'_X\right\|^2 B_z^2
\end{align*}
\]

where \( r = X^T z / n \), a column vector of correlation-like metrics of the \( p \) covariates with \( z \), denote \( B_X = X^T w / n \), a column vector of average differences in the \( p \) covariates between treatment and control, \( A = n(X^T X)^{-1} \), a symmetric matrix, \( B'_X := A^{1/2} B_X \), \( r' := A^{1/2} r \) and \( B_z \) is the same as in the univariate case, the average difference in \( z \) between treatment and control. Note that \( B'_X B'_X \) is the Mahalanobis distance between the average covariate values in the treatment group and the average covariate values in the control group.

We can show that \( g \) simplifies to \( \frac{B_z - B'_X r'}{1 - B'_X B'_X} \) in the univariate case (the expression in Table 2). Note that this estimator is not a function of \( \beta \)! This is a convenient result of covariate adjustment.

The \( \text{MSE}_w[\hat{\beta}_{LR} | z] \) is the expectation of \( (\hat{\beta}_T - \beta_T)^2 = g^2 \). This expectation is difficult to express in closed form. We instead take a geometric series approximation,

\[
g = \frac{B_z - B'_X r'}{1 - B'_X B'_X} = (B_z - B'_X r') \left( 1 + \left\| B'_X\right\|^2 + O \left( \left\| B'_X\right\|^4 \right) \right)
\]

We can use asymptotic notation to expand \( g^2 \) and then approximate it

\[
g^2 = (B_z - B'_X r')^2 \left( 1 + \left\| B'_X\right\|^2 + O \left( \left\| B'_X\right\|^4 \right) \right)^2 \\
= (B_z - B'_X r')^2 + 2 \left\| B'_X\right\|^2 B_z^2 \left( 1 + O \left( \left\| B'_X\right\|^2 \right) \right)
\]

Recall that our target is \( \text{MSE}_w[\hat{\beta}_T | z] = \mathbb{E}_w[g^2] \). The expectation of the first term can be written as

\[
\begin{align*}
\mathbb{E}_w[(B_z - B'_X r')^2] &= \mathbb{E}_w[(w^T (I - P) z)^2] \\
&= \mathbb{E}_w\left[(z(I - P))^\top w w^T (I - P) z\right] \\
&= z^\top (I - P) \Sigma_w (I - P) z \\
&= z^\top G z
\end{align*}
\]
where \( G := (I - P)\Sigma_W(I - P) \). This term can alternatively be expressed as \( z_{\perp}^\top \Sigma_W z \) where \( z_{\perp} \) is defined to be the component of \( z \) orthogonal to the column space of \( X \).

The expectation of the second term is:

\[
\mathbb{E}_w \left[ 2 \|B_X\|^2 B_z^2 \right] = 2\mathbb{E}_w \left[ \|B_X\|^2 B_z^2 \right] \\
= 2\mathbb{E}_w \left[ B_z \frac{1}{n} w^\top P w B_z \right] \\
= \frac{2}{n^3} \mathbb{E}_w \left[ z_{\perp}^\top w w^\top P w w^\top z \right] \\
= \frac{2}{n^3} z_{\perp}^\top D z
\]

where \( D := \mathbb{E}_w [ww^\top Pww^\top] \), an expectation of a homogeneous quartic form that cannot be simplified further. Putting this all together,

\[
\text{MSE}_w[\hat{\beta}^{LR}_T | z] = \frac{1}{n^2} z^\top G z + \frac{2}{n^3} z_{\perp}^\top D z \\
= z^\top R z
\]

where the determining matrix of the quadratic form is \( R := G + \frac{2}{n} D \).

5.4 The Expectation of the MSE for \( \hat{\beta}^{LR}_T \)

We find the expectation over \( z \) as

\[
\mathbb{E}_z \left[ \text{MSE}_w[\hat{\beta}^{LR}_T | z] \right] = \frac{1}{n^2} \mathbb{E}_z [z^\top R z] = \frac{\sigma^2}{n^2} \text{tr} [R]
\]

where the equality comes from Assumptions 2.3 and 2.4 and an application of Petersen & Pedersen (2012, Equation 318).

\[
\text{tr} [R] = \text{tr} [G] + \frac{2}{n} \text{tr} [D] \\
= \text{tr} [(I - P)\Sigma_W(I - P)] + \frac{2}{n} \text{tr} [\mathbb{E}_w [ww^\top Pww^\top]] \\
= \text{tr} [(I - P)\Sigma_W] + \frac{2}{n} \text{tr} [\mathbb{E}_w [ww^\top Pww^\top]] \\
= n - \text{tr} [P\Sigma_W] + \frac{2}{n} \text{tr} [ww^\top Pww^\top P] \\
= n - \text{tr} [P\Sigma_W] + \frac{2}{n} \mathbb{E}_w [tr [ww^\top P]] \\
= n - \text{tr} [P\Sigma_W] + 2\mathbb{E}_w [tr [ww^\top P]] \\
= n - \text{tr} [P\Sigma_W] + 2\mathbb{E}_w [w^\top P] \\
= n - \text{tr} [P\Sigma_W] + 2\text{tr} [P]\Sigma_W \\
= n + \text{tr} \left[ X (X^\top X)^{-1} X^\top \Sigma_W \right]
\]
\[
= n + \text{tr} \left[ (X^T X)^{-1} X^T \Sigma W X \right] \\
= n + \text{tr} \left[ (X^T X)^{-\frac{1}{2}} X^T \Sigma W X (X^T X)^{-\frac{1}{2}} \right] \\
= n + \frac{1}{n} \text{tr} \left[ A^\frac{1}{2} X^T X A^\frac{1}{2} \right] \\
= n + \text{tr} \left[ X_\perp^T \Sigma W X_\perp \right]
\]

Let \( X_\perp := X \left( X^T X \right)^{-\frac{1}{2}} \) be the orthogonalization of \( X \). Thus,

\[
E_z \left[ \text{MSE}_w \left[ \hat{\beta}^{LR}_T | z \right] \right] = \frac{\sigma_z^2}{n} + \frac{\sigma_z^2}{n^2} \text{tr} \left[ X_\perp^T \Sigma W X_\perp \right]
\]

where the trace term can more intuitively be expressed as:

\[
\text{tr} \left[ X_\perp^T \Sigma W X_\perp \right] = x_{\perp_1}^T \Sigma W x_{\perp_1} + \ldots + x_{\perp_p}^T \Sigma W x_{\perp_p} \\
= E_w \left[ B_x^2 \right] + \ldots + E_w \left[ B_{x\perp_p}^2 \right]
\]

meaning the sum of imbalances squared of the each of the orthogonalized dimensions of the column space of \( X \).

### 5.5 The Standard Error of the MSE for \( \hat{\beta}^{DM}_T \)

This section is heavily adapted from Kapelner et al. (2019, Appendix 6.6).

Section 5.1 derived the quadratic form of the MSE. The variance with respect to \( z \) can be calculated straightforwardly using Petersen & Pedersen (2012, eq. 319) when assuming that the fourth moment of \( z \) is finite (Assumption 2.5) and do not depend on \( X \) (Assumption 2.6) as

\[
\text{Var}_z \left[ \text{MSE}_w[\hat{\beta}_T | z, x] \right] = \frac{(\sigma_z^2)^2}{n^4} \left( n \kappa_z + 2 ||\Sigma W||_F^2 + \frac{4}{\sigma_z^2} \beta^T X^T \Sigma W X \beta + \gamma_z 1_n^T \Sigma W X \beta \right),
\]

where \( \kappa_z \) is the excess kurtosis in \( Z \) and \( \gamma_z := E[z^3] \) and we prove in sec. 5.6 that this last term with \( \gamma_z \) is zero if we assume 5.1 that all assignments are forced balance.

**Assumption 5.1 (Forced Balance).** For all \( w \in \mathbb{W}, w^T 1_n = 0 \).

Since the rerandomization strategy in the text employed BCRD as the base strategy, this assumption was implicit throughout the paper.

### 5.6 A Proof that the Last MSE Term is Zero

This section is heavily adapted from Kapelner et al. (2019, Appendix 6.7).

We wish to demonstrate that \( 1_n^T \Sigma W X \beta = \beta^T X^T \Sigma W 1_n = 0 \). By the forced balance assumption (5.1), \( E_w[1_n^T w | X, \beta] = \text{Var}_w[1_n^T w | X, \beta] = 0 \) since every \( w \) is balanced. Then, \( \text{Var}_w[1_n^T w | X, \beta] = E_w[(1_n^T w)^2 | X, \beta] = 1_n^T \Sigma W 1_n = 0 \).
Note that \( \Sigma_W = \sum_{i=1}^{n} \lambda_i v_i v_i^\top \) where the \( \lambda_1 \geq \ldots \geq \lambda_n \geq 0 \) and \( v_i \)'s are its eigenvalues and eigenvectors respectively. Since \( \Sigma_W \) is a variance-covariance matrix, it is symmetric implying that its eigenvalues are all non-negative. We can then write \( 1_n^\top \Sigma_W 1_n = \sum_{i=1}^{n} \lambda_i \left( v_i^\top 1_n \right)^2 = 0 \). This means that \( \lambda_i \left( v_i^\top 1_n \right)^2 = 0 \) for all \( i \). In order for this to be true, for every \( i \) either \( \lambda_i = 0 \) or \( v_i^\top 1_n = 0 \).

We now examine just the term \( \Sigma_W 1_n \) which can be written as \( \sum_{i=1}^{n} \lambda_i v_i v_i^\top 1_n \). For all \( i \) either \( \lambda_i \) or \( v_i^\top 1_n \) is zero rendering the “middle” \( v_i \) irrelevant. Thus \( \Sigma_W 1_n = 0_n \) and \( \beta^\top X^\top \Sigma_W 1_n = \beta^\top X^\top 0_n = 0 \).

### 5.7 The Standard Error of the MSE for \( \hat{\beta}_T^{LR} \)

By Assumptions 2.3 and 2.4 and an application of Petersen & Pedersen (2012, Equation 319),

\[
\text{Var}_z \left[ \frac{1}{n^2} z^\top R z \right] = \frac{\sigma_z^2}{n^4} \left( 2 \text{tr} \left[ R^2 \right] + \kappa_z \sum_{i=1}^{n} R_{i,i}^2 \right)
\]

where \( \kappa_z \) denotes excess kurtosis and \( R_{i,i} \) are the diagonal entries of \( R \) that we cannot simplify further. We evaluate the trace term below:

\[
\text{tr} \left[ R^2 \right] = \left\| G + \frac{2}{n} D \right\|_F^2 = \text{tr} \left[ \left( G + \frac{2}{n} D \right) \left( G + \frac{2}{n} D \right) \right] = \text{tr} \left[ G^2 + 4 \frac{n}{n^2} GD + \frac{4}{n^2} D^2 \right] = \text{tr} \left[ G^2 \right] + 4 \text{tr} \left[ GD \right] + 4 \frac{n^2}{n^2} \text{tr} \left[ D^2 \right]
\]

Putting this all together, we find that

\[
\text{SE}_z \left[ \text{MSE}_w \left[ \hat{\beta}_T | z, X \right] \right] = \frac{\sigma_z^2}{n^2} \sqrt{\frac{2}{n} \left( \left\| (I - P) \Sigma_W \right\|_F^2 + \text{tr} \left[ GD \right] + 4 \frac{n^2}{n^2} \text{tr} \left[ D^2 \right] \right) + \kappa_z \sum_{i=1}^{n} R_{i,i}^2}
\]

We now prove some bounds on some of these terms so we can interpret them more easily.

\[
\text{tr} \left[ D^2 \right] \leq \text{tr} \left[ D \right]^2 = n^2 \text{tr} \left[ X^\top \Sigma_W X \right]^2
\]
where the first inequality is a trace inequality for symmetric matrices and the second equality was shown in App. 5.4. Also,

$$\text{tr}[GD] \leq \sqrt{\text{tr}[G^2]\text{tr}[D^2]} \leq \text{tr}[D] \sqrt{\text{tr}[G^2]} = n\text{tr}[X^\top \Sigma W X] \|(I - P)\Sigma W\|_F$$

where the first inequality is Cauchy-Schwartz, the second is the trace inequality used above and the equality is then by substitutions.

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