Stratifying Online Field Experiments Using the Pigeonhole Design

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Practitioners and academics have long appreciated the benefits that experimentation brings to firms. For online web-facing firms, however, it still remains challenging in handling heterogeneity when experimental units arrive sequentially in online field experiments. In this paper, we study a novel online experimental design problem, which we refer to as the “Online Stratification Problem.” In this problem, experimental units with heterogeneous covariate information arrive sequentially and must be immediately assigned into either the control or the treatment group, with an objective of minimizing the total discrepancy, which is defined as the minimum weight perfect matching between the two groups. To solve this problem, we propose a novel experimental design approach, which we refer to as the “Pigeonhole Design.” The pigeonhole design first partitions the covariate space into smaller spaces, which we refer to as pigeonholes, and then, when the experimental units arrive at each pigeonhole, balances the number of control and treatment units for each pigeonhole. We analyze the theoretical performance of the pigeonhole design and show its effectiveness by comparing against two well-known benchmark designs: the match-pair design and the completely randomized design. We conduct extensive simulations to study the numerical performance of the different designs and conclude with practical suggestions.

1. Introduction

The design of experiments has long provided tremendous benefits to firms, especially in the technology sector (Kohavi et al. 2007, 2009, Bakshy et al. 2014, Lewis and Rao 2015, Kohavi et al. 2020, Li et al. 2021, Wager and Xu 2021, Johari et al. 2021, 2022). Most large technology firms develop their own tools to run field experiments to improve their software products and services, and a growing number of smaller companies purchase such tools from third-party analysts that offer full-stack integration (Thomke 2020). These tools typically enable the businesses to run “A/B tests,” in which the experimenter compares the standard offering of some policy “A” to a new version of the policy “B”, by splitting users into the “control” and the “treatment” groups. By
comparing the outcomes from these two groups, the experimenter discovers how much the new
version is better or worse than the standard version, which is referred to as the “treatment effect.”
Such simple tools have been widely adopted by a variety of online web-facing companies, including
“search engines (e.g., Bing, Google, Yandex), online retailers (e.g., Amazon, eBay, Etsy), media
service providers (e.g., Netflix), social networking services (e.g., Facebook, LinkedIn, Twitter), and
travel services (e.g., Airbnb, Booking.com, Lyft, Uber)” (Gupta et al. 2019). These tools have
brought tremendous value to the firms throughout their product development processes (Koning
et al. 2019).

Practitioners and academics have widely recognized one challenge in the design of experiments
in handling heterogeneity. Heterogeneity refers to the scenario when the same version of treatment
creates different levels of treatment effects across users with different characteristics. For example,
a newer version of an online display advertisement might have a different effect on click through
rates for younger people compared to older people. One method to address heterogeneity is via
“stratification”, which is also referred to as “blocking” (Fisher 1936, Cochran and Cox 1957, Cox
1958, Chase 1968, Matts and Lachin 1988, Imbens 2011, Athey and Imbens 2017, Imbens and Rubin
2015). Typically, in a stratified experiment, all users are characterized into several different strata,
such that within each stratum, users’ characteristics are similar. Then, assuming all the strata are
fixed, the experimenter randomly assigns half of the users from each stratum to receive control, and
the other half from each stratum to receive treatment. This simple approach has been considered
to be the gold standard in handling heterogeneity in randomized control trials (Rubin 2008), and
has been extensively studied from an optimal experimental design perspective (Rosenbaum 1989,
Greedy et al. 2004, Imai et al. 2009, Lu et al. 2011, Higgins et al. 2016, Bai 2019, Harshaw et al.
2019).

For online web-facing firms, however, such a simple stratified experiment is not always feasible.
In an online field experiment, the characteristics of the users are not known in advance. Instead,
the characteristics are sequentially revealed as the users arrive in an online fashion. Upon a user’s
arrival, the experimenter must immediately decide if the user is assigned to the control or the
treatment group based on this user’s characteristics, without knowing the characteristics of the
future arriving users. It is the uncertainty of future users’ characteristics that hinders the usage of
the well studied designs of stratified experiments.

In this paper, we study a novel online experimental design problem, which we refer to as the
“Online Stratification Problem.” To solve this problem, we propose a novel experimental design
approach, which we refer to as the “Pigeonhole Design”. We analyze the theoretical performance of the pigeonhole design against two well-known benchmark designs of experiments and show the effectiveness of the pigeonhole design.

1.1. The Online Stratification Problem

In the online stratification problem, the experimenter is given in advance a fixed budget of experimental units, who are the users to this online platform. During the experiment, a fixed number of users with unknown characteristics arrive one by one. Upon the arrival of each user, the experimenter must irrevocably assign each user into either the control or the treatment group, with the objective of minimizing the total discrepancy between the user characteristics of these two groups, which is defined as the size of a minimum weight perfect matching \cite{BertsimasTsitsiklis1997}.

To the best of our knowledge, the online stratification is similar but distinct to a few problems in the literature.

1. Online Vector Balancing. This line of literature follows the work of \cite{Spencer1977}. Recent works have studied a variant of this problem under the stochastic arrival model \cite{Bansal2020,Alweiss2021,Bansal2021}. In an online vector balancing problem, users with unknown vector information arrive one by one. Upon arrival, the vector information is revealed, and the decision maker must irrevocably assign a positive or negative sign \(\pm\). The objective is to minimize the \(L_\infty\) norm of the total signed prefix-sum.

Our problem is closely related to the online vector balancing problem, but with the following two distinctions. First, the online vector balancing problem allows the number of users who receive the negative sign to be different from the number of users who receive the positive sign. In contrast, our problem requires the control and treatment groups to have equal size, which is an omnipresent assumption in the experimental design literature \cite{Rosenbaum1989,Greevy2004,Lu2011,Harshaw2019}. Note that the online vector balancing problem can be adapted via augmenting the covariate space, such that the number of users in two groups are equal. So this is a minor distinction.

Second, the objective functions are different. The online vector balancing problem minimizes the total signed prefix-sum, whereas our online stratification problem minimizes the size of the minimum weight perfect matching. See Figure 1 for an illustrator. As shown in Figure 1, there are 8 users \((A_1, A_2, B_1, B_2, C_1, C_2, D_1, D_2)\) whose covariates are in a 2-dimensional space. Under our online stratification objective, one optimal design could be matching \((A_1, A_2)\) into a pair, ...,
Figure 1  An illustrator of the difference between the online vector balancing objective and the online stratification objective.

$(D_1, D_2)$ into a pair. Thus, the optimal design selects exactly one from each pair into the control group, and exactly the other from each pair into the treatment group. On the other hand, under the online vector balancing objective, one optimal design (not necessarily unique) could be assigning negative signs to $A_1, A_2, C_1, C_2$, i.e., into the control group, and positive signs to $B_1, B_2, D_1, D_2$, i.e., into the treatment group. Such a design could possibly lead to imbalance between the two groups, as the geometric center may not fully capture the locations of all users.

2. Online Experimental Design under $D_A$-Optimality. This line of literature follows the work of Atkinson (1982, 1999). Recently, Bhat et al. (2020) revisits this problem by articulating the tension between online algorithms and experimental design, which has greatly motivated our work.

In this problem, there are several prognostic factors that are assumed to impact the potential outcomes through a linear model, including the treatment status. We refer to such prognostic factors as covariate information, and treatment status is one of them. Users with unknown covariate information arrive one by one, and the covariate information is revealed upon the arrival of one user. The experimenter must irrevocably administer control or treatment to this user, which determines the value of a single binary indicator among the covariates. The objective is the $D_A$-optimality, which refers to minimizing the variance of the Ordinary Least Squares (OLS) estimator on some certain covariates.

Our problem is closely related to the online $D_A$-optimal experimental design problem as well, with the following three distinctions. First, the online $D_A$-optimal experimental design problem allows the number of users in the control and treatment groups to be different whereas our online
stratification problem requires the numbers to be the same. Second, the objective functions are different. The online $D_A$-optimal experimental design problem uses an OLS estimator to estimate the effects of treatment by postulating a linear dependence of the potential outcomes on the covariates. The objective is to minimize the variance of the OLS estimator on some certain covariates, e.g., on the treatment indicator. In contrast, our objective is the size of the minimum weight perfect matching. Third, the models of the arrival sequence are different. The model in Atkinson (1982) assumes that the covariate information is part of the decision making. The model in Bhat et al. (2020) assumes a stochastic arrival sequence drawn from an elliptical distribution with finite second order moment. An implication of choosing this model is that the optimal design will be deterministic, and there is no randomization in the optimal design. In contrast, we model the arrival sequence to be adversarial. Our model has the flexibility to extend to the stochastic arrival setting, which potentially improves our results.

3. Online Bipartite Matching. This line of literature follows the works of Karp et al. (1990), Mehta et al. (2007), and has been summarized in the textbook of Mehta (2013). In an online bipartite matching problem, one side of the bipartite graph, usually referred to as the resources, is known in advance and endowed with fixed capacities. The other side of the bipartite graph, usually referred to as the users, arrives in a sequential fashion. Upon arrival, one user must be immediately matched to one of the adjacent resources, and earns an immediate reward that is equal to the weight of the created edge. The objective is to maximize the total sum of rewards accumulated over the horizon. While the online bipartite matching problem typically has a maximization objective, some works have discussed finding the minimum weight matching (Kalyanasundaram and Pruhs 1993). Recent works have extensively studied a number of other variants, e.g., under the stochastic IID model (Feldman et al. 2009, Devanur et al. 2013, Alaei et al. 2012, Jaillet and Lu 2014), under the random order model (Goel and Mehta 2008), and allowing for delays (Ashlagi et al. 2019).

Our problem is intrinsically different from the online bipartite matching problem in the following two aspects. First, in an online bipartite matching problem, one side of the graph (the resource side) is given in advance. But in the online stratification problem, both sides are the users and arrive one by one. Second, the rewards in an online bipartite matching problem are generated immediately when users are matched to resources. The core trade-off lies in balancing immediate rewards and potential future rewards, and an assignment executed in a previous period only makes an impact on the future rewards through the remaining resources. But in the online stratification problem, while we make an assignment decision immediately upon the arrival of a user, the discrepancy is
calculated at the end of the horizon. As a result, the impact of an assignment executed in an early period will not be fully understood until the end of the horizon.

1.2. The Pigeonhole Design

To solve the online stratification problem, we propose a pigeonhole design that works in the following two stages. In the first stage, the pigeonhole design partitions the covariate space into smaller spaces, which we refer to as pigeonholes. We administer assignments based on the covariates. When arriving users are routed to pigeonholes, we make the number of treatment and control users as balanced as possible by sequentially matching the arrived users in pairs. In the second stage, we ignore the covariate information and only administer assignments based on the overall imbalance across the control and treatment groups.

To the best of our knowledge, the pigeonhole design is similar but distinct to a few experimental design methods in the literature.

1. Matched-Pair Design. The idea of the matched-pair design, or more generally, stratification, has been well studied from the beginning of the experimental design literature (Fisher 1936). The matched-pair design is a limiting case in which each strata only has two experimental users (Chase 1968, Athey and Imbens 2017, Imbens and Rubin 2015). In a matched-pair design, there is an even number of users, and all the users are grouped into size-two pairs according to some criterion. From each pair of the two users, one is randomly administered control and the other is administered treatment. Other than the criterion considered in this work of finding the minimum weight perfect matching, there are many other criteria in deciding how to pair the users, including minimizing the maximum within-pair distance (Higgins et al. 2016), minimizing the (generalized) Mahalanobis distance (Diamond and Sekhon 2013), and minimizing the risk function (Bai 2019). Since the matched-pair design requires information about all the users, this design has not been well adapted to the online setting when users arrive one by one.

2. Completely Randomized Design. The idea of completely randomized design has been well studied from the beginning of the experimental design literature (Fisher 1936). It is one of the most basic sources of randomness in a randomized experiment. In a completely randomized design, a fixed number (usually half of total population) of users are randomly selected to administer control while the remaining users are assigned to treatment. Since randomization can be determined and fixed before running the experiment, this design can be easily implemented in the online setting (Efron 1971).
3. **Biased Coin Design.** This line of literature is pioneered by the work of Efron (1971), and has been subsequently generalized to covariate-adaptive versions as in Pocock and Simon (1975), Atkinson (1982, 1999). In a biased coin design, each time the next user arrives, the experimenter flips a biased coin to administer control (if tails) and treatment (if heads). The head-up probability of the coin can depend on the heads and tails in the observations collected so far. One remarkable special case of the biased coin design is the completely randomized design, where the biased coin flipping always tends to balance the number of control and treatment assignments. In the generalization to covariate-adaptive versions, there are a fixed number of prognostic factors and the experimenter suggests head-up probabilities that depend on a generic cost function of the covariate imbalance. As commented in Bhat et al. (2020), the biased coin designs and their covariate-adaptive versions “can be regarded as myopic policies ... that only consider the immediate impact of an allocation decision but not the impact on future decisions.” Specifically for the covariate-adaptive versions, as commented in Rosenberger and Sverdlov (2008), Rosenberger and Lachin (2015), “very little is known about their theoretical properties.”

4. **Matching-On-The-Fly.** Recently, Kapelner and Krieger (2014) proposes the idea of maintaining a reservoir to match units. Whenever the next user arrives, if there is no good match with the reservoired users, measured in the Mahalanobis distance, then flip a fair coin to determine the assignment. If there is a good match with one of the reservoired users, then both of them are determined to be a pair and removed from the reservoir. Such a heuristic idea is creative, yet there is no mathematical formulation of the objective, and no theoretical analysis of this method’s quality.

### 1.3. Performance Guarantees and Analytical Techniques

In this paper, we analyze the performance of the matched-pair design, the completely randomized design, and the pigeonhole design whose discrepancies are summarized in Table 1. First, the

| Dimension of Covariates | $p = 1$ | $p \geq 2$ |
|-------------------------|---------|----------|
| Matched-Pair Design     | $\Theta(1)$ | Theorem 1 | $\Theta\left(T^{\frac{p-1}{p}}\right)$ | Theorem 4 |
| Completely Randomized Design | $\Theta\left(T^{\frac{1}{2}}\right)$ | Theorem 2 | $\Omega\left(T^{\frac{p-1}{p}}\right)$ | Theorem 5 |
| Pigeonhole Design       | $O\left(T^{\frac{1}{2}}(\log T)^{\frac{1}{2}}\right)$ | Theorem 3 | $O\left(T^{\frac{p-1}{p}}(\log T)^{\frac{1}{2}}\right)$, $p = 2$ | Theorem 6 |
|                         |         |          | $O\left(T^{\frac{p-1}{p}}\right)$, $p \geq 3$ |          |

In this table, $T$ stands for the total number of experimental population; $p$ stands for the dimension of covariate information.
matched-pair design serves as a benchmark that any online design of experiments cannot achieve. This is because the matched-pair design uses all the covariate information which would not be available to the online designs, as it is sequentially revealed over time. Second, the completely randomized design serves as a naive benchmark by not using any covariate information at all. The resulting expected discrepancy is larger. Third, and most importantly, the pigeonhole design as we propose in this paper has a performance in between the matched-pair design and the completely randomized design.

Table 1 also summarizes the discrepancies of the three designs under two cases: the single-dimensional case and the multi-dimensional cases. Our analysis suggests that the discrepancy will increase as the dimension increases, which coincides with the recognition that finding matching estimators becomes more challenging when the dimensions grow larger.

As outlined in Table 1 in the single-dimensional case, the matched-pair design has the smallest discrepancy in the order of $\Theta(1)$, which serves as a benchmark for all online designs. The completely randomized design has a much larger expected discrepancy in the order of $\Theta(T^{\frac{1}{2}})$. The pigeonhole design achieves an expected discrepancy in the order of $O(T^{\frac{1}{4}(\log T)^{\frac{1}{2}}})$, which improves upon the benchmark of the completely randomized design. The simulation results that we will show in Section 7 verify the theoretical analyses. The pigeonhole design significantly outperforms the completely randomized design in the single-dimensional case.

Moving to the multi-dimensional case, the matched-pair design has the smallest discrepancy, in the order of $\Theta(T^{\frac{p-1}{p}})$. This discrepancy increases as the dimension increases, showing the hardness of this problem. The completely randomized design has an expected discrepancy in the order of $\Omega(T^{\frac{p-1}{p}})$, as it cannot perform better than the matched-pair design. The pigeonhole design, surprisingly, achieves an expected discrepancy in the order of $\tilde{O}(T^{\frac{p-1}{p}})$, which closely matches the performance of the matched-pair design. This suggests that the pigeonhole design is near optimal with only up to logarithmic factors. Even though not depicted in the theoretical gaps, the simulation results that we will show in Section 7 suggests that the pigeonhole design significantly outperforms the completely randomized design again in the multi-dimensional case.

Next, we highlight our analytical techniques.

1.3.1. Coupling Arguments in the Single-Dimensional Case. In the single-dimensional case, the matched-pair design, which is an offline policy, always achieves a discrepancy less than 1.

To show that the completely randomized design achieves an expected discrepancy in the order of $\Theta(T^{\frac{1}{2}})$, it only suffices to create an arrival sequence to show the $\Omega(T^{\frac{1}{2}})$ part. In order to show
the $O(T^{\frac{1}{2}})$ part, we introduce a counting idea to write the discrepancy as an algebraic expression that explicitly depends on the covariates of all the users. Then we identify the worst-case arrival sequence and find the associated discrepancy.

The pigeonhole design that we propose achieves a smaller discrepancy, in the order of $O\left(T^{\frac{1}{3}}(\log T)^{\frac{1}{2}}\right)$. The pigeonhole design works by matching in pairs as many users as possible that arrive at one pigeonhole. For those unmatched users at each pigeonhole, we introduce a coupling method that shows the assignment of these users can be viewed as coming from a coupling stochastic process that mimics the completely randomized design. The pigeonhole design strikes a balance between the discrepancies generated from the matched users and the unmatched users. There is a balancing parameter that can be tuned in practice to reflect the balance (or imbalance).

1.3.2. **Challenges in the Multi-Dimensional Case.** Performing matching in the multi-dimensional case is more challenging than in the single-dimensional case. For the matched-pair design, unlike in the single-dimensional case where there exists a much simplified structure, we have to solve a combinatorial optimization problem to find the discrepancy. Instead of explicitly calculating the discrepancy, we instead characterize the order of the discrepancy. We first find an arrival sequence in which the matched-pair design has at least $\Omega(T^{\frac{p}{p-1}})$ discrepancy. Then we introduce a new method to first find the average discrepancy along each pair of users, and then show that we are unable to pack more users into the unit hypercube, thus finishing the proof by contradiction.

For the completely randomized design, since it is challenging to find the minimum weight perfect matching in the multi-dimensional case, it is challenging then to provide an upper bound for its expected discrepancy. Instead, we show that for a special family of arrival sequences, we can calculate the order of its discrepancy by applying a novel induction method.

Our pigeonhole design in the multi-dimensional case follows the same intuition as in the single-dimensional case. It is a surprising result that the discrepancy of the pigeonhole design in the multi-dimensional case achieves the optimal order, i.e. it has the same order as the matched-pair design does, even though the matched-pair design is endowed with full knowledge of all the covariate information of the arrival sequence. Our pigeonhole design in the multi-dimensional case relies on the same coupling technique, which uses the analysis of the completely randomized design under the family of instances we have defined earlier.
1.4. Roadmap

The paper is structured as follows. In Section 2, we introduce the online stratification problem which we study in this paper. In Section 3, we first introduce the matched-pair design, then distinguish the single-dimensional and multi-dimensional cases, and finally show the performance of the matched-pair design in the single-dimensional case as in Theorem 1. In Section 4, we introduce the completely randomized design and show the performance of the completely randomized design in the single-dimensional case as in Theorem 2. In Section 5, we introduce the pigeonhole design, outline the intuitions of how to design pigeonholes, and show the performance of one pigeonhole design in the single-dimensional case as in Theorem 3. In Section 6, we show the performances of the three designs in the multi-dimensional cases as in Theorems 4–6. In Section 7, we run numerical simulations to show strong numerical performance of the pigeonhole design. Finally, we conclude the paper by providing practical suggestions for firms to run online experiments using the pigeonhole design, and by pointing out three limitations that could lead to future research directions.

2. The Online Stratification Problem

Consider the following experimental design problem for an online platform. Let there be a discrete, finite time horizon of T periods, where we assume T to be an even number. In practice, T is typically known and given in advance, which reflects the size of the experimental budget. For example, at online search engines, online retailers, and travel service providers, T is typically determined in advance by the product managers who are testing their new products.

At any point in time, \( t \in [T] := \{1, 2, \ldots, T\} \), one user arrives at the platform. Each arriving user is associated with a covariate, \( x_t \), from some \( p \)-dimensional space \( S \). In this paper, we normalize the covariate space to be \( S = [0, 1]^p \) by properly re-scaling the support of each dimension to \([0, 1]\), because such a re-scaling does not change our results with respect to the dependence on T. Each dimension reflects a unit of important covariate information that the experimenter needs to consider. For example, at Yahoo! Front Page (Lewis 2010), the covariate(s) could either be one important Key Performance Index (KPI) such as the “browsing type,” or a combination of several user demographics. In this paper, we model the covariates to be adversarially chosen from the covariate space \([0, 1]^p\), which is often referred to as an adversarial arrival model. Such an adversarial arrival typically reflects the non-predictable nature of the future arriving users, and has been widely adopted in the online algorithms literature (Mehta 2013, Buchbinder and Naor 2009).

Upon the arrival of one user \( t \), the experimenter observes the covariate information of the user, \( x_t \), and then must immediately and irrevocably administer an intervention \( W_t \in \{0, 1\} \) to this user.
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t, without knowing the covariates from the future arriving users. For example, at Yahoo! Front Page [Lewis 2010], the assignment of control or treatment must be determined within 0.01 seconds when one user arrives. Following convention, we say that user \( t \) is assigned to the control group when \( W_t = 0 \); user \( t \) is assigned to the treatment group when \( W_t = 1 \). We adopt the convention that \( W_t \) stands for a random assignment, and that \( w_t \) stands for a realization.

Out of a total of \( T \) users, there must be half of them that are assigned to the control group, and the other half assigned to the treatment group. As commented by Pocock and Simon (1975), “it is desirable to have the treatment groups of equal size.” This half-half assignment typically reflects the ignorance of magnitudes of the control and the treatment groups, and has been widely assumed in the experimental design literature [Wu 1981; Li 1983; Rosenbaum 1989; Greevy et al. 2004; Lu et al. 2011; Abadie and Imbens 2012; Bai 2019; Basse et al. 2019; Harshaw et al. 2019; Xiong et al. 2019; Bojinov et al. 2020; Candogan et al. 2021]. In A/B testing terminology, we denote \( A \) to be the set of users in the control group, and \( B \) to be the set of users in the treatment group. The two groups must form a partition of all the users, \( A, B \subseteq \{T\}, A \cup B = \{T\}, A \cap B = \emptyset \), and each group must have half of the total users \( |A| = |B| = T/2 \). Denote \( \mathcal{M} \) to be the set of all possible partitions.

In an online stratification problem, the experimenter aims at finding a (possibly randomized) sequential assignment policy such that the total discrepancy between the users in the control group and the users in the treatment group is minimized. We define the discrepancy as follows. For any pair of users \( t \in A \) and \( t' \in B \), the discrepancy between users \( i \) and \( j \) is

\[
d_{i,j'} = \|x_i - x_{j'}\|_2.
\]

For two fixed groups of users \( A \) and \( B \), the discrepancy between \( A \) and \( B \) is the minimum weight perfect matching (Bertsimas and Tsitsiklis 1997, Chapter 7.8) between groups \( A \) and \( B \), formally defined as

\[
d_{A,B} = \min_y \sum_{t \in A} \sum_{t' \in B} d_{i,j'} y_{t,t'} \tag{1}
\]

\[
s.t. \quad \sum_{t' \in B} y_{t,t'} = 1, \forall t \in A,
\]

\[
\sum_{t \in A} y_{t,t'} = 1, \forall t' \in B,
\]

\[
y_{t,t'} \in \{0, 1\}, \forall t \in A, t' \in B,
\]

\[1\] In the original paper they refer to “control” as one version of treatment. So “two treatment groups” refers to the control and treatment groups in our paper.
where \( y_{t,t'} \) is a binary variable that takes value 1 if users \( t \) and \( t' \) are matched. For any random assignment policy, if the policy induces a distribution of the two groups of users \((A,B)\), then we define the expected discrepancy to be the expectation of \( d_{A,B} \) where randomness is coming from the distribution induced by the policy. The minimum weight perfect matching has been extensively studied in the operations research literature (Ahuja et al. 1988, Bertsimas and Tsitsiklis 1997, Schrijver 2003), and has been well recognized in the statistics literature to serve as a viable objective function for matching estimators without replacement (Rosenbaum 1989, Greevy et al. 2004, Lu et al. 2011, Dehejia and Wahba 2002, Abadie and Imbens 2012).

We analyze the online stratification problem when \( T \) is relatively large. As \( T \) is larger, the discrepancy usually gets larger as well. So we primarily focus on the dependence of the discrepancies with respect to \( T \) as the performance metric of this paper. For example, at online search engines, online retailers, and travel service providers, a typical sample size is at the scale of \( 100K \sim 1M \).

We distinguish between an online design and an offline design. We define an online design \( \mu \) to be a collection of functions, \( \mu = (\mu_1, \mu_2, ..., \mu_T) \), such that \( \mu_1(x_1) : S \rightarrow [0,1] \) for \( t = 1 \), and \( \mu_t(x_1, x_2, ..., x_t, w_1, w_2, ..., w_{t-1}) : S^t \times \{0,1\}^{t-1} \rightarrow [0,1] \) for \( t \geq 2 \). In words, an online design only takes as input the covariate information of the users arrived up to the current period, as well as the treatment assignments to the users up to the previous period. Each function \( \mu_t \) maps the information space to a treatment probability. The treatment assignment is then determined by \( \Pr(W_t = 1) = \mu_t, \) and \( \Pr(W_t = 0) = 1 - \mu_t \). In contrast to an online design, we define an offline design \( \nu \) to be a collection of functions, \( \nu = (\nu_1, \nu_2, ..., \nu_T) \), such that \( \nu_t(x_1, x_2, ..., x_T) : S^T \rightarrow [0,1] \). In words, an offline design takes as input the covariate information of all users, as if there were a clairvoyant oracle that revealed all the future information. Though our primary focus is on the online designs of experiments, the optimal offline design, which we refer to as the matched-pair design in Section 3, will serve as a benchmark for comparison.

3. The Matched-Pair Design

If there were a clairvoyant oracle that revealed all the user characteristics to the experimenter before users arrived, the experimenter could leverage all such information to design the following experiment, which is one version of the well-known matched-pair design (Rosenbaum 1989, Greevy et al. 2004, Lu et al. 2011).
Figure 2  An illustrator of the matched-pairs in a single dimension. The $A$ stands for users in the control group; whereas $B$ stands for users in the treatment group.

**Definition 1 (Matched-Pair Design).** In a matched-pair design, the experimenter first solves the following problem,

$$(A^*, B^*) = \arg \min_{(A,B) \in \mathcal{M}} d_{A,B},$$

and finds the solution $y^*$ to the minimum weight perfect matching between $A^*$ and $B^*$ as in (1). Second, recall that $y_{t,t'}^*$ is a binary variable that takes value 1 if users $t$ and $t'$ are matched. For each pair of users $t, t' \in [T]$ such that $y_{t,t'}^* = 1$, randomly administer control to one user and treatment to the other, with probability $1/2$ each.

By definition, the above matched-pair design has the smallest discrepancy among any possible offline designs. As an online design is contained in the offline design family, the matched-pair design also serves as a benchmark for the online designs, i.e., no online design can achieve a smaller discrepancy than the matched-pair design.

To solve (2) and find the matched-pair design, we distinguish two cases in the covariate space: the single-dimensional case, $p = 1$, and the multi-dimensional case, $p \geq 2$. When $p = 1$, it is easy to see that the matched-pair design has a discrepancy of no more than 1. The matched-pair design easily solves (2) and proceeds in the following way: first, rearrange all users from the smallest to the largest in the covariate space and group them in size-two pairs; second, for the two users in each pair, randomly administer control to one user and treatment to the other, with probability $1/2$ each. This design has a provable guarantee as stated in Theorem 1. See Figure 2 for an illustration.

**Theorem 1.** When $p = 1$, the matched-pair design has a discrepancy less than or equal to 1.

The proof of Theorem 1 is essentially following the rearrangement argument that we made above. The complete proof is deferred to Section B in the Appendix.

While the discrepancy of a matched-pair design is very small in the single-dimensional case, it is not the same in the multi-dimensional case. When $p \geq 2$, there does not exist such a small-to-large ordering in the covariate space so the procedure in the single-dimensional case does not work when
it comes to multiple dimensions. In fact, there is an intrinsic difference between the single and multi-dimensional cases. In the multi-dimensional case, the discrepancy will usually increase as the total number of users increases, which is different from the result we see in Theorem 1. Moreover, even finding an optimal solution to (2) will be computationally more challenging.

Since the single and multi-dimensional cases are different, we first focus on the single-dimensional case in this section as well as in Sections 4 and 5. We will discuss the multi-dimensional case in Section 6 after we build enough intuition.

4. The Completely Randomized Design

In Section 3 we have learned that the matched-pair design achieves the smallest discrepancy, by using the knowledge of all users’ covariates. In the online stratification problem, however, this is not feasible. Nonetheless, there is another well-known design of experiments, the completely randomized design, that is feasible for the online setting.

**Definition 2 (Completely Randomized Design).** Out of a total of $T$ users, a completely randomized design randomly selects $T/2$ users as the control group $A$, and the other $T/2$ users as the treatment group $B$. Upon the arrival of a user $t$, administer control if $t \in A$, and treatment if $t \in B$, regardless of user $t$’s covariate information.

Since a completely randomized design does not use any covariate information in administering control and treatment assignments, it is a feasible online design. As expected, it has a larger discrepancy compared to the matched-pair design. We illustrate using the following example.

**Example 1.** Let there be 4 users, with single-dimensional covariates $x_1 = 0.1, x_2 = 0.7, x_3 = 0.4, x_4 = 0.9$.

Under a matched-pair design, we rearrange the four users from the smallest to the largest in the covariate space, $x_1 \leq x_3 \leq x_2 \leq x_4$. Then we match users $\{1, 3\}$ in one pair and $\{2, 4\}$ in one pair. Within each pair, we randomly administer control and treatment. The above matched-pair design has a discrepancy of 0.5.

Under a completely randomized experiment: with probability $1/6$, $A = \{1, 2\}, B = \{3, 4\}, d_{A,B} = 0.5$; with probability $1/6$, $A = \{1, 3\}, B = \{2, 4\}, d_{A,B} = 1.1$; with probability $1/6$, $A = \{1, 4\}, B = \{2, 3\}, d_{A,B} = 0.5$; with probability $1/6$, $A = \{2, 3\}, B = \{1, 4\}, d_{A,B} = 0.5$; with probability $1/6$, $A = \{2, 4\}, B = \{1, 3\}, d_{A,B} = 1.1$; with probability $1/6$, $A = \{3, 4\}, B = \{1, 2\}, d_{A,B} = 0.5$. So in expectation, the discrepancy is equal to 0.7, which is larger than the discrepancy from a matched-pair design.
Next, we formally show in Theorem 2 that the expected discrepancy of a completely randomized design is indeed larger than that of a matched-pair design when \( p = 1 \).

**Theorem 2.** When \( p = 1 \), the completely randomized design has an expected discrepancy in the order of \( \Theta(T^{\frac{1}{2}}) \).

We explain the main idea of the proof of Theorem 2 here in an unrigorous way, and defer the detailed proof to Section C in the Appendix.

**Sketch Proof of Theorem 2.** We first show the \( \Omega(T^{\frac{1}{2}}) \) part in the \( p = 1 \) case by constructing an instance \( x^* \) of the arrival sequence. Let the covariates of the first \( \frac{T}{2} \) users be equal to 0, i.e., \( x^*_t = 0, \forall 1 \leq t \leq \frac{T}{2} \); let the covariates of the last \( \frac{T}{2} \) users be equal to 1, i.e., \( x^*_t = 1, \forall \frac{T}{2} + 1 \leq t \leq T \). In Lemma 5, we show that in this instance \( x^* \), the completely randomized design has an expected discrepancy of \( \frac{1}{2\sqrt{\pi}} \sqrt{T} \).

Next, we turn to the \( O(T^{\frac{1}{2}}) \) part. We introduce Lemma 6 to show that the completely randomized design in the \( p = 1 \) case is invariant to permutations of the arrival sequence. For any two sequences \( x', x'' \), if there exists a one-to-one correspondence \( \sigma: [T] \rightarrow [T] \), such that \( \forall t \in [T], x'_t = x''_{\sigma(t)} \), then the expected discrepancy of the completely randomized design will be the same for these two arrival sequences \( x' \) and \( x'' \). Intuitively, this is because the completely randomized design, when determining the assignment of each user, completely randomizes the indices of the users without using any covariate information of the other users. With this permutation-invariant observation, and given that we focus on the \( p = 1 \) case, we are able to focus only on the arrival sequences that are ordered from the smallest to the largest.

Finally, to conclude the \( O(T^{\frac{1}{2}}) \) part, we introduce Lemma 7 to show that, among all possible arriving sequences, the sequence \( x^* \), with the first half users equal to zero and the second half users equal to one, is the one that has the largest expected discrepancy. This shows that the expected discrepancy of the completely randomized design is in the order of \( O(T^{\frac{1}{2}}) \). □

We emphasize here that Theorem 2 suggests an expected discrepancy exactly in the order of \( \Theta(T^{\frac{1}{2}}) \). This is both an upper bound and a lower bound. This result suggests that, while the completely randomized experiment leads to an expected discrepancy that does not increase linearly as the total number of users increases, it is still unavoidable that the expected discrepancy is of the square root order.

By comparing the matched-pair design to the completely randomized design, we make the following two observations. On one hand, the matched-pair design, though infeasible to the online
setting, fully uses all the knowledge of users’ covariates. As a result, the discrepancy is very small. On the other hand, the completely randomized design, feasible for the online setting, does not use any covariate information at all. These two observations motivate the following question: is there an adaptive design of the experiment whose performance is in between? We will provide an affirmative answer in Section 5.

5. The Pigeonhole Design

In this section we introduce the Pigeonhole Design, a new experimental design method, that adaptively administers control and treatment assignments to the online users. We will first introduce what a pigeonhole design is and how to design the pigeonholes. Then we will provide intuitions regarding why and how it improves the completely randomized design. We conclude this section by analyzing the discrepancy of the pigeonhole design.

First, we start with the intuition of the pigeonhole design. The pigeonhole design partitions the covariate space. We refer to the smaller, partitioned spaces as pigeonholes. In each pigeonhole, we wish to make the number of control and treatment users as balanced as possible, by sequentially matching the users who arrive at the same pigeonhole in pairs. The discrepancy of each pair of users will be no larger than the diameter of this pigeonhole. However, under the adversarial arrival setting, it is impossible to guarantee that the number of control and treatment users are exactly equal in each pigeonhole. A simple example is that the adversary chooses an odd number of users to arrive at each pigeonhole. As there can exist only one extra user in each pigeonhole, we have to match these extra users across different pigeonholes. This would require some extra balancing efforts in the last few periods, which we refer to as the balancing periods.

Now we are ready to formally describe the pigeonhole design. Let the covariate space be $S$. Define a $K$-partition of $S$ to be $\mathcal{P}(S) = \{S_1, S_2, \ldots, S_K\}$, such that $\bigcup_{k=1}^K S_k = S$ and that $S_k \cap S_{k'} = \emptyset, \forall k, k' \in [K]$. These sets $\{S_k\}_{k \in [K]}$ are referred to as the pigeonholes. Since a pigeonhole design adaptively administers control and treatment assignments, we use the following notations, $n_{k,0}^0$ and $n_{k,1}^1$, to denote the number of control and treatment users in the $k$-th pigeonhole after the arrival of user $t$. Denote $n_{k,0}^0 = n_{k,1}^1 = 0, \forall k \in [K]$, to reflect that no users have arrived yet at the beginning of the entire horizon. Let a balancing parameter be $\beta \in [0, 1]$, and we refer to the last $\lceil \beta T \rceil$ periods as the balancing periods. For any partition $\mathcal{P}(S)$ and any balancing parameter $\beta$, define the pigeonhole design as follows.
Definition 3 (Pigeonhole Design). A pigeonhole design takes as input a partition of the covariate space \( P(S) \) and a balancing parameter \( \beta \).

Upon the arrival of user \( t \), if user \( t \) is among the first \( T - \lceil \beta T \rceil \) users, i.e., \( t \leq T - \beta T \), find the associated pigeonhole \( k \) such that \( x_t \in S_k \). If there are fewer control users in this pigeonhole than treatment users, i.e., \( n_{k,t-1}^0 < n_{k,t-1}^1 \), administer control to user \( t \); if there are fewer treatment users than control users, i.e., \( n_{k,t-1}^0 > n_{k,t-1}^1 \), administer treatment to user \( t \); if there are equal numbers of control and treatment users, i.e., \( n_{k,t-1}^0 = n_{k,t-1}^1 \), administer control or treatment with probability 1/2 each.

If user \( t \) is among the last \( \lceil \beta T \rceil \) users, i.e., \( t > T - \beta T \), ignore the covariate information of user \( t \) and purely balance the control and treatment users. If the absolute difference between the total number of control and treatment users is smaller than the remaining periods, i.e., \( |\sum_{k \in K} (n_{k,t-1}^0 - n_{k,t-1}^1)| < T - t + 1 \), then administer control or treatment with probability 1/2 each; otherwise, administer control or treatment that reduces the absolute difference.

Example 2 shows how a pigeonhole design sequentially administers control and treatment assignments.

Example 2 (Example 1 Continued). Let there be 4 users, \( x_1 = 0.1, x_2 = 0.7, x_3 = 0.4, x_4 = 0.9 \). In a pigeonhole design, suppose we choose the pigeonholes to be \( S_1 = [0, 0.5), S_2 = [0.5, 1] \), and the balancing parameter to be \( \beta = 1/4 \).

This pigeonhole design works as follows. In the first three periods, we sequentially match users in pairs. When \( x_1 = 0.1 \in S_1 \) arrives, there is no user in \( S_1 \). So we randomly administer control or treatment. Suppose \( w_1 = 1 \), then we administer treatment. When \( x_2 = 0.7 \in S_2 \) arrives, there is no user in \( S_2 \). So we randomly administer control or treatment. Suppose \( w_2 = 0 \), then we administer control. When \( x_3 = 0.4 \) arrives, there is one more user in the treatment group (1 in treatment, 0 in control) in \( S_1 \). So \( w_3 = 0 \) means we administer control. The last period belongs to the balancing period. Note that, in total, there are more users in the control group than in the treatment group (1 in treatment, 2 in control). So \( w_4 = 1 \) means we administer treatment to the last user.

Under this trajectory of randomness, this pigeonhole design turns out to have a small discrepancy equal to 0.5.

The performance of a pigeonhole design critically depends on how the pigeonhole is devised, in the following two aspects. First, since the arrival sequence is adversarially chosen, the pigeonholes
should be uniformly split. Otherwise, the adversary could control the arrival sequence to all go into the largest pigeonhole, thus increasing the discrepancy of the design. Second, the number of pigeonholes should be neither too small nor too big. If there is only one single pigeonhole that is the entire covariate space, i.e., $K = 1$ and $S_1 = S$, then this is the biased coin design with parameter equal to 1 as proposed in [Efron 1971]. However, when there is only one pigeonhole, the pigeonhole design does not consider covariate information at all, so it will lead to a large discrepancy. On the other hand, when there are too many pigeonholes, the adversary can make every pigeonhole have an odd number of users. So each pigeonhole will have one unpaired user. These unpaired users will have to be paired across different pigeonholes, thus causing a large discrepancy.

In order to choose the correct number of pigeonholes, we first illustrate by the following very simple design in the $p = 1$ single-dimensional case that achieves $O(T^{\frac{1}{2}})$ expected discrepancy. In this design, we equally divide the covariate space $[0, 1]$ into $T^{\frac{1}{2}}$ pigeonholes with the length of each pigeonhole being $T^{-\frac{1}{2}}$. Consider the first $T - T^{\frac{1}{2}}$ arriving users. For every two users that arrive at the same pigeonhole, we match them in pairs. For each pair of users matched in each pigeonhole, the discrepancy is no more than the length of the pigeonhole $T^{-\frac{1}{2}}$. Therefore, the total discrepancy for the first $(T - T^{\frac{1}{2}})$ users that are matched in this way is no more than $T^{-\frac{1}{2}}(T - T^{\frac{1}{2}}) = T^{\frac{1}{2}} - 1$. However, among the first $(T - T^{\frac{1}{2}})$ users, there are at most $T^{\frac{1}{2}}$ of them that remain unpaired. This is because there are $T^{\frac{1}{2}}$ pigeonholes and there is at most one user in each pigeonhole that remains unpaired. Next, observe that there are $T^{\frac{1}{2}}$ users to arrive in the balancing periods. No matter what their covariates are, we match them in pairs with the $T^{\frac{1}{2}}$ unpaired users, each pair generating at most 1 discrepancy. The total discrepancy generated during such balancing periods is at most $T^{\frac{1}{2}}$. Therefore, the total discrepancy is at most

$$T^{\frac{1}{2}} - 1 + T^{\frac{1}{2}} = 2T^{\frac{1}{2}} - 1.$$  

By the pigeonhole design outlined above, we can achieve a $\Theta(\sqrt{T})$ discrepancy. Can we improve the above pigeonhole design to achieve some smaller discrepancy? The answer is affirmative. Before diving into details, we introduce what to improve in the above pigeonhole design.

Observe that after first $T - T^{\frac{1}{2}}$ arriving users, there will be at most $T^{\frac{1}{2}}$ users that remain unpaired, one from each pigeonhole. If we take a closer look at these users, we actually randomly assign them into either the control or the treatment group with half probability each. Therefore, there exist certain probabilities that two adjacent users are assigned to different groups, and we can match them in a pair.
Algorithm 1 The Pigeonhole Design when \( p = 1 \)

1: **Initialize:** \( \eta \leftarrow -\frac{2}{3}, \beta \leftarrow T^{\frac{1}{2}-1} \). \( P(S) \leftarrow \{ [0,T^{-\eta}), [T^{-\eta}, 2T^{-\eta}), \ldots, [1-T^{-\eta}, 1] \} \).

2: **for** \( t = 1, 2, \ldots, T - \lfloor \beta T \rfloor \)** do

3: **if** One of the control or treatment group has \( \frac{T}{2} \) units **then**

4: Assign \( x_t \) to the other group.

5: **else**

6: Observe \( x_t \) and find \( I_k \in P(S) \) such that \( x_t \in I_k \).

7: **if** There is even number of units in \( I_k \) **then**

8: Assign \( x_t \) to control or treatment group with half probability each.

9: **else**

10: Assign \( x_t \) to the group which has less units in interval \( I_k \).

11: **end if**

12: **end if**

13: **end for**

14: **for** \( t = T - \lfloor \beta T \rfloor + 1, \ldots, T \)** do

15: **if** One of the control or treatment group has \( \frac{T}{2} \) units **then**

16: Assign \( x_t \) to the other group.

17: **else**

18: Assign \( x_t \) to control or treatment group with half probability each.

19: **end if**

20: **end for**

In Theorem 3 and the discussions below, we describe in detail how to leverage the randomness in the assignment of users to suggest a better pigeonhole design.

**Theorem 3.** Fix any \( \eta \in (0, 1) \). When \( p = 1 \), the pigeonhole design using a uniform pigeonhole \( P(S) = \{ [0,T^{-\eta}), [T^{-\eta}, 2T^{-\eta}), \ldots, [1-T^{-\eta}, 1] \} \) combined with a balancing parameter \( \beta = T^{\frac{1}{2}-1} \) has an expected discrepancy in the order of \( O \left( T^{1-\eta} + T^{\frac{1}{2}} (\log T)^{\frac{1}{2}} \right) \).

**Corollary 1.** When \( \eta = \frac{2}{3} \), the pigeonhole design using a uniform pigeonhole and an associated balancing parameter has an expected discrepancy in the order of \( O \left( T^{\frac{1}{2}} (\log T)^{\frac{1}{2}} \right) \).
To make it precise, the pigeonhole design as in Theorem 3 can be described using Algorithm 1. We explain the main idea of the proof of Theorem 3 here in an unrigorous way, and defer the detailed proof to Section D in the Appendix.

**Sketch Proof of Theorem 3.** Now that we have built the intuition that uniform pigeonholes are preferable in hedging against adversarial arrival sequences, the most important decision is how many pigeonholes we should split. Suppose the length of each pigeonhole is $T^{-\eta}$; then the number of pigeonholes is $T^{\eta}$. We analyze the discrepancy generated from using $T^{\eta}$ many pigeonholes, by considering the following two perspectives.

On one hand, consider the first $(1 - \beta)T$ arriving users. We match every pair of users that arrive at the same pigeonhole. If the adversary makes an even number of users arrive at each pigeonhole and there are no unpaired users, the discrepancy of the first $(1 - \beta)T$ arriving users is at least $T^{-\eta}(1 - \beta)T$, which is in the order of $O(T^{1-\eta})$. This shows that the length of each pigeonhole should be as small as possible to reduce the discrepancy generated from the first phase.

On the other hand, however, the adversary could make an odd number of users arrive at each pigeonhole, leaving a total number of $T^{\eta}$ unpaired users. If all such unpaired users are in one group, they will result in large imbalance between the two groups. In order not to leave such unpaired users all in one group, we use randomization to balance the users. Due to concentration of probability, with high probability the difference between the two groups of users will be upper bounded by $2T^{\frac{\eta}{2}}(\log T)^{\frac{1}{2}}$. Using a coupling technique, we show that these many unmatched users will create discrepancy in the order of $O(T^{\frac{\eta}{2}}(\log T)^{\frac{1}{2}})$. Therefore, the number of pigeonholes should be small, which is equivalent to saying that the length of each pigeonhole should be large.

The above two perspectives suggest a trade-off between having small and large pigeonholes, and we balance these two aspects by selecting $\eta = \frac{2}{3}$, which leads to $O(T^{\frac{1}{2}}(\log T)^{\frac{1}{2}})$ discrepancy. □

Theorem 3 and Corollary 1 suggest that, through properly splitting the pigeonholes, the pigeonhole design can achieve an expected discrepancy in the order of $O(T^{1-\eta})$. This is a reduction from the $\Theta(T^{1/2})$ expected discrepancy obtained by the completely randomized design.

6. **Analyzing Different Designs in the Multi-Dimensional Case**

So far we have seen that, in the single-dimensional case, the pigeonhole design has a smaller discrepancy than the completely randomized design. Yet the pigeonhole design still has a larger discrepancy than the matched-pair design, which has a small, negligible discrepancy.

In this section, we will analyze the discrepancies of the three aforementioned designs in the multi-dimensional case. Note that Definitions 1–3 of the three designs are general. Our definitions
of three designs all hold in the multi-dimensional case. It is their theoretical performances and the associated analyses that will be different in the multi-dimensional case.

In the multi-dimensional case, the discrepancies generated from the three designs are much different from the single-dimensional case. As shown in Theorem 4, even the matched-pair design has a non-negligible discrepancy in the order of $\Theta(T^{\frac{n-1}{p}})$. As shown in Theorem 5, the completely randomized design has an expected discrepancy in the order of $\Omega(T^{\frac{n-1}{p}})$, as it cannot perform better than the matched-pair design. Surprisingly, as shown in Theorem 6, the pigeonhole design achieves an expected discrepancy in the order of $O(T^{\frac{n-1}{p}}(\log T)^{\frac{3}{2}})$ when $p = 2$; and in the order of $O(T^{\frac{n-1}{p}})$ when $p \geq 3$. The performance of the pigeonhole design closely matches that of the matched-pair design.

6.1. The Matched-Pair Design in the Multi-Dimensional Case

Unlike in the single-dimensional case, where the minimum weight perfect matching can be easily found by matching the closest users in pairs, the matched-pair design in the multi-dimensional case needs to solve problem (2). In fact, in the multi-dimensional case, not only is the matched-pair design more challenging to find, but the discrepancy of the design is also much larger. We first describe Theorem 4.2 in Bai et al. (2021), which suggests an upper bound on the discrepancy of the matched-pair design,

**Lemma 1 (Theorem 4.2, (Bai et al. 2021)).** When $p \geq 2$, the matched-pair design has a discrepancy in the order of $O(T^{\frac{n-1}{p}})$.

Next, we introduce Theorem 4 below to for a lower bound on the discrepancy, which illustrates the hardness of matched-pair designs in the multi-dimensional case.

**Theorem 4.** When $p \geq 2$, the matched-pair design has a discrepancy in the order of $\Theta(T^{\frac{n-1}{p}})$.

We explain the main idea of the proof of Theorem 4 here in an unrigorous way, and defer the detailed proof to Section E in the Appendix.

**Sketch proof of Theorem 4.** We essentially prove the $\Omega(T^{\frac{n-1}{p}})$ part. We construct an arrival sequence such that the discrepancy on this sequence is $\Omega(T^{\frac{n-1}{p}})$. First, evenly split the covariate space $[0,1]^p$ into $T$ smaller hypercubes, such that each hypercube has edge length $T^{-\frac{1}{p}}$. Then, let the covariate of each user be at the center of each smaller hypercube, respectively. In this sequence, the distance between the covariates of any two users is at least $T^{-\frac{1}{p}}$. There is a total of $T/2$ pairs of users. Therefore, the discrepancy is at least $T^{-\frac{1}{p}} \cdot T = T^{\frac{n-1}{p}}$. Combining with Lemma 1 we finish the proof.  □
This discrepancy increases with respect to $T$, and increases as the dimension $p$ increases. This coincides with the intuition from the statistics literature, that the dimension of the covariate information “plays an important role in the properties of matching estimators” \cite{abadie_targeted_2006}. Theorem \ref{thm:multi_dim} suggests that the discrepancy in the multi-dimensional case is intrinsically different from, and larger than, in the single-dimensional case.

### 6.2. The Completely Randomized Design in the Multi-Dimensional Case

In the multi-dimensional case, the performance of the completely randomized design is challenging to analyze. We only know that the expected discrepancy of the completely randomized design is at least in the order of $\Omega \left( T^{\frac{p-1}{p}} \right)$, as it cannot be smaller than that of the matched-pair design.

We introduce the following Theorem \ref{thm:completely_randomized} but the proof is simply omitted.

**Theorem 5.** When $p \geq 2$, the completely randomized design has an expected discrepancy in the order of $\Omega \left( T^{\frac{p-1}{p}} \right)$.

Even though we are unable to clearly derive the upper bound of the expected discrepancy for the completely randomized design, we can still calculate the expected discrepancy under a special family of arrival sequences. This result will be helpful in analyzing the expected discrepancy of the pigeonhole design.

We construct the family of arrival sequences as follows. First, we split the $p$-dimensional unit hypercube into $T$ smaller hypercubes, each with edge-length $T^{-\frac{1}{p}}$. With all the smaller hypercubes given, let there be exactly one user in each smaller hypercube. Mathematically, the family of arrival sequences can be defined as follows. First, for any set $X$, denote $X^p$ to be the $p$-ary Cartesian power of $X$, i.e., $X^p = X \times X \times \cdots \times X = \{(x_1, \ldots, x_p) \mid x_i \in X \text{ for every } i \in \{1, \ldots, p\} \}$. Then, the family of arrival sequences is defined to be

$$X^{(T)} = \left\{ (x_1, x_2, \ldots, x_T) \mid \forall X \in \left\{ [0, T^{-\frac{1}{p}}), [T^{-\frac{1}{p}}, 2T^{-\frac{1}{p}}), \ldots, [1 - T^{-\frac{1}{p}}, 1] \right\}^p, \exists t, \text{s.t. } x_t \in X, \text{ and } \forall t' \neq t, x_{t'} \notin X \right\}.$$

Under such a family of arrival sequences, the expected discrepancy of the completely randomized design can be upper bounded.

**Lemma 2.** For any $x \in X$, the expected discrepancy of the completely randomized design under arrival sequence $x$ is:

- in the order of $O \left( T^{-\frac{p-1}{p}} \log T \right)$ when $p = 2$;
• in the order of $O\left(\frac{T^{p-1}}{p}\right)$ when $p \geq 3$.

The proof of Lemma 2 is by induction, and is deferred to Section F in the Appendix. Again, note that Lemma 2 is only for a special family of arrival sequences, but not for all the arrival sequences. An upper bound for any arrival sequences still remains unclear.

6.3. The Pigeonhole Design in the Multi-Dimensional Case

In the multi-dimensional case, the performance of the pigeonhole design closely matches that of the matched-pair design. When $p = 2$, the gap is up to logarithmic factors; when $p \geq 3$, there is no gap in the order.

Recall that for any set $X$, $X^p$ is the $p$-ary Cartesian power of $X$.

**Theorem 6.** Fix any $\phi \in (0, 1)$, and any $c > 1$. The pigeonhole design using a uniform pigeonhole $P(S) = \left\{[0, c^\frac{1}{p} T^{-\phi}), [c^\frac{1}{p} T^{-\phi}, 2c^\frac{1}{p} T^{-\phi}), \ldots, [1 - c^\frac{1}{p} T^{-\phi}, 1]\right\}^p$ combined with a balancing parameter $\beta = T^{\frac{p\phi}{2} - 1}$ has an expected discrepancy:

- in the order of $O\left(\frac{T^{1-\phi}}{p} + T^{(p-1)\phi} (\log T)^{\frac{3}{2}} + T^{\frac{p\phi}{2}} (\log T)^{\frac{1}{2}}\right)$ when $p = 2$;
- in the order of $O\left(\frac{T^{1-\phi}}{p} + T^{(p-1)\phi} + T^{\frac{p\phi}{2}} (\log T)^{\frac{1}{2}}\right)$ when $p \geq 3$.

**Corollary 2.** When $\phi = \frac{1}{p}$, the pigeonhole design using a uniform pigeonhole and an associated balancing parameter has an expected discrepancy:

- in the order of $O\left(\frac{T^{p-1}}{p} (\log T)^{\frac{3}{2}}\right)$ when $p = 2$;
- in the order of $O\left(\frac{T^{p-1}}{p}\right)$ when $p \geq 3$.

To make it precise, the pigeonhole design as in Theorem 6 can be described using Algorithm 2. We explain the main idea of the proof of Theorem 6 here in an unrigorous way, and defer the detailed proof to Section G in the Appendix.

**Sketch proof of Theorem 6.** We consider the following three perspectives. First, consider the first $T - \beta T$ arriving users. We match every pair of users that arrive at the same pigeonhole, with at most one user unmatched from each pigeonhole. For the matched users, we show that the discrepancy is in the order of $O(T^{1-\phi})$.

Second, there are $T^{p\phi}$ many unmatched users. For all the unmatched users, they are randomly assigned to either the control or the treatment group. If there are exactly the same number of users that are assigned into the control group as into the treatment group, we use a coupling technique to show that these $T^{p\phi}$ many unmatched users will have an expected discrepancy in the order of $\tilde{O}(T^{(p-1)\phi})$. 
Algorithm 2 The Pigeonhole Design when $p \geq 2$

1: Input: $c > 1$.

2: Initialize: $\phi \leftarrow \frac{1}{p}$, $\beta = T^{\frac{\phi}{2} - 1}$. $P(S) = \left\{ [0, c^\frac{1}{p} T^{-\phi}), [c^\frac{1}{p} T^{-\phi}, 2c^\frac{1}{p} T^{-\phi}), \ldots, [1 - c^\frac{1}{p} T^{-\phi}, 1] \right\}^p$.

3: for $t = 1, 2, \ldots, T - \lceil \beta T \rceil$ do

4: if One of the control or treatment group has $\frac{T}{2}$ units then
5: Assign $x_t$ to the other group.
6: else
7: Observe $x_t$ and find the unique $X_k \in P(S)$ such that $x_t \in X_k$.
8: if There is even number of units in $X_k$ then
9: Assign $x_t$ to control or treatment group with half probability each.
10: else
11: Assign $x_t$ to the group that has less units in $X_k$.
12: end if
13: end if
14: end for

15: for $t = T - \lceil \beta T \rceil + 1, \ldots, T$ do
16: if One of the control or treatment group has $\frac{T}{2}$ units then
17: Assign $x_t$ to the other group.
18: else
19: Assign $x_t$ to control or treatment group with half probability each.
20: end if
21: end for

Third, there might not be exactly the same number of users that are assigned into the control group as into the treatment group. But due to concentration of probability, with high probability the difference between the two groups of users will be upper bounded by $2T^{\frac{\phi}{2}} (\log T)^{\frac{1}{2}}$. Together with the last $\beta T$ users, they have a discrepancy that can be upper bounded by $\tilde{O} \left( T^{\frac{\phi}{2}} \right)$.

The above three perspectives suggest a trade-off between having small and large pigeonholes, and we strike a balance by selecting $\phi = \frac{1}{p}$, which leads to $\tilde{O} \left( T^{\frac{p-1}{p}} \right)$ discrepancy. □

It is worth noting that, with low probability, the following event happens before period $T - \beta T$: that one of the control or treatment group reaches $T/2$ in size, and the algorithm starts to assign all the other users into the opposite group. See steps 4 and 5 in Algorithm 2. When this happens,
the difference between the two groups of users is $\beta T = \sqrt{T} = T^{\frac{\phi}{2}}$ when $\phi = \frac{1}{p}$. So this happens with probability $O(\frac{1}{T})$. When it happens, the discrepancy can be upper bounded by $\frac{T}{2}\sqrt{p}$. Therefore, the contribution to the expectation of discrepancy conditional on this low-probability event is $O(1)$, which does not increase the order of the discrepancy. The details of discrepancy analysis given on low probability can also be found in appendix C.

7. Simulation Study

In Sections 3–6, we have analyzed the performance of the matched-pair design, the completely randomized design, and the pigeonhole design. We have shown theoretically that the pigeonhole design outperforms the completely randomized design. In this section, we run simulations to show numerically that the pigeonhole design outperforms the completely randomized design as a benchmark. We show the simulation results under $p = 1$ and $p \geq 2$ separately.

7.1. Simulation Results in the Single-Dimensional Case

7.1.1. Simulation Setup. In the single-dimensional case, we consider three setups. The first setup is when the arrival sequence consists of $T/2$ many zeros and $T/2$ many ones. We generate one instance of the arrival sequence by randomly permuting $T/2$ many zeros and ones, such that it is not necessary that all zeros arrive before all ones.

The second setup is when the arrival sequence is deterministically generated according to $x_t = (t - 1)/(T - 1), \forall t \in [T]$. All the user covariates are equally located along the single-dimensional unit interval.

The third setup is when the arrival sequence is randomly generated. All the user covariates are independently and identically generated from a uniform distribution, i.e., $x_t \sim U[0, 1], \forall t \in [T]$. We generate one instance of the arrival sequence from the uniform distribution.

In all the three setups, we find the expected discrepancy of the completely randomized design and the pigeonhole design by repeating each of them 1000 times. Note that, even though the pigeonhole parameters as suggested by Algorithm 1 are designed for the adversarial arrival sequence, they still perform well for the arrival sequences described in the above three setups. As we will show in the subsequent section, the pigeonhole design parameterized in this way still significantly outperforms the completely randomized design in all three setups.

7.1.2. Simulation Results. The simulation results in the three setups described in Section 7.1.1 are given in Figures 3–5. In these figures, the solid black curve stands for the discrepancy of the matched-pair design; the solid red curve stands for the expected discrepancy of the completely randomized design; and the solid blue curve stands for the discrepancy of the pigeonhole design.
randomized design; the solid green curve stands for the expected discrepancy of the pigeonhole design as described in Algorithm 1 using a balancing parameter; the dashed green curve stands for the expected discrepancy of the pigeonhole design without a balancing parameter, i.e., $\beta = 0$ (this is a valid pigeonhole design as lines 3–4 in Algorithm 1 ensure feasibility).

We first focus on Figure 3, the simulation results in the first setup. The discrepancy of the matched-pair design is always 0. This is because the matched-pair design can always match every two zeros in pairs, and every two ones in pairs. The expected discrepancy of the completely randomized design increases with respect to $T$, which is consistent with the results in Theorem 2. In particular, as suggested by Lemma 5, this first setup is the worst-case arrival sequence for the completely randomized design. So the expected discrepancy in Figure 3 is larger than the expected discrepancy in Figures 4 and 5. The expected discrepancies of the pigeonhole designs are much smaller than the completely randomized design. The performance of the pigeonhole design without using a balancing parameter even outperforms that using a balancing parameter, and has almost zero expected discrepancy.

Next, we focus on Figure 4, the simulation results in the second setup. The discrepancy of the matched-pair design is always close to a constant 0.5. This is because the matched-pair design always matches two adjacent users into one pair, and there are $T/2$ many such pairs, each with a length of $1/(T - 1)$. The expected discrepancy of the completely randomized design increases...
Figure 4  (Expected) discrepancy in the single-dimensional case, when the arrival sequence is equally located along the unit interval.

with respect to $T$, which is consistent with the results in Theorem 2. Similar to the first setup, the expected discrepancies of the pigeonhole designs are much smaller than the completely randomized design. But the performance of the pigeonhole design fluctuates as $T$ increases. This is because the parity (odd or even) of the number of users that fall into the same pigeonhole changes due to rounding. When odd, it generates cross-pigeonhole discrepancies. Note also that although the arrival sequence in this setup is not the worst case for the pigeonhole design (because of the randomness of pigeonhole design, it is hard to exactly find one worst case), this arrival sequence does make the expected discrepancy of the pigeonhole design larger than in the first setup. This is because the pigeonhole design performs much better if there are many users whose covariates are close to each other and belong to the same pigeonhole.

Finally, we focus on Figure 5 the simulation results in the third setup. The discrepancy of the matched-pair design does not increase as $T$ increases, and is close to a constant 0.5. Since a uniformly random arrival sequence (as in the third setup) is similar to a sequence that is deterministically equally located (as in the second setup), the performance of the matched-pair design in the third setup is similar to the performance in the second setup, especially when $T$ is large. The expected discrepancy of the completely randomized design increases with respect to $T$, which is consistent with the results in Theorem 2. For similar reasons, the performance of the completely
randomized design in the third setup is similar to the performance in the second setup. Moving on to the pigeonhole design, the expected discrepancies of the pigeonhole designs are much smaller than in the completely randomized design. But unlike in the second setup, the expected discrepancy smoothly increases with respect to $T$. This is because the sequence is random, so the parity (odd or even) of the number of users that fall into the same pigeonhole is less affected by rounding issues.

7.2. Simulation Results in the Multi-Dimensional Case

7.2.1. Simulation Setup. In the multi-dimensional case, we consider only one setup when the arrival sequence is randomly generated. All the user covariates are uniformly, independently and identically generated from the unit hypercube, i.e., $x_t \sim U[0,1]^p, \forall t \in [T]$. We generate one instance of the arrival sequence from the uniform distribution. We run multiple simulations under different values of $p \in \{2, 5, 20\}$ to test the performance when the dimension increases.

Similar to Section 7.1, we find the expected discrepancy of the completely randomized design and the pigeonhole design by repeating each of them 1000 times. Note that, even though the pigeonhole parameters as suggested by Algorithm 2 are designed for the adversarial arrival sequence, they still perform well when the arrival sequence is randomly generated. As we will show in the subsequent section, the pigeonhole design parameterized in this way still outperforms the completely randomized design. However, the performance gaps become smaller as the dimension $p$ increases.
7.2.2. Simulation Results. The simulation results under different dimensions are given in Figures 6–8. In these figures, the solid black curve stands for the discrepancy of the matched-pair design; the solid red curve stands for the expected discrepancy of the completely randomized design; the solid green curve stands for the expected discrepancy of the pigeonhole design as described in Algorithm 2, using a balancing parameter; the dashed green curve stands for the expected discrepancy of the pigeonhole design without a balancing parameter, i.e., $\beta = 0$.

In the multi-dimensional case, in order to find the minimum weight perfect matching for the matched-pair design, we solve problem (2) in Gurobi 9.1. by implementing the formulation below. This formulation has been discussed by Derigs (1988), where the author proposed shortest path based heuristics to solve the problem. For any two distinct indices $t < t' \in [T]$, let $y_{t,t'}$ be a binary decision variable that takes value 1 if users $t$ and $t'$ are matched. There are a total of $\frac{T(T-1)}{2}$ many decision variables. Recall that $d_{t,t'} = \|x_t - x_{t'}\|_2$ is the discrepancy between users $t$ and $t'$. Then we solve

$$\min \sum_{t=1}^{T-1} \sum_{t'=t+1}^{T} d_{t,t'} y_{t,t'}$$

s.t. $\sum_{t' < t} y_{t',t} + \sum_{t' > t} y_{t,t'} = 1, \forall t \in [T]$, $y_{t,t'} \in \{0, 1\}, \forall t < t' \in [T]$. 

![Figure 6](image.png)

(Expected) discrepancy in the multi-dimensional case $p = 2$, when the arrival sequence is uniformly and randomly generated.
Figure 7  (Expected) discrepancy in the multi-dimensional case $p = 5$, when the arrival sequence is uniformly and randomly generated.

Figure 8  (Expected) discrepancy in the multi-dimensional case $p = 20$, when the arrival sequence is uniformly and randomly generated.

The completely randomized design and the pigeonhole design can be evaluated easily using the formulation in [1].
From Figures 6 - 8, we see that the matched-pair design, the completely randomized design, and the two pigeonhole designs all increase as $T$ increases. The pigeonhole designs outperform the completely randomized design. It seems that the performance of the matched-pair design and the pigeonhole designs increase in the same order, which is consistent with Theorems 4 and 6.

By comparing across Figures 6 - 8, we see that as $p$ increases, the performance gaps decrease. When $p = 20$, the gap between the completely randomized design and the pigeonhole design becomes negligible. This suggests that matching in the dimension is challenging. However, in cases when there are many binary covariates, the discrepancy is significantly reduced, and the pigeonhole design significantly outperforms the completely randomized design when there are many such binary covariates. We will discuss this issue in Section 8.1.

8. Practical Suggestions, Limitations, and Future Research Directions

In this paper, we have considered the problem of designing online experiments, when experimental units with heterogeneous covariate information arrive sequentially and must be immediately assigned into either the control or the treatment group, with an objective of minimizing the total discrepancy. To solve this problem, we have proposed the use of the pigeonhole design. In a pigeonhole design, we first partition the covariate space into smaller spaces, and then balance the number of control and treatment units when they arrive at the same pigeonhole. In both single-dimensional and multi-dimensional cases, we have shown strong theoretical performance of the pigeonhole design, compared to the completely randomized design as a benchmark. In the multi-dimensional case, the theoretical performance of the pigeonhole design even closely matches that of the match-pair design. We have run simulation results to demonstrate the strength of the pigeonhole design. Below we conclude by providing practical suggestions for using a pigeonhole design, and by pointing out three limitations of our paper that suggest further research directions.

8.1. Practical Suggestions

When a firm decides to use a pigeonhole design, they have to make multiple decisions to ensure that the results are reliable. First, the firm must determine the possible user covariates using substantive domain knowledge, which adequately captures the impact on the objective of evaluation; see Kohavi et al. (2020) for a discussion of metric definition strategies.

Second, after the covariates are determined, the firm must use in-depth knowledge of the covariate information to describe the covariates as binary, categorical, or continuous. Categorical covariates can be represented using multiple binary covariates when the number of categories is small; can be
treated as continuous covariates when the categories are granular enough. For the binary covariates, the pigeonhole design partitions the pigeonholes differently on these dimensions. Suppose among the $p$ dimensions, there are $q < p$ dimensions whose covariates are binary. Then, on the binary dimensions, we partition the covariate space to be $[0, \frac{1}{2}] \cup (\frac{1}{2}, 1]$. Recall that $c > 1$. For the remaining $(p - q)$ dimensions, we uniformly partition the covariate space into smaller (hyper)cubes with edge length $(c \cdot 2^n)^{\frac{1}{p-q}} T^{\frac{1}{p-q}}$. Under such a partition, the expected discrepancy of the pigeonhole design is $T^{p-2q-1}$, which corresponds to the results in Theorem 6 when $(p - q)$ is the number of continuous covariates. In other words, the existence of a number of binary covariates does not hurt the performance of the pigeonhole design. We recommend that whenever possible, the firm distinguishes binary covariates and continuous covariates.

8.2. Limitations and Future Research Directions

We point out three limitations of our paper. First, we make the control group and treatment group to have the same number of users. Although this is a widely adopted assumption to make, especially in the literature of matching without replacement, this is not desirable in many applications when treatment assignments are costly. It would require a new objective function, e.g., minimizing the total discrepancy plus variance (Bertsimas et al. 2015), or some more modeling assumptions on the user covariate information (Bhat et al. 2020). We defer this to future research.

Second, it remains unknown if the balancing parameter $\beta$ is necessary in the pigeonhole design. In the numerical simulations, we find that even if we delete line 15–20 in Algorithm 2 and change line 3 to run a for loop from $t = 1$ to $T$, the discrepancy is also in the same order, and in many cases even slightly improving the performance when there is a balancing parameter. In other words, if we do not leverage the balancing periods but instead balance the experiment whenever the control or the treatment group reaches a size of $T/2$, the pigeonhole design still achieves a comparable performance. Therefore, whether a balancing parameter is necessary remains to be answered.

Third, this paper considers the user covariates to be adversarially chosen. It remains unknown if there will be better designs of experiments when user covariates are drawn from a known random distribution that can be estimated from historical data. The associated pigeonholes would be different under such an user arrival model.

References

Abadie A, Imbens GW (2006) Large sample properties of matching estimators for average treatment effects. *Econometrica* 74(1):235–267.
Abadie A, Imbens GW (2012) A martingale representation for matching estimators. *Journal of the American Statistical Association* 107(498):833–843.

Ahuja RK, Magnanti TL, Orlin JB (1988) Network flows.

Alaei S, Hajiaghayi M, Liaghat V (2012) Online prophet-inequality matching with applications to ad allocation. *Proceedings of the 13th ACM Conference on Electronic Commerce*, 18–35.

Alweiss R, Liu YP, Sawhney M (2021) Discrepancy minimization via a self-balancing walk. *Proceedings of the 53rd Annual ACM SIGACT Symposium on Theory of Computing*, 14–20.

Ashlagi I, Burq M, Dutta C, Jaillet P, Saberi A, Sholley C (2019) Edge weighted online windowed matching. *Proceedings of the 2019 ACM Conference on Economics and Computation*, 729–742.

Athey S, Imbens GW (2017) The econometrics of randomized experiments. *Handbook of economic field experiments*, volume 1, 73–140 (Elsevier).

Atkinson AC (1982) Optimum biased coin designs for sequential clinical trials with prognostic factors. *Biometrika* 69(1):61–67.

Atkinson AC (1999) Optimum biased-coin designs for sequential treatment allocation with covariate information. *Statistics in medicine* 18(14):1741–1752.

Bai Y (2019) Optimality of matched-pair designs in randomized controlled trials. *Available at SSRN 3483834*.

Bai Y, Romano JP, Shaikh AM (2021) Inference in experiments with matched pairs. *Journal of the American Statistical Association* 1–12.

Bakshy E, Eckles D, Bernstein MS (2014) Designing and deploying online field experiments. *Proceedings of the 23rd international conference on World wide web*, 283–292.

Bansal N, Jiang H, Meka R, Singla S, Sinha M (2021) Online discrepancy minimization for stochastic arrivals. *Proceedings of the 2021 ACM-SIAM Symposium on Discrete Algorithms (SODA)*, 2842–2861 (SIAM).

Bansal N, Jiang H, Singla S, Sinha M (2020) Online vector balancing and geometric discrepancy. *Proceedings of the 52nd Annual ACM SIGACT Symposium on Theory of Computing*, 1139–1152.

Basse G, Ding Y, Toulis P (2019) Minimax crossover designs. *arXiv preprint arXiv:1908.05531*.

Bertsimas D, Johnson M, Kallus N (2015) The power of optimization over randomization in designing experiments involving small samples. *Operations Research* 63(4):868–876.

Bertsimas D, Tsitsiklis JN (1997) *Introduction to linear optimization*, volume 6 (Athena Scientific Belmont, MA).

Bhat N, Farias VF, Moallemi CC, Sinha D (2020) Near-optimal ab testing. *Management Science* 66(10):4477–4495.

Blyth CR (1980) Expected absolute error of the usual estimator of the binomial parameter. *The American Statistician* 34(3):155–157.
Bojinov I, Simchi-Levi D, Zhao J (2020) Design and analysis of switchback experiments. *Available at SSRN 3684168*.

Buchbinder N, Naor J (2009) *The design of competitive online algorithms via a primal-dual approach* (Now Publishers Inc).

Candogan O, Chen C, Niazadeh R (2021) Near-optimal experimental design for networks: Independent block randomization. *Available at SSRN*.

Chase G (1968) On the efficiency of matched pairs in bernoulli trials. *Biometrika* 55(2):365–369.

Cochran WG, Cox GM (1957) Experimental designs. *John Willey and Sons. Inc., New York 546–568*.

Cox DR (1958) Planning of experiments. .

Dehejia RH, Wahba S (2002) Propensity score-matching methods for nonexperimental causal studies. *Review of Economics and statistics* 84(1):151–161.

Derigs U (1988) Solving non-bipartite matching problems via shortest path techniques. *Annals of Operations Research* 13(1):225–261.

Devanur NR, Jain K, Kleinberg RD (2013) Randomized primal-dual analysis of ranking for online bipartite matching. *Proceedings of the twenty-fourth annual ACM-SIAM symposium on Discrete algorithms*, 101–107 (SIAM).

Diamond A, Sekhon JS (2013) Genetic matching for estimating causal effects: A general multivariate matching method for achieving balance in observational studies. *Review of Economics and Statistics* 95(3):932–945.

Efron B (1971) Forcing a sequential experiment to be balanced. *Biometrika* 58(3):403–417.

Feldman J, Mehta A, Mirrokni V, Muthukrishnan S (2009) Online stochastic matching: Beating 1-1/e. *2009 50th Annual IEEE Symposium on Foundations of Computer Science*, 117–126 (IEEE).

Fisher RA (1936) Design of experiments. *Br Med J* 1(3923):554–554.

Goel G, Mehta A (2008) Online budgeted matching in random input models with applications to adwords. *SODA*, volume 8, 982–991 (Citeseer).

Greevy R, Lu B, Silber JH, Rosenbaum P (2004) Optimal multivariate matching before randomization. *Biostatistics* 5(2):263–275.

Gupta S, Kohavi R, Tang D, Xu Y, Andersen R, Baksy E, Cardin N, Chandran S, Chen N, Coey D, et al. (2019) Top challenges from the first practical online controlled experiments summit. *ACM SIGKDD Explorations Newsletter* 21(1):20–35.

Harshaw C, Sävje F, Spielman D, Zhang P (2019) Balancing covariates in randomized experiments with the gram-schmidt walk design. *arXiv preprint arXiv:1911.03071*.

Higgins MJ, Sävje F, Sekhon JS (2016) Improving massive experiments with threshold blocking. *Proceedings of the National Academy of Sciences* 113(27):7369–7376.
Hoeffding W (1994) Probability inequalities for sums of bounded random variables. *The collected works of Wassily Hoeffding*, 409–426 (Springer).

Imai K, King G, Nall C (2009) The essential role of pair matching in cluster-randomized experiments, with application to the mexican universal health insurance evaluation. *Statistical Science* 24(1):29–53.

Imbens GW (2011) Experimental design for unit and cluster randomid trials. *International Initiative for Impact Evaluation Paper*.

Imbens GW, Rubin DB (2015) *Causal inference in statistics, social, and biomedical sciences* (Cambridge University Press).

Jaillet P, Lu X (2014) Online stochastic matching: New algorithms with better bounds. *Mathematics of Operations Research* 39(3):624–646.

Johari R, Koomen P, Pekelis L, Walsh D (2021) Always valid inference: Continuous monitoring of a/b tests. *Operations Research*.

Johari R, Li H, Liskovich I, Weintraub GY (2022) Experimental design in two-sided platforms: An analysis of bias. *Management Science*.

Kalyanasundaram B, Pruhs K (1993) Online weighted matching. *Journal of Algorithms* 14(3):478–488.

Kapelner A, Krieger A (2014) Matching on-the-fly: Sequential allocation with higher power and efficiency. *Biometrics* 70(2):378–388.

Karp RM, Vazirani UV, Vazirani VV (1990) An optimal algorithm for on-line bipartite matching. *Proceedings of the twenty-second annual ACM symposium on Theory of computing*, 352–358.

Kohavi R, Crook T, Longbotham R, Frasca B, Henne R, Ferres JL, Melamed T (2009) Online experimentation at microsoft. *Data Mining Case Studies* 11(2009):39.

Kohavi R, Henne RM, Sommerfield D (2007) Practical guide to controlled experiments on the web: listen to your customers not to the hippo. *Proceedings of the 13th ACM SIGKDD international conference on Knowledge discovery and data mining*, 959–967.

Kohavi R, Tang D, Xu Y (2020) *Trustworthy online controlled experiments: A practical guide to a/b testing* (Cambridge University Press).

Koning R, Hasan S, Chatterji A (2019) Experimentation and startup performance: Evidence from a/b testing. Technical report, National Bureau of Economic Research.

Lewis RA (2010) Where’s the “wear-out?”: Online display ads and the impact of frequency. *Massachusetts Institute of Technology Typescript*.

Lewis RA, Rao JM (2015) The unfavorable economics of measuring the returns to advertising. *The Quarterly Journal of Economics* 130(4):1941–1973.

Li H, Zhao G, Johari R, Weintraub GY (2021) Interference, bias, and variance in two-sided marketplace experimentation: Guidance for platforms. *arXiv preprint arXiv:2104.12222*.
Li KC (1983) Minimaxity for randomized designs: some general results. *The Annals of Statistics* 225–239.

Lu B, Greevy R, Xu X, Beck C (2011) Optimal nonbipartite matching and its statistical applications. *The American Statistician* 65(1):21–30.

Matts JP, Lachin JM (1988) Properties of permuted-block randomization in clinical trials. *Controlled clinical trials* 9(4):327–344.

Mehta A (2013) Online matching and ad allocation.

Mehta A, Saberi A, Vazirani U, Vazirani V (2007) Adwords and generalized online matching. *Journal of the ACM (JACM)* 54(5):22–es.

Pocock SJ, Simon R (1975) Sequential treatment assignment with balancing for prognostic factors in the controlled clinical trial. *Biometrics* 103–115.

Rosenbaum PR (1989) Optimal matching for observational studies. *Journal of the American Statistical Association* 84(408):1024–1032.

Rosenberger WF, Lachin JM (2015) *Randomization in clinical trials: theory and practice* (John Wiley & Sons).

Rosenberger WF, Sverdlov O (2008) Handling covariates in the design of clinical trials. *Statistical Science* 23(3):404–419.

Rubin DB (2008) Comment: The design and analysis of gold standard randomized experiments. *Journal of the American Statistical Association* 103(484):1350–1353.

Schrijver A (2003) *Combinatorial optimization: polyhedra and efficiency*, volume 24 (Springer Science & Business Media).

Spencer J (1977) Balancing games. *Journal of Combinatorial Theory, Series B* 23(1):68–74.

Thomke SH (2020) *Experimentation works: The surprising power of business experiments* (Harvard Business Press).

Wager S, Xu K (2021) Experimenting in equilibrium. *Management Science* .

Wu CF (1981) On the robustness and efficiency of some randomized designs. *The Annals of Statistics* 1168–1177.

Xiong R, Athey S, Bayati M, Imbens GW (2019) Optimal experimental design for staggered rollouts. Available at SSRN 3483934.
Appendices

A. Useful Results

Here are existing results that we will refer to in this paper. We first review the Hoeffding’s inequality (Hoeffding 1994).

**Lemma 3 (Hoeffding’s Inequality, Hoeffding (1994)).** Let $H(n)$ be a binomial random variable with probability $p$ and trial $n$, then

$$P(|H(n) - pn| \leq \sqrt{n \log n}) \geq 1 - \frac{2}{n^2}.$$ 

**Lemma 4 (Binomial Mean Absolute Deviation, Equation 2.4 in Blyth (1980)).** Let $X$ be a Binomial distribution with $n$ trials and success probability $p$, then we have

$$E[|X - np|] = \sqrt{\frac{2p(1-p)}{\pi}} n + O(n^{-\frac{1}{2}}).$$

B. Proof of Theorem 1

**Proof of Theorem 1.** Suppose the adversary chooses input $(x_1, x_2, ..., x_T)$. As the matched-pair design considers the offline problem, the decision maker knows $(x_1, x_2, ..., x_T)$ at the beginning. Let $(x'_1, x'_2, ..., x'_T)$ be smallest-to-largest rearrangement of $(x_1, x_2, ..., x_T)$ such that

$$x'_1 \leq x'_2 \leq ... \leq x'_T.$$

The matched-pair design matches $(x'_t, x'_{t+1})$ into a size-two pair for any odd $t$. Therefore, the discrepancy under the input $(x_1, x_2, ..., x_T)$ is

$$\sum_{\tau=1}^{\frac{T}{2}} (x_{2\tau} - x_{2\tau-1}) \leq x_T - x_1 \leq 1.$$ 

So the total discrepancy will be no more than 1. □

C. Proof of Theorem 2

For any arrival sequence $x$, let $\text{ALG}^c(x)$ be the expected discrepancy incurred by a completely randomized design when the arrival sequence is $x$.

Let $V$ be the (random) set of indices that the completely randomized design selects to assign into the control group. As a result, $(\mathbb{T} \setminus V)$ is the set of indices that the completely randomized design selects to assign into the treatment group. We denote $\mathcal{V}$ to be the set that contains all possible $V$. 

We know that the size of $\mathcal{V}$ is $|\mathcal{V}| = \binom{T}{T/2}$. In addition, since we select $V$ randomly, the probability for any $V \in \mathcal{V}$ to be selected is $\frac{1}{\binom{T}{T/2}}$.

For any arrival sequence $\mathbf{x}$ and any set $V \in \mathcal{V}$, denote $\text{Dis}(\mathbf{x}, V)$ to be the (deterministic) discrepancy incurred by a completely randomized design when the arrival sequence is $\mathbf{x}$ and when the realized set of indices is $V$. We can take expectation over $V$ and have the following,

$$\text{ALG}^C(\mathbf{x}) = E_V[\text{Dis}^C(\mathbf{x}, V)].$$

We first introduce the following three Lemmas that help us prove Theorem 2.

**Lemma 5.** Let the arriving instance $\mathbf{x}^*$ be $(0, 0, ..., 0, 1, 1, ..., 1)$, which contains $\frac{T}{2}$ many zeros and $\frac{T}{2}$ many ones. The expected discrepancy on this arrival sequence $\mathbf{x}^*$ is $\text{ALG}^C(\mathbf{x}^*) = \frac{1}{2\sqrt{\pi}} \sqrt{T} + O(T^{-\frac{1}{2}})$.

**Proof of Lemma 5.** The completely randomized design select $\frac{T}{2}$ users from $T$ users randomly. Given that the $T$ users consists of $\frac{T}{2}$ many zeros and $\frac{T}{2}$ many ones, if we select $H$ many zeros to the control group, then we automatically select $\frac{T}{2} - H$ many ones to the control group. Therefore, the total discrepancy can be calculated by

$$E \left[ \left| H - \left( \frac{T}{2} - H \right) \right| \right] = \frac{1}{2} E \left[ \left| H - \frac{T}{4} \right| \right].$$

Observe that $H$ follows a binomial random variable with $\frac{T}{2}$ trials and success probability $\frac{1}{2}$. In addition, $E[H] = \frac{T}{4}$. By equation 2.4 in Blyth (1980) (re-stated using our notations in Lemma 4), we have $E \left[ \left| H - \frac{T}{4} \right| \right] = \frac{1}{2\sqrt{\pi}} \sqrt{T} + O(T^{-\frac{1}{2}})$. □

**Lemma 6.** Consider two arriving sequences $\mathbf{x}'$ and $\mathbf{x}''$. If there exists an one-to-one correspondence $\sigma : [T] \rightarrow [T]$, such that $\forall \ t \in [T]$, $x'_t = x''_{\sigma(t)}$, then the expected discrepancy of the completely randomized design will be the same on these two arrival sequences $\mathbf{x}'$ and $\mathbf{x}''$, i.e.,

$$\text{ALG}^C(\mathbf{x}') = \text{ALG}^C(\mathbf{x}'').$$

**Proof of Lemma 6.** Recall that, we use $V$ for the (random) set of indices that the completely randomized design selects to assign into the control group. And recall that we denote $\text{Dis}(\mathbf{x}, V)$ to be the (deterministic) discrepancy incurred by a completely randomized design when the arrival sequence is $\mathbf{x}$ and when the realized set of indices is $V$. Then we have,

$$\text{ALG}^C(\mathbf{x}') = E_V[\text{Dis}(\mathbf{x}', V)] = \frac{1}{\binom{T}{T/2}} \sum_{V \in \mathcal{V}} \text{Dis}(\mathbf{x}', V),$$
ALG$^C(x'') = E_V[\text{Dis}(x'', V)] = \frac{1}{\binom{T}{T/2}} \sum_{V \in \mathcal{V}} \text{Dis}(x'', V).

Now denote $\sigma(V) = \{U \subseteq [T] \mid \forall t \in V, \sigma(t) \in U; \text{ and } \forall t \in U, \sigma^{-1}(t) \in V\}$. In words, $\sigma(V)$ is the set of indices to receive control after permutation $\sigma(\cdot)$. Since $\sigma(\cdot)$ is an one-to-one correspondence, we know that $\mathcal{V}$ is not only the set that contains all possible $V$, but also the set that contains all possible $\sigma(V)$. In addition, since we select $V$ randomly, the probability for any $\sigma(V) \in \mathcal{V}$ to be selected is $\frac{1}{\binom{T}{T/2}}$.

Therefore, for any $V \in \mathcal{V}$,

$$\text{Dis}(x', V) = \text{Dis}(x'', \sigma(V)).$$

If we add them all together,

$$\sum_{V \in \mathcal{V}} \text{Dis}(x', V) = \sum_{\sigma(V) \in \mathcal{V}} \text{Dis}(x'', \sigma(V)) = \sum_{V \in \mathcal{V}} \text{Dis}(x'', V).$$

This suggests that

$$\text{ALG}^C(x') = \text{ALG}^C(x''),$$

which completes the proof. □

**Lemma 7.** For all possible arriving instances $x \in [0, 1]^T$, we have

$$\max_{x \in [0, 1]^T} \text{ALG}^C(x) = \text{ALG}^C(x^*),$$

where $x^* = (0, 0, ..., 0, 1, 1, ..., 1)$, which contains $\frac{T}{2}$ many zeros and $\frac{T}{2}$ many ones.

**Proof of Lemma 7.** Consider any arrival sequence $x = (x_1, x_2, \ldots, x_T)$. Due to Lemma 6 we have that the discrepancy of $\text{ALG}^C$ does not change under any permutation $\sigma(\cdot)$. Therefore, we can sort the users in $x$ from the smallest to the largest, i.e., $x_1 \leq x_2 \leq \ldots \leq x_T$.

Next, we select $\frac{T}{2}$ users from $(x_1, x_2, \ldots, x_T)$ randomly. There are $|\mathcal{V}| = \binom{T}{T/2}$ possible cases. We have

$$\text{ALG}^C(x) = \frac{1}{\binom{T}{T/2}} \sum_{V \in \mathcal{V}} \text{Dis}(x, V).$$

Now we wish to expand

$$\sum_{V \in \mathcal{V}} \text{Dis}(x, V) = \sum_{t=1}^{T} \xi_t x_t,$$

where $\xi_t \in \mathbb{Z}$ is an abstract notation that counts how many times (out of a total of $\binom{T}{T/2}$ many selections of $V$) user $t$ is matched to another user with a larger index (negative number stands for
the number of time matched to another user with a smaller index). Note that we have ordered
\(x_1 \leq x_2 \leq \ldots \leq x_T\). For any \(V\), denote \(\sigma_s(V) = \{t | (T - t + 1) \in V\}\). Then for any \(t \in [T]\), whenever user \(t\) is matched to a user with a larger index under \(V\), we know that user \((T - t + 1)\) is matched to a user with a smaller index under \(\sigma_s(V)\). As a result, for any \(t \in [T]\), \(\xi_t = -\xi_{T+1-t}\).

Therefore, we have
\[
ALG^C(x) = \frac{1}{(T/2)} \sum_{t=1}^{T} \xi_t x_t \\
= \frac{1}{(T/2)} \sum_{t=1}^{T} \xi_t (x_{T-t+1} - x_t) \\
\leq \frac{1}{(T/2)} \sum_{t=1}^{T} |\xi_t| (1 - 0) \\
= \frac{1}{(T/2)} \sum_{t=1}^{T} |\xi_t|.
\]
The equality sign holds if and only if \(x_t = 1\) for all \(t > \frac{T}{2}\) and \(x_t = 0\) for all \(t \leq \frac{T}{2}\). Under this case, \((x_1, x_2, \ldots, x_T) = x^*\), and \(\max_{x \in [0,1]^T} ALG^C(x) = ALG^C(x^*)\). \(\Box\)

Proof of Theorem 3  For any instance of arrival sequence \(x\), denote \(ALG^C(x)\) to be the expected discrepancy of the completely randomized design on sequence \(x\). Let \([0,1]^T\) be the set that contains all possible arrival inputs. By Lemma 5, we find an arriving instance \(x^*\) such that \(ALG^C(x^*) = \frac{1}{2\sqrt{\pi}} \sqrt{T} + O(T^{-\frac{1}{2}})\). This suggests that the discrepancy of the completely randomized design is at least \(\frac{1}{2\sqrt{\pi}} \sqrt{T}\).

Next, we show that the upper bound of the discrepancy is also in the same order. First, by Lemma 6, we have the completely randomized design under \(p = 1\) is permutation-invariant to the arriving sequence. Second, Lemma 7 shows that among all possible arriving instances in \([0,1]^T\), \(x^*\) has the largest discrepancy. Therefore, combining this result with Lemma 5, we know that the discrepancy of any completely randomized design is bounded by
\[
\max_{x \in [0,1]^T} ALG^C(x) = ALG^C(x^*) = \frac{1}{2\sqrt{\pi}} \sqrt{T} + O(T^{-\frac{1}{2}}).
\]
Combining the lower bound and the upper bound we show that the completely randomized design has an expected discrepancy in the order of \(\Theta(T^{\frac{1}{2}})\). \(\Box\)

D. Proof of Theorem 3

Proof of Theorem 3  Consider the case when the length of each pigeonhole is \(T^{-\eta}\) and there are \(T^\eta\) many pigeonholes, i.e., \(P(S) = \{[0, T^{-\eta}), [T^{-\eta}, 2T^{-\eta}), \ldots, [1 - T^{-\eta}, 1]\}\). We analyze the expected discrepancy that come from the following two components.
**Component 1:** Consider the first \((1 - \beta)T\) arriving users. Following the procedure in Definition 3, we sequentially match the arrived users at the same pigeonhole in pairs, while leaving at most one unmatched user from each pigeonhole. Denote the set of time indices for the matched users to be \(T_M\); denote the set of time indices for the unmatched users to be \(T_U\). We first focus on \(T_M\), the matched users. The discrepancy on \(T_M\), the matched users, is upper bounded by 

\[ T - \eta (1 - \beta)T, \]

which is in the order of \(O(T^{1-\eta})\).

**Component 2:** Next, we focus on \(T_U\), the unmatched users, together with the last \(\beta T\) users. Let there be \(T_U = |T_U|\) many unmatched users.

Case 1: \(T_U < T^{\frac{\eta}{2}}\). In this case, together with the last \(\beta T = T^{\frac{\eta}{2}}\) users, the total discrepancy is no larger than \(T^{\frac{\eta}{2}}\). So combining both components, the total expected discrepancy is in the order of \(O(T^{1-\eta} + T^{\frac{\eta}{2}})\).

Case 2: \(T_U \geq T^{\frac{\eta}{2}}\). Recall that there are \(T^{\eta}\) many pigeonholes. So we know that \(T_U \leq T^{\eta}\). We can index the pigeonholes with one unmatched users from the smallest to largest, i.e., \(i \in \{1, 2, \ldots, T_U\}\). Let \(p_i, q_i, \forall i \in \{1, 2, \ldots, T_U\}\) be the (random) number of unmatched users in the \(i\)-th smallest indexed pigeonhole that is assigned into the control and the treatment group, respectively. We know \(p_i, q_i \in \{0, 1\}\), and \(p_i + q_i = 1\). As each unmatched user is randomly assigned to the control or the treatment group, we have \(E[p_i] = E[q_i] = \frac{1}{2}\) so \(\sum_{i=1}^{T_U} p_i = \sum_{i=1}^{T_U} q_i = T_U\). By Hoeffding’s inequality, we have with probability at least \(1 - \frac{2}{T_U}\),

\[
\sum_{i=1}^{T_U} p_i, \sum_{i=1}^{T_U} q_i \in \left[ \frac{1}{2}T_U - \sqrt{T_U \log T_U}, \frac{1}{2}T_U + \sqrt{T_U \log T_U} \right].
\]

With above, we can define the following probability event \(E_0\), which happens with probability at least \(1 - \frac{2}{T_U}\).

\[
E_0 = \left\{ \left| \sum_{i=1}^{T_U} (p_i - q_i) \right| \leq 2 \sqrt{T_U \log T_U} \right\}.
\]

In words, \(E_0\) is the event that the absolute value of difference of number of users between the control and the treatment group is less than or equal to \(2 \sqrt{T_U \log T_U}\).

If event \(E_0\) does not happen, the discrepancy can still be bounded by \(T/2\). So in expectation, the low probability event contributes no more than \(\frac{T}{T_U} \leq \frac{T}{T^{\eta}} = T^{1-\eta}\) discrepancy.

Conditioned on \(E_0\), we define a coupling of two stochastic processes. First, we define a stochastic process \(Z\) as follows: for every \(i \in \{1, 2, \ldots, T_U\}\), \(Z_i = 1\) with probability 0.5, and \(Z_i = 0\) with probability 0.5. The assignment of all the unmatched users follows \(Z\). Second, we define a stochastic
process \( Y \) as follows: we randomly “select” \( T_U - \sqrt{T_U \log T_U} \) indices from \( \{1, 2, \ldots, T_U\} \). On the “selected” indices, \( Y \) follows completely randomized design, i.e., we randomly pick \( \frac{1}{2} T_U - \sqrt{T_U \log T_U} \) indices and assign \( Y_i = 1 \), and the other \( \frac{1}{2} T_U - \sqrt{T_U \log T_U} \) indices are assigned \( Y_i = 0 \). On the \( 2\sqrt{T_U \log T_U} \) many indices that are not “selected”, we set \( Y_i = 1 \) with probability 0.5, and \( Y_i = 0 \) with probability 0.5. Conditional on the high probability event \( E_0 \), \( Y \) is a coupling process of \( Z \).

This is because a completely randomized design is a Bernoulli design conditional on the numbers of control and treatment units being fixed.

Now that we have the coupling, we can view the assignments of the \( T_U \) many unmatched users as if they were generated from the process \( Y \) as we have defined above. There are two components of users that we analyze separately. First, in process \( Y \), there are \( T_U - 2\sqrt{T_U \log T_U} \) many users that are assigned based on the completely randomized design. Due to Theorem 2, we know that the total discrepancy between these users can be upper bounded by

\[
\frac{1}{2\sqrt{\pi}} \left( \frac{1}{2} T_U - \sqrt{T_U \log T_U} \right)^\frac{1}{2} \leq \frac{1}{2\sqrt{\pi}} \left( \frac{1}{2} T_U \right)^\frac{1}{2} \leq \frac{1}{2\sqrt{\pi}} \left( \frac{1}{2} T^n \right)^\frac{1}{2},
\]

which is in the order of \( O(T^\frac{2}{3}) \).

Second, in process \( Y \), there are \( 2\sqrt{T_U \log T_U} \) many users that are assigned into either the control group or the treatment group with probability 0.5 each. On these users, together with the last \( \beta T \) users, we match them in any arbitrary fashion. The discrepancy between each pair is no more than 1. Therefore, the total discrepancy can be upper bounded by

\[
\frac{1}{2} (2\sqrt{T_U \log T_U} + \beta T) \leq \frac{1}{2} (2\sqrt{T^n \log T^n} + \beta T) = \frac{1}{2} (2\sqrt{T^n \log T^n} + T^\frac{2}{3}),
\]

which is in the order of \( O(T^\frac{2}{3}(\log T)^\frac{1}{3}) \). The second inequality above is because we select \( \beta = T^\frac{2}{3} - 1 \).

Finally, combining both components, the total expected discrepancy is in the order of

\[
O \left( T^{1-\eta} + T^2 + T^\frac{2}{3}(\log T)^\frac{1}{3} \right) = O \left( T^{1-\eta} + T^2 \right) \].

**Proof of Corollary 2.** From Theorem 3 the total expected discrepancy is in the order of

\[
O \left( T^{1-\eta} + T^2 (\log T)^\frac{1}{3} \right).
\]

If we choose \( \eta \) such that

\[
T^{1-\eta} = T^2,
\]

which implies \( \eta = \frac{2}{3} \), the pigeonhole design has an expected discrepancy in the order of

\[
O \left( T^\frac{2}{3}(\log T)^\frac{1}{3} \right). \]
E. Proof of Theorem 4

Proof of Theorem 4  To show the total discrepancy of matched-pair design is $\Theta(T^{p-1})$, we only need to prove the $\Omega(T^{p-1})$ part.

We prove by constructing an arrival sequence such that the discrepancy on this sequence is $\Omega(T^{p-1})$. Consider the following sequence. We evenly split the covariate space $[0,1]^p$ into $T$ smaller hypercubes, such that each hypercube has edge length $T^{-\frac{1}{2}}$. Then, we let the covariate of each user to be at the center of each smaller hypercube, respectively.

By construction, the distance between the covariates of any two users is at least $T^{-\frac{1}{2}}$. There are a total of $T/2$ pairs of users. Therefore, the discrepancy is at least $T^{-\frac{1}{2}} \cdot T = T^{\frac{p-1}{2}}$. So the matched-pair design has a discrepancy in the order of $\Omega(T^{p-1})$. Combining with Lemma 1, we finish the proof. □

F. Proof of Lemma 2

Proof of Lemma 2  Recall that we construct the family of arrival sequences as follows. First, we split the $p$-dimensional unit hypercube to $T$ smaller hypercubes, each with edge-length $T^{-\frac{1}{2}}$. Second, let there be exactly one user in each smaller hypercube. Mathematically, let the family of arrival sequences be

$$\mathcal{X}^{(T)} = \left\{ (x_1, x_2, \ldots, x_T) \left| \forall X \in \left\{ [0, T^{-\frac{1}{2}}), [T^{-\frac{1}{2}}, 2T^{-\frac{1}{2}}), \ldots, [1 - T^{-\frac{1}{2}}, 1] \right\}^p, \exists t, s.t. x_t \in X, \text{ and } \forall t' \neq t, x_{t'} \notin X \right\}.$$

First, we show that when $p = 2$, for any $T$, the following holds:

$$\forall x^{(T)} \in \mathcal{X}^{(T)}, ALG^C(x^{(T)}) \leq \sqrt{2} \sqrt{T} \log T \sqrt{\log T}. \quad (3)$$

We prove this for any $T = 2^i$ by induction on $i \in \mathbb{N}$. First, when $T = 2^2$, we have $ALG^C(x) \leq 2\sqrt{2} \leq \sqrt{2} \sqrt{4} \log 4 + \sqrt{4} \log 4$. The first inequality is because there are 2 pairs and each pair contributes at most $\sqrt{2}$ discrepancy.

Suppose (3) holds for $i = i_0 \in \mathbb{N}$, i.e., (3) holds for $2^{2i_0} = T_0$. We show that for $i = i_0 + 1$, i.e., for $2^{2(i_0+1)} = 2^2T_0$, the inequality (3) also holds. Consider the new family of arrival sequences $\mathcal{X}^{(2^2T_0)}$, and one arrival sequence $x^{(2^2T_0)} \in \mathcal{X}^{(2^2T_0)}$. There are a total of $2^2T_0$ users. And there are $2^2T_0$ small squares each with edge length $\frac{1}{4}T_0^{-\frac{1}{2}}$. There is exactly one user in each small square.

For the unit square with edge length 1, we cut it by half in each dimension. Then, there are $2^2$ squares each with edge length $\frac{1}{2}$, which we refer to as the “good-squares”. In each such good-square, the arrival sequence $x^{(2^2T_0)}$ has $T_0$ users that are evenly distributed. If we apply completely
randomized design in each good-square, we have that the expected discrepancy in such good-square is $\frac{1}{2}\sqrt{2}\sqrt{T_0}\log T_0$. This is because all distances are shrunked by a half. However, as we apply completely randomized design in the unit square, it does not necessarily guarantee that the number of users between control and treatment group are the same in each good-square. By Lemma 3, we know that with probability at least $(1 - \frac{2}{T_0^2})^2$, the absolute difference between the number of control and treatment users is bounded by $\sqrt{T_0}\log T_0$ in every good-square.

Conditional on the low probability event, which happens with probability at most $\frac{2}{T_0^2} \cdot 2^2$ due to union bound, the discrepancy can be upper bounded by $\frac{2}{T_0^2} \cdot 2^2 = \frac{2^4}{T_0} \leq 2^2 = 4$, where the inequality is due to $T_0 \geq 2^2$.

Next, conditional on the high probability event, suppose in good-square $i, i \in \{1, 2, 3, 4\}$, there is an imbalanced number of control and treatment users of no more than $\sqrt{T_0}\log T_0$ in every good-square. Then, we randomly pick no more than $\sqrt{T_0}\log T_0$ users in the group with more users and denote as $R_i$. For all the users that are not in $R_i$ but in good-square $i$, we make a minimum weight perfect matching, whose discrepancy is upper bounded by the discrepancy of a completely randomized design. In each good-square, the expected discrepancy on the number of users that are matched can be upper bounded by $\frac{1}{2}\sqrt{2}\sqrt{T_0}\log T_0\sqrt{\log T_0}$. There are 4 such squares, and so the expected discrepancy is

$$4 \cdot \frac{1}{2}\sqrt{2}\sqrt{T_0}\log T_0\sqrt{\log T_0} = 2\sqrt{2}\sqrt{T_0}\log T_0\sqrt{\log T_0}.$$  

Note that we still have no more than $\sqrt{T_0}\log T_0$ users in each $R_i$, we match them randomly. The total discrepancy of users in $R_i$ can be bounded by $\frac{2^2\sqrt{T_0}\log T_0}{2} \cdot \sqrt{2}$. Therefore, the total discrepancy of completely randomized design under $x^{(2^2T_0)}$ is upper bounded by

$$2\sqrt{2}\sqrt{T_0}\log T_0\sqrt{\log T_0} + 2\sqrt{2}\sqrt{T_0}\log T_0 + 4 = 2\sqrt{2}\sqrt{T_0}\log T_0(\log T_0 + 1) + 4$$

$$\leq 2\sqrt{2}\sqrt{T_0}\log T_0(\log T_0 + \log 4)$$

$$= 2\sqrt{2}\sqrt{4T_0}\log 4T_0 \log 4T_0$$

Second, we show that when $p \geq 3$, for any $T$, the following holds:

$$\forall x^{(T)} \in \mathcal{X}^{(T)}, \text{ALG}^C(x^{(T)}) \leq \sqrt{pT^{\frac{p+1}{p}}} + \sqrt{T}\log T \log T.$$  

(4)
We prove this for any $T = 2^p$ by induction on $i \in \mathbb{N}$. First, when $T = 2^p$, we have $\text{ALC}^C(\mathbf{x}) \leq \sqrt{p}2^{p-1} = \sqrt{p}T^{\frac{p-1}{p}} \leq \sqrt{p}T^{\frac{p-1}{p}} + \sqrt{T}\log T\log T$. The first inequality is because there are $2^{p-1}$ many pairs and each pair contributes at most $\sqrt{p}$ discrepancy.

Suppose (4) holds for $i = i_0 \in \mathbb{N}$, i.e., (4) holds for $2^{i_0}p = T_0$. We show that for $i = i_0 + 1$, i.e., for $2^{(i_0+1)p} = 2^pT_0$, the inequality (4) also holds. Consider the new family of arrival sequences $\mathcal{X}^{(2^pT_0)}$, and one arrival sequence $\mathbf{x}^{(2^pT_0)}\in\mathcal{X}^{(2^pT_0)}$. There are a total of $2^pT_0$ users. And there are $2^pT_0$ small hypercubes each with edge length $\frac{1}{2}T_0^{\frac{1}{p}}$. There is exactly one user in each small hypercube.

For the unit hypercube with edge length 1, we cut it by half in each dimension. Then, there are $2^p$ hypercubes each with edge length $\frac{1}{2}$, which we refer to as the “good-cubes”. In each such good-cube, the arrival sequence $\mathbf{x}^{(2^pT_0)}$ has $T_0$ users that are evenly distributed. If we apply completely randomized design in each good-cube, we have that the expected discrepancy in such good-cube is $\frac{1}{2}\sqrt{p}T_0^{\frac{p-1}{p}} + \frac{1}{2}\sqrt{T_0}\log T_0\log T_0$. This is because all distances are shrunk by a half. However, as we apply completely randomized design in the unit hypercube, it does not necessarily guarantee that the number of users between control and treatment group are the same in each good-cube. By Lemma 3, we know that with probability at least $(1 - \frac{2}{T_0})^p$, the absolute difference between the number of control and treatment users is bounded by $\sqrt{T_0}\log T_0$ in every good-cube.

Conditional on the low probability event, which happens with probability at most $\frac{2}{T_0^p}\cdot 2^p$ due to union bound, the discrepancy can be upper bounded by $\frac{2^pT_0}{2}$. So the contribution to the total expected discrepancy can be upper bounded by $\frac{2^pT_0}{2}\cdot 2^p\cdot 2^pT_0 = \frac{2^{2p}T_0}{2} \leq 2^p$, where the inequality is due to $T_0 \geq 2^p$.

Next, conditional on the high probability event, suppose in good-cube $i, i \in \{1, 2, ..., 2^p\}$, there is an imbalanced number of control and treatment users. Then, we randomly pick no more than $\sqrt{T_0}\log T_0$ users in the group with more users and denote as $R_i$. For all the users that are not in $R_i$ but in good-cube $i$, we make a minimum weight perfect matching, whose discrepancy is upper bounded by the discrepancy of a completely randomized design. In each good-cube, the expected discrepancy on the number of users that are matched can be upper bounded by $\frac{1}{2}\sqrt{p}T_0^{\frac{p-1}{p}} + \frac{1}{2}\sqrt{T_0}\log T_0\log T_0$. There are $2^p$ such cubes, and so the expected discrepancy is

$$2^{p-1}\sqrt{p}T_0^{\frac{p-1}{p}} + 2^{p-1}\sqrt{T_0}\log T_0\log T_0 = \sqrt{p}(2^pT_0)^{\frac{p-1}{p}} + 2^{p-1}\sqrt{T_0}\log T_0\log T_0.$$
\[
\sqrt{p}(2^pT_0) - \frac{1}{p} + 2^{p-1} \sqrt{T_0 \log T_0} \log T_0 + 2^{p-1} \left( \sqrt{p} \sqrt{T_0 \log T_0} + 2 \right) 
\leq \sqrt{p}(2^pT_0) - \frac{1}{p} + 2^{p-1} \sqrt{T_0 \log (2^pT_0) \log T_0} + 2^{p-1} \log (2^pT_0)
\]

where the inequality holds when \( p \geq 3 \). □

G. Proof of Theorem 6

Proof of Theorem 6. Fix \( c \) to be any positive real number that is greater than 1, i.e., \( c > 1 \).
Consider the case when the edge length of each pigeonhole is \( c \frac{1}{p} T^{-\phi} \) and there are \( \frac{1}{c} T^{\phi} \) many pigeonholes, i.e., \( \mathcal{P}(S) = \{ [0, c \frac{1}{p} T^{-\phi}), [T^{-\phi}, 2c \frac{1}{p} T^{-\phi}), \ldots, [1 - c \frac{1}{p} T^{-\phi}, 1] \}^p \). We analyze the expected discrepancy that come from the following two components.

Component 1: Consider the first \((1 - \beta)T\) arriving users. Following the procedure in Definition 3, we sequentially match the arrived users at the same pigeonhole in pairs, while leaving at most one unmatched user from each pigeonhole.

With low probability, the following event happens before period \( T - \beta T \), that one of the control or the treatment group reaches \( T/2 \) in size, the algorithm starts to assign all the other users into the opposite group. See steps 4 and 5 in Algorithm 2. When this happens, the difference between the two groups of users is \( \beta T = \sqrt{T} = T^{\frac{\phi}{2}} \) when \( \phi = \frac{1}{p} \). So this happens with probability \( O \left( \frac{\log T}{T} \right)^2 \).

When it happens, the discrepancy can be upper bounded by \( \frac{T}{2} \sqrt{p} \). Therefore, the contribution to the expectation of discrepancy conditional on this low probability event is \( O \left( \frac{\log T}{T} \right)^2 \), which does not increase the order of the discrepancy.

With at least \( \Omega \left( 1 - \frac{(\log T)^2}{T} \right) \) probability, neither the control or the treatment group reaches \( T/2 \) in size by period \( T - \beta T \). Recall that we sequentially match users at the same pigeonhole in pairs, while leaving at most one unmatched user from each pigeonhole. Denote the set of matched users to be \( T_M \); denote the set of unmatched users to be \( T_U \). We first focus on \( T_M \) the matched users. Since the diameter of each pigeonhole is \( c \frac{1}{p} \sqrt{p}T^{-\phi} \), the discrepancy on \( T_M \), the matched users, can be calculated as \( c \frac{1}{p} \sqrt{p}T^{-\phi}(T - \beta T) \). This is in order \( O(T^{1-\phi}) \).

Component 2: Next, we focus on \( T_U \) the unmatched users, together with the last \( \beta T \) users. Let there be \( T_U = |T_U| \) many unmatched users.

Case 1: \( T_U < \frac{1}{c} T^{\frac{\phi}{2}} \). In this case, together with the last \( \beta T = T^{\frac{\phi}{2}} \) users, the total discrepancy is no larger than \( \frac{1+c}{2c} T^{\frac{\phi}{2}} \). So combining both components, the total expected discrepancy is in the order of \( O \left( T^{1-\phi} + T^{\frac{\phi}{2}} \right) \).
Case 2: $T_U \geq \frac{1}{c} T^{p\phi}$. Recall that there are $\frac{1}{c} T^{p\phi}$ many pigeonholes. So we know that $T_U \leq \frac{1}{c} T^{p\phi}$.

We can index the pigeonholes with one unmatched users from the smallest to largest, i.e., $i \in \{1, 2, \ldots, T_U\}$. Let $p_i, q_i, \forall i \in \{1, 2, \ldots, T_U\}$ be the (random) number of unmatched users in the $i$-th smallest indexed pigeonhole that is assigned into the control and the treatment group, respectively. We know $p_i, q_i \in \{0, 1\}$, and $p_i + q_i = 1$. As each unmatched user is randomly assigned to the control or the treatment group, we have $E[p_i] = E[q_i] = \frac{1}{2}$ so $\sum_{i=1}^{T_U} p_i = \sum_{i=1}^{T_U} q_i = \frac{T_U}{2}$. By Hoeffding’s inequality, we have with probability at least $1 - \frac{2}{T_U}$,

$$\sum_{i=1}^{T_U} p_i, \sum_{i=1}^{T_U} q_i \in \left[\frac{1}{2} T_U - \sqrt{T_U \log T_U}, \frac{1}{2} T_U + \sqrt{T_U \log T_U}\right].$$

With above, we can define the following probability event $E_0$, which happens with probability at least $1 - \frac{2}{T_U}$,

$$E_0 = \left\{ \left| \sum_{i=1}^{T_U} (p_i - q_i) \right| \leq 2 \sqrt{T_U \log T_U} \right\}.$$

In words, $E_0$ is the event that the absolute value of difference of number of users between the control and the treatment group is less than or equal to $2 \sqrt{T_U \log T_U}$.

If event $E_0$ does not happen, the discrepancy can still be bounded by $T/2$. So in expectation, the low probability event contributes no more than $\frac{T}{T_U} \leq \frac{c^2 T^{1-p\phi}}{T_U} = c^2 T^{1-p\phi}$ discrepancy.

Conditioned on $E_0$, we define a coupling of two stochastic processes. First, we define a stochastic process $Z$ as follows: for every $i \in \{1, 2, \ldots, T_U\}$, $Z_i = 1$ with probability 0.5, and $Z_i = 0$ with probability 0.5. The assignment of all the unmatched users follows $Z$. Second, we define a stochastic process $Y$ as follows: we randomly “select” $T_U - 2 \sqrt{T_U \log T_U}$ indices from $\{1, 2, \ldots, T_U\}$. On the “selected” indices, $Y$ follows completely randomized design, i.e., we randomly pick $\frac{1}{2} T_U - \sqrt{T_U \log T_U}$ indices and assign $Y_i = 1$, and the other $\frac{1}{2} T_U - \sqrt{T_U \log T_U}$ indices are assigned $Y_i = 0$. On the $2 \sqrt{T_U \log T_U}$ many indices that are not “selected”, we set $Y_i = 1$ with probability 0.5, and $Y_i = 0$ with probability 0.5. Conditional on the high probability event $E_0$, $Y$ is a coupling process of $Z$.

This is because a completely randomized design is a Bernoulli design conditional on the numbers of control and treatment users being fixed.

Now that we have the coupling, we can view the assignments of the $T_U$ many unmatched users as if they were generated from the process $Y$ as we have defined above. There are two components of users that we analyze separately. First, in process $Y$, there are $T_U - 2 \sqrt{T_U \log T_U}$ many users that are assigned based on the completely randomized design. Due to Lemma 2 we know that the
total discrepancy between these users can be upper bounded by either the following quantity in the $p = 2$ case,
\[
\sqrt{2} \left( \frac{1}{2} T_U - \sqrt{T_U \log T_U} \right)^{p-1} \left( \log \left( \frac{1}{2} T_U - \sqrt{T_U \log T_U} \right) \right)^{\frac{1}{2}} \leq \sqrt{2} \left( \frac{1}{2} T_U \right)^{p-1} \left( \log \left( \frac{1}{2} T_U \right) \right)^{\frac{1}{2}} \\
\leq \sqrt{2} \left( \frac{1}{2^c} T^{p\phi} \right)^{p-1} \left( \log \left( \frac{1}{2^c} T^{p\phi} \right) \right)^{\frac{1}{2}},
\]
which is in the order of $O \left( T^{(p-1)\phi} (\log T)^{\frac{1}{2}} \right)$; or bounded by the following quantity in the $p \geq 3$ case,
\[
\sqrt{p} \left( \frac{1}{2} T_U - \sqrt{T_U \log T_U} \right)^{\frac{p-1}{p}} + \left( \frac{1}{2} T_U - \sqrt{T_U \log T_U} \right)^{\frac{1}{p}} \left( \log \left( \frac{1}{2} T_U - \sqrt{T_U \log T_U} \right) \right)^{\frac{3}{2}} \\
\leq \sqrt{p} \left( \frac{1}{2} T_U \right)^{\frac{p-1}{p}} + \left( \frac{1}{2} T_U \right)^{\frac{1}{p}} \left( \log \left( \frac{1}{2} T_U \right) \right)^{\frac{3}{2}} \\
\leq \sqrt{p} \left( \frac{1}{2^c} T^{p\phi} \right)^{\frac{p-1}{p}} + \left( \frac{1}{2^c} T^{p\phi} \right)^{\frac{1}{p}} \left( \log \left( \frac{1}{2^c} T^{p\phi} \right) \right)^{\frac{3}{2}},
\]
which is in the order of $O \left( T^{(p-1)\phi} \right)$.

Second, in process $Y$, there are $2\sqrt{T_U \log T_U}$ many users that are assigned into either the control group or the treatment group with probability 0.5 each. On these users, together with the last $\beta T$ users, we match them in any arbitrary fashion. The discrepancy between each pair is no more than 1. Therefore, the total discrepancy can be upper bounded by
\[
\frac{1}{2} (2\sqrt{T_U \log T_U} + \beta T) \leq \frac{1}{\sqrt{c}} T^{\frac{p\phi}{\sqrt{c}}} \sqrt{\log \left( \frac{1}{c} T^{p\phi} \right)} + \beta T = \frac{1}{\sqrt{c}} T^{\frac{p\phi}{\sqrt{c}}} \sqrt{\log \left( \frac{1}{c} T^{p\phi} \right)} + \frac{1}{2} T^{\frac{p\phi}{\sqrt{c}}},
\]
which is in the order of $O(T^{\frac{p\phi}{\sqrt{c}}} (\log T)^{\frac{1}{2}})$.

Finally, combining both components, when $p = 2$, the total expected discrepancy is in the order of $O \left( T^{1-\phi} + T^{(p-1)\phi} (\log T)^{\frac{1}{2}} + T^{\frac{p\phi}{\sqrt{c}}} (\log T)^{\frac{1}{2}} \right)$; when $p \geq 3$, the total expected discrepancy is in the order of $O \left( T^{1-\phi} + T^{(p-1)\phi} + T^{\frac{p\phi}{\sqrt{c}}} (\log T)^{\frac{1}{2}} \right)$. $\square$

**Proof of Corollary 3**. From Theorem 6 when $p = 2$, the total expected discrepancy is in the order of $O \left( T^{1-\phi} + T^{(p-1)\phi} (\log T)^{\frac{1}{2}} + T^{\frac{p\phi}{\sqrt{c}}} (\log T)^{\frac{1}{2}} \right)$; when $p \geq 3$, the total expected discrepancy is in the order of $O \left( T^{1-\phi} + T^{(p-1)\phi} + T^{\frac{p\phi}{\sqrt{c}}} (\log T)^{\frac{1}{2}} \right)$. Note that when $p \geq 2$, we have $T^{(p-1)\phi} \geq T^{\frac{p\phi}{\sqrt{c}}}$. If we choose $\phi$ such that
\[
T^{1-\phi} = T^{(p-1)\phi},
\]
then we have $\phi = \frac{1}{p}$. So when $p = 2$, the pigeonhole design has an expected discrepancy in the order of $O \left( T^{\frac{p-1}{\sqrt{c}}} (\log T)^{\frac{1}{2}} \right)$; when $p \geq 3$, the pigeonhole design has an expected discrepancy in the order of $O \left( T^{\frac{p-1}{\sqrt{c}}} \right)$. $\square$