

Hypothesis Testing in Sequentially Sampled Data: AdapRT to Maximize Power Beyond *iid* Sampling*

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Abstract

Testing whether a variable of interest affects the outcome is one of the most fundamental problems in statistics. It is often the main scientific question of interest and also ubiquitously used in variable selection. To tackle this problem, the conditional randomization test (CRT) is widely used to test the independence of a variable of interest (X) with an outcome (Y) holding some controls (Z) fixed. The CRT uses randomization or *design-based* inference that relies solely on the random *iid* sampling of (X, Z) to produce exact finite-sample p -values that are constructed using any test statistic. We propose a new method, the *adaptive randomization test* (AdapRT), that similarly tackles the independence problem but allows the data to be sequentially sampled. Like the CRT, the AdapRT relies solely on knowing the (adaptive) sampling distribution of (X, Z) , making it a *design-based* approach. Although the AdapRT allows practitioners to flexibly design adaptive experiments, the method itself does not guarantee a powerful adaptive sampling scheme. For this reason, we show the significant power increase by adaptively sampling in two illustrative settings in the latter half of this paper. We first showcase the AdapRT in a particular multi-arm bandit problem known as the normal-mean model. Under this setting, we theoretically characterize the powers of both the *iid* sampling scheme and the AdapRT and empirically find that the AdapRT can uniformly outperform the typical uniform *iid* sampling scheme that pulls all arms with equal probability. We also surprisingly find that the AdapRT can be more powerful than even the oracle *iid* sampling scheme when the signal is relatively strong. We believe that the proposed adaptive procedure is successful mainly because it stabilizes arms that may initially look like “fake” signal. We additionally showcase the AdapRT to a popular factorial survey design setting known as conjoint analysis. We similarly find the AdapRT to be more powerful than the *iid* sampling scheme both through simulations and an application to a recent conjoint study on political candidate evaluation. Lastly, we also provide a power analysis pipeline for practitioners to diagnosis the effectiveness of their proposed adaptive procedures and apply the pipeline to the two aforementioned settings.

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1 Introduction

Independence testing is ubiquitous in statistics and often the main task of interest in variable selection problems. For example, it is an important tool in causal inference for different applications (Bates et al., 2020; Ham, Imai and Janson, 2022; Candès et al., 2018). Social scientists may wonder if a political candidate’s gender may affect voting behavior while controlling for all other gender related stereotypes to isolate the true effect of gender (Ono and Burden, 2018; Arrow, 1998; Lupia and McCubbins, 2000). Biologists may be interested in the effect of a specific gene on a characteristic after holding all other genes constant (Skarnes et al., 2011).

In the independence testing problem, the main objective is to test whether a response Y is statistically affected by a variable of interest X while controlling for other variables Z . Informally speaking, the main objective is to test $Y \perp\!\!\!\perp X \mid Z$, where Z can be the empty set for an unconditional test. For the aforementioned gender example, Y is voting responses, X is the political candidate’s gender, and Z can be the candidate’s personality, party affiliation, etc. One way to approach this problem is the *model-based* approach that uses parametric or semi-parametric methods such as regression while assuming some knowledge of $Y \mid (X, Z)$. Recently, *design-based* approach has been increasingly gaining popularity (Ham, Imai and Janson, 2022; Bates et al., 2020; Bojinov and Shephard, 2019a) to tackle the independence testing problem. In an influential paper (Candès et al., 2018), the authors introduce the conditional randomization test (CRT), which uses the “Model- X ” approach to perform randomization based inference. This approach assumes nothing about the $Y \mid (X, Z)$ relationship but shifts the burden on requiring knowledge of $X \mid Z$. In exchange, the CRT has exact type-1 error control while allowing the user to propose any test statistics, including those from complicated machine learning models, to increase power. We remark that if the data was collected from an experiment, then the distribution of (X, Z) is immediately available and the CRT can be classified as a non-parametric approach to testing.

Although the “Model- X ” randomization inference approach proposed by the CRT is close to “assumption-free” in an experimental setting (or when the distribution of (X, Z) is exactly known), it does require that the sampling scheme of (X, Z) is collected independently and identically (*iid*) from some distribution. However, the *iid* assumption may not always be appropriate or desired. For example, large tech companies such as Uber or Doordash have rich experimental data that are sequentially collected, i.e., the next treatment is sampled as a function of all of its previous history (Chiara Farronato, 2018; Glynn, Johari and Rasouli, 2020). Despite this non-*iid* experimental setup, these companies are still interested in testing whether a certain treatment has any effect, i.e., the independence testing problem. *iid* sampling may also not always be desired even if one could sample with an *iid* scheme. Since obtaining large number of samples is generally difficult and costly, practitioners may want to efficiently design an experiment to powerfully detect if X impacts Y given a small sample size. Consequently, adaptively sampling may be more effective in tackling the independence problem than a typical *iid* sampling scheme. We show this is true in two different settings in the latter half of this paper and believe the intuition within should generalize to more general settings. Currently, however, the CRT does not allow an experimenter to have this flexibility due to the *iid* sampling requirement.

Given this motivation, a natural direction is to weaken the *iid* assumption in the “Model- X ” randomization inference approach and allow testing adaptively collected data. In general, regardless of using randomization based inference, parametric inference, non-parametric inference, etc., it is difficult to get a valid test for the independence testing problem when X is adaptively sampled as a function of Y . For example, even if one knew that the true function of $Y \mid X$ was linear, a parametric linear regression approach would lead to many false discoveries due to the possible “fake” dependencies induced by the adaptive procedure. In order to construct a valid test, one would need to decouple the adaptive procedure from the “true” relationship between Y and X . Consequently, to the best of our knowledge, there does not exist a general randomization inference procedure that enjoys all the same benefits as the CRT but allows for adaptively sampled data (see Section 1.2 for more details). Therefore, the main contribution of our paper is we allow sequentially

adaptive sampling schemes in the context of the “Model-X” randomization framework while enjoying all the same benefits as those enjoyed by the CRT. More specifically we assume nothing more than the CRT, i.e., knowing the distribution of (X, Z) , but allow testing for adaptively collected data while maintaining exact finite-sample p -values using any test statistic.

This extra flexibility to allow for non-*iid* sampling opens interesting avenues of research. One important question from an experimental perspective is if one should even design an adaptive experiment for tackling the independence problem. Although our contribution allows a practitioner to consider adapting, it is not obvious that adapting is helpful. However, we show through illustrative examples how adapting sampling schemes can significantly increase power compared to *iid* sampling schemes. To achieve this, we borrow ideas from the reinforcement learning literature such as those presented in popular procedures like Thompson sampling (Thompson, 1933) and Epsilon-Greedy algorithms (Sutton and Barto, 2018b). In the reinforcement learning setting, an experimenter is faced with the task of sampling the next values of (X, Z) as a function of all the previous values of (X, Z) and Y to maximize an objective (Sutton and Barto, 2018a). For example, the commonly known “multi-arm bandit” problem (Slivkins, 2019) aims to sample the next value of X , often referred to as sampling the next “arms” of X , that would give a higher value of outcome Y . In this setting, there are finite but various choices of arms the experimenter can pull, in which the primary objective is to sequentially optimize which arm to pull to produce the maximum reward.

Although the reinforcement learning literature does not concern itself with the independence testing problem, many key ideas in popular reinforcement learning procedures boils down to identifying arms of X that have strong signals. Therefore, one could expect that incorporating a sequentially adaptive sampling scheme, such as those that are used in reinforcement learning, can be helpful in answering the independence testing problem. To provide a simple naive example, consider the aforementioned multi-arm bandit problem with a typical *iid* sampling framework that pulls each arm with equal probability for all n samples. If there exists only one arm that has a weak signal, then the power, even using powerful machine learning algorithms, is relatively low. On the other hand, if the experimenter was allowed to sequentially sample, then he/she would be able to sample more from the arm with signal, where the data would clearly show more evidence of a signal, thus perhaps leading to a greater power. We indeed use these naive strategies as starting points to construct powerful adaptive procedures in Section 3 and Section 4. We now summarize our contributions.

1.1 Our Contributions

The main contribution of our paper is we allow the same “Model-X” randomization inference procedure under sequentially collected data. More specifically, we allow the data (X_t, Z_t) to be sequentially collected at time t as a function of the historical values of $X_{1:(t-1)}, Z_{1:(t-1)}, Y_{1:(t-1)}$ while still tackling the same independence problem. In this non *iid* sampling scheme, the CRT theory is insufficient to guarantee a valid finite-sample p -value. Our contribution is helpful in two different scenarios. The first scenario is *before* the data was collected, i.e., the experiment stage, which is also the focus of our paper. Our contribution now allows experimenters to flexibly use any sequentially adaptive sampling scheme to collect data and potentially increase power compared to an *iid* sampling scheme. The second scenario is *after* the data was collected, i.e., the analysis stage. Our contribution additionally allows the analyst to run the “Model-X” randomization inference approach for any sequentially collected data such as those in time series as long as the analyst knows how the data was sequentially sampled. We call our approach the AdapRT (Adaptive Randomization Test) and we remark that the AdapRT, like the CRT, does not require any knowledge of $Y | (X, Z)$ and leverages the distribution of (X, Z) . Therefore, in an experimental setting, the AdapRT can also be viewed as a non-parametric test.

In Section 2 we formally introduce the proposed method, AdapRT, and show how the AdapRT leverages the known distribution of (X, Z) to produce exact finite-sample valid p -values for any test statistic. Although

this formally allows practitioners to adaptively sample data to potentially increase power, it does not give any guidance on how to choose a reasonable adaptive scheme. Therefore, we provide a power analysis pipeline practitioners can follow in Section 2.5. We then apply this pipeline and show how the AdapRT can be more powerful than the *iid* sampling scheme given the same test statistic and sample size in two illustrative examples. We first explore in Section 3 the AdapRT in the normal-means model setting, which is a special case of the “multi-arm” bandit setting. In this section, we apply our proposed pipeline and also theoretically characterize the power to give further understanding on how adaptive schemes may help increase power under different scenarios. We postulate that adapting can significantly increase power compared to the typical uniform *iid* sampling scheme that pulls all arms with equal probability because an adaptive scheme allows the experimenter to sample more from arms that may look like potential signals but is actually not. This is useful because such a sampling scheme then stabilizes the “fake” noisy signal arms. Additionally, it is likely that the AdapRT will also down-weight arms which (with high probability) contain no signal, thus allocating more sampling budget on exploring other relevant arms. Lastly, the AdapRT can also, to some extent, mimic the oracle *iid* scheme and achieve closer-to-oracle sampling proportions on average. We also find a stronger conclusion, namely that the AdapRT can be more powerful than even the oracle *iid* sampling scheme when the signal is relatively strong (see Section 3.3 for details). We then further explore the AdapRT’s potential in a factorial survey setting - often known as conjoint analysis in Section 4. We empirically apply the proposed pipeline through simulations and to a recent conjoint application that studies whether the gender of political candidates matter given other factors (Ono and Burden, 2018). We find similar results to those presented in Section 3, where the AdapRT is significantly more powerful than the *iid* sampling scheme. Section 5 concludes with a discussion and remarks about future work.

1.2 Related Works

In this section, we put our proposed method in the context of the current literature. The AdapRT methodology is in the intersection of reinforcement learning and “Model-X” randomization inference procedures. As far as we know, our paper is the first to weaken the *iid* assumption and allow adaptive testing in the context of randomization inference when specifically tackling the independence testing problem. We remark that (Bojinov and Shephard, 2019a) considers *unconditional* randomization testing in sequentially sampled treatment assignments. However, this work does not cover the more general case of conditional randomization testing and assumes a causal inference framework under the finite-population view when the response Y is not random given the treatment (Imbens and Rubin, 2015). Our work differs in that we allow for both super-population and finite-population view and additionally generalize to the *conditional* independence testing problem for any sequentially adaptive procedures (see Section 2.2 for more details).

As mentioned above, many ideas from the reinforcement learning literature can also be useful starting points to construct a sensible adaptive procedure. For example, we find ideas from the multi-arm bandit literature, including the Thompson sampling (Thompson, 1933) and epsilon-greedy algorithms (Sutton and Barto, 2018b), to be useful when constructing the adaptive sampling scheme. Although ideas from reinforcement learning can be utilized when performing the AdapRT, the objective of independence testing is different than that of a typical reinforcement learning problem. For example, in the multi-arm bandit problem with a binary response Y , the researcher is interested in pulling arms that maximize the number of $Y = 1$ (reward). For the inference problem, the AdapRT is interested in not only pulling arms with strong reward but also the arms that give high probability to sample $Y = 0$ since they both inform that X is not independent of Y . Furthermore, in the independence testing problem, we also care about sampling the “useless” arms to use as a baseline comparison. Therefore, the “oracle” sampling policy would not only want to sample the arm with a strong signal but also sample the other “useless” arms with no signal. However, in the bandit problem, the oracle would always sample the arm with the highest reward. This difference is illustrated and

further emphasized in the theoretical analysis of the normal means bandit problem in Section 3.3.

Lastly, there also exist rich literature dealing with the appropriateness of “Model-X” and building powerful test statistics for the application of interest (Bates et al., 2020; Ham, Imai and Janson, 2022; Candès et al., 2018; Bojinov and Shephard, 2019a) when using randomization inference such as the CRT. Although this is also crucial, this is not the main focus of our paper. We assume we are given the full distribution of (X, Z) or assume the experimenter is currently deciding on how to efficiently design the experiment. Furthermore, we do not explore which test statistics may be powerful when using the AdapRT. Although this is an interesting avenue for future research and also important to increase power, the latter half of our paper approaches this problem from the design stage, i.e., how to design an effective adaptive sampling scheme before the data is even collected. In other words, we fix a reasonable test statistic that is commonly used in a typical *iid* sampling scheme and vary the possible sampling scheme namely the *iid* sampling scheme and an adaptive sampling scheme. Since our objective is to show that the AdapRT can be useful and more powerful than the typical *iid* sampling scheme, it is sufficient to show that it can beat the power of the *iid* sampling scheme with a fixed a reasonable test statistic.

1.3 The Conditional Randomization Test (CRT)

Before proposing our method, we briefly introduce the baseline *iid* sampling scheme that uses the “Model-X” randomization inference approach - the CRT. The CRT assumes that the data $(X_t, Z_t, Y_t) \stackrel{i.i.d}{\sim} f_{XZY}$ for $t = 1, 2, \dots, n$, where f_{XZY} denotes the joint probability density function (pdf) or probability mass function (pmf) of (X, Z, Y) and n is the total sample size. For brevity, we refer to both probability density function and probability mass function as pdf¹. The CRT aims to test whether the variable of interest X affects distribution of Y conditional on Z , i.e., $Y \perp\!\!\!\perp X \mid Z$. If Z is the empty set, the CRT reduces to the (unconditional) randomization test. The CRT tests $Y \perp\!\!\!\perp X \mid Z$ by creating “fake” resamples \tilde{X}_t^b for $t = 1, 2, \dots, n$ from the conditional distribution $X \mid Z$ induced by f_{XZ} , the joint pdf of (X, Z) , for $b = 1, 2, \dots, B$, where B is the Monte-Carlo parameter of choice. More formally, the fake resamples \tilde{X}_t^b are sampled in the following way,

$$\tilde{X}_t^b \sim \frac{f_{XZ}(\tilde{x}_t^b, Z_t)}{\int_z f_{XZ}(\tilde{x}_t^b, z) dz} \text{ for } t = 1, 2, \dots, n, \quad (1)$$

where the right hand side is the pdf of the conditional distribution $X \mid Z$ induced by the joint pdf f_{XZ} , lower case \tilde{x}_t^b represents the realization of random variable \tilde{X}_t^b , and each \tilde{X}_t^b is sampled *iid* for $b = 1, 2, \dots, B$ independently of X and Y . Since each sample X_t only depends on the current Z_t , the right hand side of Equation 1 is a conditional distribution that is a function of only its current Z_t . Under the conditional independence null, $Y \perp\!\!\!\perp X \mid Z$, Candès et al. show that $(\tilde{\mathbf{X}}^1, \mathbf{Z}, \mathbf{Y}), (\tilde{\mathbf{X}}^2, \mathbf{Z}, \mathbf{Y}), \dots, (\tilde{\mathbf{X}}^B, \mathbf{Z}, \mathbf{Y})$, and $(\mathbf{X}, \mathbf{Z}, \mathbf{Y})$ are exchangeable, where \mathbf{X} denotes the complete collection of (X_1, X_2, \dots, X_n) . $\tilde{\mathbf{X}}^b, \mathbf{Z}$, and \mathbf{Y} are defined similarly. This implies that any test statistic $T(\mathbf{X}, \mathbf{Z}, \mathbf{Y})$ is also exchangeable with $T(\tilde{\mathbf{X}}^b, \mathbf{Z}, \mathbf{Y})$ under the null. This key exchangeability property allows practitioners to use any test statistic T when calculating the final p -value. More formally, the CRT proposes to obtain a p -value in the following way,

$$p_{\text{CRT}} = \frac{1}{B+1} \left[1 + \sum_{b=1}^B \mathbb{1}_{\{T(\tilde{\mathbf{X}}^b, \mathbf{Z}, \mathbf{Y}) \geq T(\mathbf{X}, \mathbf{Z}, \mathbf{Y})\}} \right] \quad (2)$$

where the addition of 1 is included so that the null p -values are stochastically dominated by the uniform distribution. Due to the exchangeability of the test statistics, the p -value in Equation 2 is guaranteed to have

¹Neither the CRT nor our paper needs to assume the existence of the pdf. However, for clarity and ease of exposition, we present the data generating distribution with respect to a pdf.

exact type-1 error control, i.e., $\mathbb{P}(p_{\text{CRT}} \leq \alpha) \leq \alpha$ for all $\alpha \in [0, 1]$ under the null $Y \perp\!\!\!\perp X \mid Z$ despite the choice of T and any relationship of $Y \mid (X, Z)$. In other words, the CRT guarantees exact valid p -values because the observed test statistic $T(\mathbf{X}, \mathbf{Z}, \mathbf{Y})$ is statistically indistinguishable from a “fake” resampled test statistic $T(\tilde{\mathbf{X}}^b, \mathbf{Z}, \mathbf{Y})$ under the null. Consequently, this also allows the practitioner to ideally choose a test statistic that is powerful to distinguish the observed test statistic with the resampled fake test statistic such as the sum of the absolute value of the main effects of X from a penalized Lasso regression (Tibshirani, 1996).

2 Methodology

With the goal of tackling the independence testing problem for sequentially generated data using a “Model- X ” randomization inference approach, we now introduce our proposed method - the Adaptive Randomization Test (AdapRT).

2.1 Sequential Adaptive Sampling

We first formally present the definition of a sequentially adaptive sampling scheme.

Definition 2.1 (Sequential adaptive procedure). We say the sample $(\mathbf{X}, \mathbf{Z}, \mathbf{Y})$ follows an adaptive procedure A if the sample obeys the following sequential data generating process.

$$\begin{aligned} (X_1, Z_1) &\sim f_1^A(x_1, z_1), \quad Y_1 \sim f_Q(x_1, z_1) \\ (X_2, Z_2) &\sim f_2^A(x_2, z_2 \mid x_1, z_1, y_1), \quad Y_2 \sim f_Q(x_2, z_2) \\ &\vdots \\ (X_t, Z_t) &\sim f_t^A(x_t, z_t \mid x_1, z_1, y_1, \dots, x_{t-1}, z_{t-1}, y_{t-1}), \quad Y_t \sim f_Q(x_t, z_t), \end{aligned}$$

where lower case (x_t, z_t, y_t) denotes the realization of the random variables (X_t, Z_t, Y_t) at time t , respectively, f_t^A denotes the joint probability density function of (X_t, Z_t) given the past realizations, and f_Q denotes the probability density function of the response Y_t as a function of only the current (X_t, Z_t) .

Definition 2.1 captures a general sequential adaptive experimental setting, where an experimenter adaptively samples the next values of (X_t, Z_t) according to a procedure f_t^A that may be dependent on all the history (including the outcome) while “nature” f_Q determines the next outcome. We emphasize that f_Q is generally unknown and in most cases hard to model exactly. Figure 1 visually summarizes the sequential adaptive procedure, where we allow the next sample to depend on all the history (including the response). Although Definition 2.1 makes no assumption about the adaptive procedure f_t^A (even allowing the adaptive procedure to change across time), it does implicitly assume that the response Y has no carryover effects, i.e., f_Q is only a function of its current realizations (x_t, z_t) as there are no arrows in Figure 1 from previous (X_{t-1}, Z_{t-1}) into current Y_t . It also assumes that f_Q is stationary and does not change across time. Both of these assumptions are typically invoked in the sequential reinforcement learning literature (Shi et al., 2022; Sutton and Barto, 2018a; Bojinov and Shephard, 2019b). Our methodology naturally extends to non-stationary models, where f_Q also depends on t . However, for presentational clarity, we present our method in the common stationary scenario. Moreover, we add that our methodology and main theoretical results should naturally extend when there are simple structural carryover effects, but we leave this for future work.

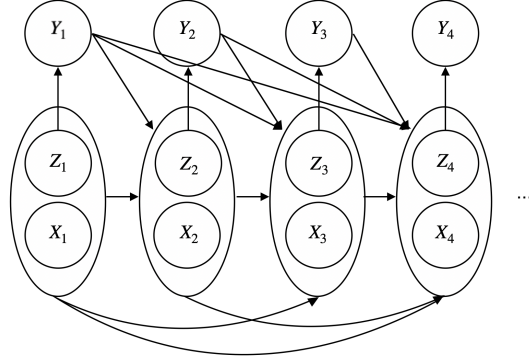


Figure 1: Schematic diagram of the Sequential Adaptive Sampling Scheme in Definition 2.1. The directed arrows denote the order in how the random variable(s) may affect the corresponding random variable(s).

Given the adaptive procedure defined in Definition 2.1, the main objective is to determine whether the variable of interest X affects Y after controlling for Z . Unlike the CRT setting, the data is no longer sampled *iid*, thus formalizing the main objective of testing $Y \perp\!\!\!\perp X \mid Z$ requires further notation. For example, in the CRT procedure, the null hypothesis of interest is formally $Y_t \perp\!\!\!\perp X_t \mid Z_t$ for all $t = 1, 2, \dots, n$. Since the data is sample *iid*, $Y_t \perp\!\!\!\perp X_t \mid Z_t$ reduces to testing $\mathbf{Y} \perp\!\!\!\perp \mathbf{X} \mid \mathbf{Z}$ using the whole data since the subscript t is irrelevant. However, for the adaptive case, $\mathbf{Y} \perp\!\!\!\perp \mathbf{X} \mid \mathbf{Z}$ is trivially false for any non-degenerate adaptive procedure A since \mathbf{X} depends on \mathbf{Y} through f_t^A . Just like the CRT, the practitioners are interested in whether X affects Y for each sample t . We now formalize this by testing the following null hypothesis H_0 against H_1 ,

$$\begin{aligned} H_0 &: f_Q(x, z) = f_Q(x', z) \text{ for all } x, x' \in \mathcal{X}, z \in \mathcal{Z} \\ H_1 &: f_Q(x, z) \neq f_Q(x', z) \text{ for some } x, x' \in \mathcal{X}, z \in \mathcal{Z} \end{aligned} \quad (3)$$

where \mathcal{X} denotes the entire domain of X that captures all possible values of X regardless of the distribution of X induced by the adaptive procedure. For example, if X is a univariate discrete variable that can take any integer values, then $\mathcal{X} = \mathbb{Z}$ even if the adaptive procedure A only has a finite support with positive probability only on values $(-1, 0, 1)$. In such a case, testing H_0 using the aforementioned adaptive procedure A will only be powerful up to the restricted support induced by A . \mathcal{Z} is defined similarly as the entire domain for Z .

We finish this subsection with a discussion of H_0 . First, H_0 captures the same notion as the CRT null of $Y \perp\!\!\!\perp X \mid Z$ because if X makes any distributional impact on Y given Z , then H_0 is false. On the other hand, if H_0 is false, then the CRT null is trivially false. Recently, Ham, Imai and Janson show that the CRT null is equivalent to testing the following causal hypothesis,

$$H_0^{\text{Causal}} : Y_t(x, z) \stackrel{d}{=} Y_t(x', z) \text{ for all } x, x' \in \mathcal{X}, z \in \mathcal{Z},$$

where $Y_t(x, z)$ is the potential outcome for individual t at values $X = x, Z = z$. The proposed H_0 implicitly already captures the causal hypothesis H_0^{Causal} because $f_Q(x, z)$, by definition, characterizes the causal relationship between (X, Z) and Y . To formally establish this in the potential outcome framework, we define $Y_t(x, z) \stackrel{i.i.d}{\sim} f_Q(x, z)$ from a super-population framework (Imbens and Rubin, 2015). Then H_0 is indeed also testing H_0^{Causal} , i.e., whether X causally impacts Y after accounting for Z . Additionally, if the researcher wishes to think in terms of the finite-population framework, i.e., conditioning on the potential outcomes and units in the sample, then only a simple modification of Definition 2.1 is needed. More specifically, we replace obtaining the response $Y_t \sim f_Q$ in Definition 2.1 from a stochastic f_Q to a fixed potential outcome

$Y_t = Y_t(x_t, z_t)$ at every time point t , where $Y_t(x_t, z_t)$ is the deterministic (non-random) potential outcome of individual t with values $X_t = x_t$ and $Z_t = z_t$. Additionally we would similarly modify H_0 to the sharp Fisher null that states $Y_t(x, z) = Y_t(x', z)$ for all $x, x' \in \mathcal{X}, z \in \mathcal{Z}$ and all individuals t in our finite population. This finite-population testing framework is the one proposed in (Bojinov and Shephard, 2019a), where the authors perform the unconditional randomization test in a sequential adaptive setting.

2.2 Adaptive Randomization Test (AdapRT)

The main contribution of this paper is that we allow the ‘‘Model-X’’ randomization inference approach when testing H_0 under a sequential adaptive setting in Definition 2.1. Since (X_t, Z_t, Y_t) are no longer sampled *iid* from some joint distribution, the main task is to construct $\tilde{\mathbf{X}}^b$ such that $(\tilde{\mathbf{X}}^b, \mathbf{Z}, \mathbf{Y})$ and $(\mathbf{X}, \mathbf{Z}, \mathbf{Y})$ are still exchangeable to ensure the validity of the p -value in Equation 2. A necessary condition for the joint distributions of $(\tilde{\mathbf{X}}^b, \mathbf{Z}, \mathbf{Y})$ and $(\mathbf{X}, \mathbf{Z}, \mathbf{Y})$ to be exchangeable is that they are equal in distribution. To achieve this, Candès et al. construct the fake resamples $\tilde{\mathbf{X}}^b$ from the conditional distribution of $X | Z$ as done in Equation 1, which directly satisfies the exchangeability criteria due to the *iid* setting of X and Z . However, in the sequential adaptive case, X_t depends on all the history including the response and it is unclear how to construct our resamples because we can not assume knowledge of f_Q .

Although there is actually not only one way to obtain valid resamples of X (further discussed in Section 2.4), we propose the most natural resampling procedure that respects our sequential adaptive setting in Definition 2.1. Before formally presenting the resampling procedure, we hint at how we construct the valid resamples $\tilde{\mathbf{X}}^b$. Similar to the CRT, the key is to create the fake copies of X by replicating the original sampling scheme of X instead conditional on \mathbf{Z}, \mathbf{Y} . For the *iid* CRT sampling scheme, this reduces to sampling X_t *iid* from the conditional distribution of $X_t | Z_t$ for all $t = 1, 2, \dots, n$. In our sequential adaptive sampling scheme, we similarly sequentially sample \tilde{X}_t by replicating the original adaptive sampling scheme of X_t conditional on \mathbf{Z}, \mathbf{Y} . Since sampling X_t does not depend on the future values of Z and Y , sampling X_t conditional on \mathbf{Z}, \mathbf{Y} reduces to sampling X_t conditional on the history as done exactly in the original adaptive sampling scheme. We now formalize this in the following definition.

Definition 2.2 (Natural Adaptive Resampling Procedure). Given data $(\mathbf{X}, \mathbf{Z}, \mathbf{Y})$, $\tilde{\mathbf{X}}^b$ follows the natural adaptive resampling procedure if $\tilde{\mathbf{X}}^b$ satisfies the following data generating process,

$$\tilde{X}_1^b \sim \frac{f_1^A(\tilde{x}_1^b, z_1)}{\int_z f_1^A(\tilde{x}_1^b, z) dz}, \tilde{X}_2^b \sim \frac{f_2^A(\tilde{x}_2^b, z_2 | \tilde{x}_1^b, z_1, y_1)}{\int_z f_1^A(\tilde{x}_1^b, z | \tilde{x}_1^b, z_1, y_1) dz}, \dots, \tilde{X}_n^b \sim \frac{f_n^A(\tilde{x}_n^b, z_n | \tilde{x}_1^b, z_1, y_1, \dots, \tilde{x}_{n-1}^b, z_{n-1}, y_{n-1})}{\int_z f_1^A(\tilde{x}_n^b, z | \tilde{x}_1^b, z_1, y_1, \dots, \tilde{x}_{n-1}^b, z_{n-1}, y_{n-1}) dz},$$

for $b = 1, 2, \dots, B$ independently condition on (\mathbf{Z}, \mathbf{Y}) , where \tilde{x}_t^b are dummy variables representing \tilde{X}_t^b .

Similar to Equation 1, Definition 2.2 formalizes how each \tilde{X}_t is sequentially sampled from the conditional distribution of $X_t | (X_{1:(t-1)}, Z_{1:t}, Y_{1:(t-1)})$. We call this the natural adaptive resampling procedure (NARP) because at each time t the fake resamples \tilde{X}_t^b are sampled from the original sequential adaptive distribution of X_t conditional on $Z_{1:t}$ and $Y_{1:(t-1)}$. Just like the CRT, Definition 2.2 requires one to sample from a conditional distribution. For this practically important consideration, we propose another alternative where the experimenter, at each time t , samples Z_t first and then samples the variable of interest X_t from $X_t | Z_{1:t}, Y_{1:(t-1)}$ at every time step (as opposed to simultaneously sampling (X_t, Z_t) from a joint distribution). This alternative procedure loses very little generality but allows the NARP in Definition 2.2 to directly sample from the already available conditional distribution. We refer to this as the convenient adaptive sampling scheme.

Unfortunately resampling from the NARP does not come for free. Recall that we require our resampled $\tilde{\mathbf{X}}^b$ to be exchangeable with \mathbf{X} conditional on (\mathbf{Z}, \mathbf{Y}) . A necessary condition of exchangeability requires the

joint distribution of $(\tilde{\mathbf{X}}, \mathbf{Y}, \mathbf{Z})$ be the same as that of $(\mathbf{X}, \mathbf{Y}, \mathbf{Z})$. In particular, the following distributional relationship is always true for any t when assuming the NARP,

$$\tilde{X}_{1:(t-1)} \perp\!\!\!\perp Z_t \mid (Y_{1:(t-1)}, Z_{1:(t-1)}), \quad (4)$$

because $\tilde{X}_{1:(t-1)}$ is a random function of only $(Y_{1:(t-1)}, Z_{1:(t-1)})$. Equation 4 shows that Z_t is independent of previous fake resamples of X . To satisfy the exchangeability criteria, we also need the same distributional relationship in Equation 4 to be satisfied by the original sampling scheme of \mathbf{X} . This leads to the following natural assumption where Z can not depend on previous X , which turns out to be both sufficient and necessary to ensure validity of using the AdapRT to test H_0 as formally stated in Theorem 2.1 and Theorem 2.2.

Assumption 1 (Z can not adapt to previous X). For each $t = 1, 2, \dots, n$ we have by basic rules of probability $f_t^A(x_t, z_t \mid x_{1:(t-1)}, z_{1:(t-1)}, y_{1:(t-1)}) = g_t^A(x_t \mid x_{1:(t-1)}, z_{1:(t-1)}, y_{1:(t-1)}, z_t)h_t^A(z_t \mid x_{1:(t-1)}, z_{1:(t-1)}, y_{1:(t-1)})$, where g_t^A, h_t^A denotes the conditional and marginal density functions induced by the joint probability density function of f_t^A respectively. We say an adaptive procedure A satisfies Assumption 1 if $h_t^A(z_t \mid x_{1:(t-1)}, z_{1:(t-1)}, y_{1:(t-1)})$ does not depend on $x_{1:(t-1)}$.

Assumption 1 states that the sequential adaptive procedure A does not allow Z_t to depend on the history of X . Although this does restrict our adaptive procedure, it is crucial that each X_t and Z_t are allowed to adapt by looking at its own previous values and the previous responses.

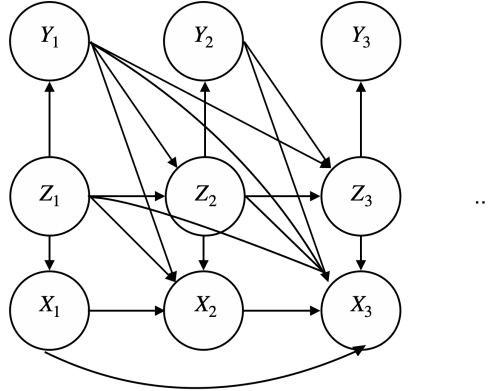


Figure 2: Schematic diagram of the convenient adaptive sampling scheme that satisfies Assumption 1. As before, the directed arrows denote the order in how the random variable(s) may affect the corresponding random variable(s).

We visually summarize Assumption 1 and a more convenient, but not necessary, way to conduct a restricted adaptive sampling scheme in Figure 2. Figure 2 shows a set of arrows from Z_t into X_t as opposed to them being simultaneously generated as in Figure 1 to allow the proposed NARP in Definition 2.2 to conveniently sample directly from the already available conditional distribution. We emphasize that this is a mere practical convenience and not necessary for the general the AdapRT procedure to work. Assumption 1 is also satisfied in Figure 2 as there exist no arrows from any $X_{t'}$ into Z_t for $t' < t$. Before stating our main theorem, we summarize the AdapRT procedure in Algorithm 1. We note that although the p -value calculation of p_{AdapRT} in Equation 5 is similar to p_{CRT} , the resamples \tilde{X}^b are different in the two procedures. We now state the main theorem that gives the validity of using the AdapRT for testing H_0 .

Algorithm 1: AdapRT p -value

Input: Adaptive procedure A , test statistic T , total number of resamples B ;

Given an adaptive procedure A , obtain n samples of $(\mathbf{X}, \mathbf{Z}, \mathbf{Y})$ according to the sequential adaptive procedure in Definition 2.1

for $b = 1, 2, \dots, B$ **do**

 └ Sample $\tilde{\mathbf{X}}^{(b)}$ according to the NARP in Definition 2.2;

Output:

$$p_{\text{AdapRT}} := \frac{1}{B+1} \left[1 + \sum_{b=1}^B \mathbb{1}_{\{T(\tilde{\mathbf{X}}^b, \mathbf{Z}, \mathbf{Y}) \geq T(\mathbf{X}, \mathbf{Z}, \mathbf{Y})\}} \right] \quad (5)$$

Theorem 2.1 (Valid p -values under the AdapRT). Suppose the adaptive procedure A follows the adaptive procedure in Definition 2.1 and satisfies Assumption 1. Further suppose that the resampled $\tilde{\mathbf{X}}^b$ follows the NARP in Definition 2.2 for $b = 1, 2, \dots, B$ conditionally independent of (\mathbf{Z}, \mathbf{Y}) . Then the p -value p_{AdapRT} in Algorithm 1 for testing H_0 is a valid p -value. Equivalently, $\mathbb{P}(p_{\text{AdapRT}} \leq \alpha) \leq \alpha$ for any $\alpha \in [0, 1]$.

Remark 1. We note that p_{AdapRT} is also a valid p -value condition on \mathbf{Y} and \mathbf{Z} .

The proof of Theorem 2.1 is in Appendix A. This theorem is the main result of this paper, which allows testing of H_0 for sequentially collected data through randomization inference. Moreover, since this result is valid for any adaptive sampling scheme, it opens new possibilities to analyze which adaptive procedures may lead to better power. Before concluding this section, as alluded before, we state formally in Theorem 2.2 that our assumption is indeed necessary to establish the exchangeability of $(\mathbf{X}, \mathbf{Z}, \mathbf{Y})$ and $(\tilde{\mathbf{X}}^b, \mathbf{Z}, \mathbf{Y})$ if we follow the natural adaptive procedure in Definition 2.2.

Theorem 2.2 (Necessity of Assumption). For any adaptive procedure A , if the resampled $\tilde{\mathbf{X}}^b$ follows the natural adaptive resampling procedure in Definition 2.2 and $(\mathbf{X}, \mathbf{Z}, \mathbf{Y})$ and $(\tilde{\mathbf{X}}^b, \mathbf{Z}, \mathbf{Y})$ are exchangeable, then Assumption 1 is necessary.

The proof is in Appendix A.

2.3 Multiple Testing

So far we have introduced our proposed method to test H_0 for a single variable of interest X conditional on Z . However, the practitioner may be interested in testing multiple H_0 for different variables of interest.

To formalize this, denote $X = (X^1, X^2, \dots, X^p)$ to contain p variables of interest, each of which can also be multidimensional. Informally speaking, our objective is to perform p tests of $Y \perp\!\!\!\perp X^j \mid X^{-j}$ for $j = 1, 2, \dots, p$, where X^{-j} denotes all variables in X except X^j . Given a fixed j , our proposed methodology in Section 2.1-2.2 can be used to test any single one of these hypothesis. The main issue with directly extending our proposed methodology for testing on all $j = 1, 2, \dots, p$ variables is that Assumption 1 does not allow X^{-j} to depend on previous X^j but X^j may depend on previous X^{-j} . This asymmetry may cause this assumption to hold when testing for X^j but also not hold when testing for $X^{j'}$ for $j \neq j'$. For example, suppose we are testing $Y \perp\!\!\!\perp X^1 \mid X^{-1}$ and allow X^1 to depend on the history of X^2 . This would satisfy Assumption 1, but Assumption 1 would be violated when testing for $Y \perp\!\!\!\perp X^2 \mid X^{-2}$. In order to satisfy Assumption 1 for all variables of interest simultaneously, we modify our procedure such that each X_t^j is independent of $X_t^{j'}$ for all j, j' and $t' \leq t$. In other words, we force each X_t^j to be sampled according to its

own history $X_{1:(t-1)}^j$ and the history of the response but not the history and current values of $X^{j'}$ for $j \neq j'$ and for every j . We formalize this in following assumption.

Assumption 2 (Each X^j do not adapt to other $X^{j'}$). For each $t = 1, 2, \dots, n$ suppose each $X_t = (X_t^1, X_t^2, \dots, X_t^p)$ are sampled according to a sequential adaptive sampling scheme A : $X_t \sim f_t^A(x_t^1, x_t^2, \dots, x_t^p \mid x_{1:(t-1)}^{-j}, x_{1:(t-1)}^j, y_{1:(t-1)})$. We say an adaptive procedure A satisfies Assumption 2 if f_t^A can be written into following factorized form,

$$f_t^A(x_t^1, x_t^2, \dots, x_t^p \mid x_{1:(t-1)}^{-j}, x_{1:(t-1)}^j, y_{1:(t-1)}) = \prod_{j=1}^p f_{t,j}^A(x_t^j \mid x_{1:(t-1)}^j, y_{1:(t-1)}^j)$$

with every $f_{t,j}^A(\cdot \mid x_{1:(t-1)}^j, y_{1:(t-1)}^j)$ being a valid probability measure for all possible values of $(x_{1:(t-1)}^j, y_{1:(t-1)}^j)$.

Assumption 2 states that X^j can not adapt and be dependent on any of the other $X^{j'}$ for every j . This assumption is sufficient to satisfy Assumption 1 when testing H_0 for any X^j , thus leading to a valid p -value for every X^j simultaneously when using the proposed AdapRT scheme in Algorithm 1. Although our framework gives valid p -values for each of the multiple tests, we need to further account for multiple testing issues. For example, one naive way to control the false discovery rate is to use the Benjamini Hochberg procedure (Benjamini and Hochberg, 1995). Since this is not the focus of our paper, we leave the multiple testing issue to future research.

2.4 Discussion of the Natural Adaptive Resampling Procedure

Keen readers may argue the NARP is merely a practical choice but an unnecessary one, thus no longer needing Assumption 1. Since we only need $(\mathbf{X}, \mathbf{Z}, \mathbf{Y})$ and $(\tilde{\mathbf{X}}^b, \mathbf{Z}, \mathbf{Y})$ to be exchangeable under the null, one could try to find a way to resample $\tilde{\mathbf{X}}^b$ to allow this exchangeability. Exchangeability requires $(\mathbf{X}, \mathbf{Z}, \mathbf{Y})$ and $(\tilde{\mathbf{X}}^b, \mathbf{Z}, \mathbf{Y})$ to be equal in distribution. Consequently, if one could sample the entire data vector $\tilde{\mathbf{X}}$ from the conditional distribution of $\mathbf{X} \mid (\mathbf{Z}, \mathbf{Y})$, then this construction of $\tilde{\mathbf{X}}$ would satisfy the required distributional equality. In general, however, it is well known that it is difficult to sample from a complicated graphical model Wainwright, Jordan et al. (2008). To further illustrate this difficulty, we show how constructing valid resamples $\tilde{\mathbf{X}}^b$ for even two time periods may be difficult without assuming Assumption 1 with the following equation.

$$\begin{aligned} & P(X_1 = x_1, X_2 = x_2 \mid Z_1 = z_1, Z_2 = z_2, Y_1 = y_1, Y_2 = y_2) \\ &= \frac{P(X_2 = x_2 \mid X_1 = x_1, Z_1 = z_1, Z_2 = z_2, Y_1 = y_1)P(Z_2 = z_2 \mid X_1 = x_1, Y_1 = y_1, Z_1 = z_1)P(X_1 = x_1 \mid Z_1 = z_1)}{\int_x P(Z_2 = z_2 \mid X_1 = x, Y_1 = y_1, Z_1 = z_1)dP(X_1 = x \mid Z_1 = z_1)} \\ &\propto P(X_2 = x_2 \mid X_1 = x_1, Z_1 = z_1, Z_2 = z_2, Y_1 = y_1) \left[P(Z_2 = z_2 \mid X_1 = x_1, Y_1 = y_1, Z_1 = z_1)P(X_1 = x_1 \mid Z_1 = z_1) \right] \end{aligned}$$

This follow directly from elementary probability calculations. Since any valid construction of $\tilde{\mathbf{X}}^b$ must have that $P(\tilde{X}_1 = x_1, \tilde{X}_2 = x_2 \mid Z_1 = z_1, Z_2 = z_2, Y_1 = y_1, Y_2 = y_2) = P(X_1 = x_1, X_2 = x_2 \mid Z_1 = z_1, Z_2 = z_2, Y_1 = y_1, Y_2 = y_2)$, the above equation shows that it is generally hard to construct valid resamples due to the normalizing constant in the denominator of the second line. We further note that Assumption 1 bypasses this problem because $P(Z_2 = z_2 \mid X_1 = x_1, Y_1 = y_1, Z_1 = z_1)$ is now independent of the condition $X_1 = x_1$. Therefore, the denominator in the second line is always $P(Z_2 = z_2 \mid X_1 = x_1, Y_1 = y_1, Z_1 = z_1)$, cancelling out with the numerator. Consequently, the entire expression above reduces to $P(X_2 = x_2 \mid X_1 = x_1, Z_1 = z_1, Z_2 = z_2, Y_1 = y_1)P(X_1 = x_1 \mid Z_1 = z_1)$, which is equivalent to sequentially sampling from the original sampling scheme.

Although, sampling from a distribution that is known up to a proportional constant has been extensively studied in Markov Chain Monte Carlo (MCMC) literature (see for instance Liu (2001)) all reasonable methods will nevertheless introduce extra computational burden to an already computationally expensive algorithm that requires $B + 1$ resamples and computation of test statistic T . Furthermore, it is unclear how “approximate” draws from the desired distribution in a MCMC algorithm may impact the exact validness of the p -values. This problem may be exacerbated when the sample size n is large. The above equation only demonstrates the problem for only two time steps, $n = 2$. For most reasonable scenarios the sample size $n \gg 2$. Since our resamples depend on the previous resamples, it may be harder to precisely obtain valid samples using MCMC methods since the errors could exponentially accumulate. Putting all this together, we choose to use the NARP along with Assumption 1 as the proposed method because it avoids these complications and leave the possibility for different resampling procedures for future research.

2.5 Pipeline for Practitioners: Choosing a Powerful Adaptive Procedure

We conclude this section with a general guideline to practitioners on how they may determine if an adaptive scheme is reasonable. Although the AdapRT described in Algorithm 1 allows a practitioner to test H_0 with a sequential adaptive procedure, the method itself does not give any hints on how a practitioner can create a reasonable adaptive procedure A to more powerfully reject H_0 . Unfortunately, there is no general theoretical guideline that will allow a class of adaptive schemes to always be more powerful than a standard *iid* data collection because the power depends on the alternative hypothesis, i.e., the true model of f_Q . Although we propose some adaptive procedures that work well under certain scenarios in Section 3 and 4, we leave the exploration of optimal adaptive schemes for specific applications for future research. Instead, we present a general power analysis pipeline practitioners can follow to determine whether a certain adaptive procedure can be helpful. To readers already familiar with standard power analysis, they may skip this section.

Since both the *iid* sampling procedure and the AdapRT procedure have exactly valid p -values, we can measure the “goodness” of an adaptive sampling scheme with respect to the statistical power of the test. The power of both the *iid* and the adaptive procedure will depend on a given test statistic T and the true model f_Q . The power of the AdapRT will additionally be dependent on the proposed adaptive procedure. Our goal is to present a pipeline to determine whether the power of a proposed adaptive procedure will be higher than that of a standard *iid* sampling scheme given a fixed sample size n and the same test statistic T . Although we provide theory on how to determine the power of a specific adaptive procedure under a normal-means model in Section 3, it is in general difficult to theoretically characterize power, especially for a complicated adaptive scenario. Therefore, we propose the practitioner run a power analysis given a guess of f_Q , \hat{f}_Q , based on domain expertise.

For concreteness, consider the motivating bandit example where a practitioner wants to determine if a treatment with multiple levels has any effect on the response. The practitioner can make an guess of the true model \hat{f}_Q such as a simple linear model with a weak main effect on a few levels of X . Suppose further there is only an experimental budget of $n = 50$. Since the practitioner is interested in determining which experimental sampling scheme will be optimal for detecting a signal (if any), the practitioner can first empirically obtain the power of a baseline *iid* sampling scheme. To do this, he/she can sample each treatment level *iid* uniformly and obtain the corresponding response Y from \hat{f}_Q for a sample size of 50. Given this sample, the practitioner can obtain one CRT based p -value p_{CRT} given a reasonable test statistic such as the sum squared of the coefficients of X from a linear regression. He/she can then empirically repeat this whole process, for example 1,000 times, to empirically obtain a power estimate of this typical uniform *iid* sampling scheme. Lastly, the practitioner can repeat this for the AdapRT with a proposed adaptive sampling scheme to compare the power. Additionally, if the practitioner has multiple adaptive procedures of interest, then he/she can obtain the empirical power for all the proposed adaptive schemes.

Algorithm 2: Pipeline to Practitioners

Input: \hat{f}_Q , test statistic T , adaptive procedures A_1, A_2, \dots, A_m , standard *iid* sampling scheme, total number of p -values P , significance level α ;

for $i = 1, 2, \dots, P$ **do**

- Sample data (\mathbf{X}, \mathbf{Z}) from a standard *iid* sampling scheme and obtain \mathbf{Y} from \hat{f}_Q
- Obtain p -value p_{CRT} for the *iid* sampling scheme with the CRT procedure and test statistic $T(\mathbf{X}, \mathbf{Z}, \mathbf{Y})$
- for** $j = 1, 2, \dots, m$ **do**
 - Sample data $(\mathbf{X}^j, \mathbf{Z}^j, \mathbf{Y}^j)$ from a sequential adaptive sampling scheme A_j and \hat{f}_Q
 - Obtain m p -values p_{AdapRT} for each adaptive sampling scheme, where the j th p -value corresponding to adaptive sampling scheme A_j is computed using Equation 5 and test statistic $T(\mathbf{X}^j, \mathbf{Z}^j, \mathbf{Y}^j)$ and the fake resamples obtained from the NARP in Definition 2.2.

Output: Empirical power for each sampling scheme, calculated as the proportion of P p -values less than α .

This power analysis pipeline will allow the practitioners to empirically diagnosis whether the proposed adaptive procedures are helpful in increasing power given a guess of the true model. Unfortunately, this pipeline leads to an accurate diagnosis only if \hat{f}_Q is close to the truth. To mitigate the reliance on specifying the correct f_Q , the practitioner can repeat this procedure for several different specifications and parameter values of \hat{f}_Q . For example, \hat{f}_Q can vary between both linear and non-linear models with weak, medium, and strong main effects. If the results show a specific adaptive procedure A that uniformly dominates other sampling schemes across all (or most) the different specifications, then the practitioner should be more comfortable with employing the adaptive sampling scheme in the real experiment. Lastly, we note that this proposed pipeline may be computationally expensive especially if the practitioner wants to try many specifications of \hat{f}_Q and many different adaptive procedures.

We summarize our proposed guideline in Algorithm 2. We denote m to be the total number of proposed adaptive schemes, which can also differ by only by a single adaptive parameter for the same class of adaptive schemes. For example, in the ϵ -greedy adaptive scheme (Sutton and Barto, 2018b), the practitioner can vary different values of ϵ since it is not clear which ϵ may be optimal for a particular alternative hypothesis f_Q . We emphasize again that although Algorithm 2 requires the practitioner to have a guess of the true model \hat{f}_Q , the practitioner can run Algorithm 2 for a class of different \hat{f}_Q for robustness. Lastly, P is the total number of Monte-Carlo p -values that the practitioner wishes to compute. Reasonable values of P is 500 – 1,000. For the remainder of the paper, we demonstrate Algorithm 2 under various common settings of interest to show an adaptive sampling scheme can indeed be helpful in increasing power

3 AdapRT in Normal Means Model

In this section, we explore the AdapRT under the well-known normal-means setting James and Stein (1961). Using local asymptotic power analysis, we theoretically characterize the power of the typical (uniform) *iid* sampling scheme and a naive, but still insightful, two stage adaptive sampling scheme.

We first introduce the normal-means setting, the sampling schemes we consider, and the test statistic in Section 3.1. We then present two main theorems, Theorem 3.1 and Theorem 3.2, that characterize the asymptotic power of both the *iid* and adaptive sampling schemes respectively under local alternatives of

$O(n^{-1/2})$ distance in Section 3.2. Finally, we numerically evaluate Theorem 3.1 and Theorem 3.2 to illustrate when the adaptive sampling scheme leads to an increase of power. Using these theoretical characterizations of power, we also concretely showcase the proposed pipeline in Section 2.5 by illustrating when adapting is helpful for this setting in Section 3.3. Lastly, we attempt to postulate the main reasons for why an adaptive sampling scheme is more powerful than an *iid* sampling scheme in Section 3.4.

3.1 Normal Means Model

Formally, the normal-means model is characterized by the following model.

$$f_Q = Y \mid (X = j) \sim \mathcal{N}(\theta_j, 1), \quad \text{for } j \in \mathcal{X} := \{1, 2, \dots, p\},$$

where j refers to the p different possible integer values of X . We refer to the different values of X as different arms. Our task is to characterize power under the alternative, i.e., when at least one arm of X has a different mean than that of the other arms. For simplicity we consider an alternative where only one arm has a positive non-zero mean while the remaining $p - 1$ arms have zero mean. This leads to the following one-sided alternative.

$$H_1^{\text{NMM}} : \text{there exists only one } j^* \text{ such that } \theta_{j^*} = h > 0 \text{ and } \theta_j = 0, \forall j \neq j^*,$$

As usual, our null assumes that X does not affect Y in any way, i.e., all arms have the same mean.

$$H_0^{\text{NMM}} : \theta_j = 0, \forall j \in \{1, 2, \dots, p\}.$$

Given a budget of n samples, our task is to come up with a reasonable adaptive sampling scheme that leads to a higher power than that of the typical uniform *iid* sampling scheme. Because we do not use a fully adaptive procedure for this setting but a simplified two step adaptive procedure, in we use subscript i instead of t to denote the sample index for this section. We now introduce the typical uniform *iid* sampling scheme.

Definition 3.1 (Normal Means Model: *iid* Sampling Scheme with Weight Vector q). We call a sampling scheme *iid with weight vector* $q = (q_1, q_2, \dots, q_p)$ if each sample of $\mathbf{X} = (X_1, X_2, \dots, X_n)$ is sampled independently and

$$\mathbb{P}(X_i = j) = q_j, \text{ for any } i \in 1, 2, \dots, n \text{ and } j \in \mathcal{X}. \quad (6)$$

We note that this definition is more general than the classical uniform *iid* sampling scheme, in which $q = (1/p, 1/p, \dots, 1/p)$. We further denote $\mathbf{X} \sim \mathcal{M}(q)$ to compactly describe the *iid* sampling scheme for \mathbf{X} . With a slight abuse of notation, we also use $X_i \sim \mathcal{M}(q)$ to denote the above distribution of X_i .

Despite the simplicity of the normal-means setting, analysing the power of a fully adaptive procedure is generally theoretically infeasible. For example, if every sample is dependent on the previous history, no central limit theorems will allow any distributional statements due to this heavy dependence. To make the problem theoretically tractable, we consider a naive “two stage” adaptive procedure. The first stage is an exploration stage that follows the typical *iid* sampling scheme while the second stage is again another *different iid* sampling scheme that adapts based on the first stage’s data. More specifically, the second stage will adapt by reweighting the probability of pulling each arm by a function of the sample mean. Under the alternative we consider, we expect the arm with the true signal will on average have a higher sample means, thus we can exploit this in the second stage. Furthermore, the adaptive procedure will also detect arms that, by chance, lead to a higher sample mean. In such a case, we can additionally identify these “fake” signal arms and sample more to “de-noise” these arms. We note that this two-stage adaptive scheme does not utilize the full potential of an adaptive sampling scheme, but we show that even a simple two stage adaptive scheme such as this can lead to insightful gains and conclusions. We formally summarize the two stage adaptive sampling scheme in Definition 3.2.

Definition 3.2 (Normal Means Model: Two Stage Adaptive Sampling Scheme). An adaptive sampling scheme is called a *two stage adaptive sampling scheme* with *exploration parameter* ϵ , *reweighting function* f and *scaling parameter* t if (\mathbf{X}, \mathbf{Y}) are sampled by the following procedure. First, for $1 \leq i \leq \lfloor n\epsilon \rfloor$,

$$\begin{aligned} X_i &\stackrel{iid}{\sim} \mathcal{M}(q), \text{ for } 1 \leq i \leq \lfloor n\epsilon \rfloor; \\ Y_i &\stackrel{iid}{\sim} f_Q(x_i). \end{aligned}$$

Second, for each $j \in \mathcal{X}$, we compute the sample mean for each arm using the $\lfloor n\epsilon \rfloor$ samples from the first stage,

$$\bar{Y}_j^{\text{F}} := \frac{\sum_{i=1}^{\lfloor n\epsilon \rfloor} Y_i \mathbb{1}_{X_i=j}}{\sum_{i=1}^{\lfloor n\epsilon \rfloor} \mathbb{1}_{X_i=j}},$$

in which the superscript ‘‘F’’ stands for the first stage. Third, we calculate a reweighting vector $Q \in \mathbb{R}^p$ as a function of \bar{Y}_i^{F} 's that captures the main adaptive step,

$$Q_j = \frac{f(t\sqrt{n} \cdot \bar{Y}_j^{\text{F}})}{\sum_{k=1}^p f(t\sqrt{n} \cdot \bar{Y}_k^{\text{F}})}. \quad (7)$$

Finally, sample the second batch of samples using the new weighting vector, namely, for $\lfloor n\epsilon \rfloor + 1 \leq i \leq n$

$$\begin{aligned} X_i &\stackrel{iid}{\sim} \mathcal{M}(Q); \\ Y_i &\stackrel{iid}{\sim} f_Q(x_i). \end{aligned}$$

We comment that $f(\cdot)$ denotes the adaptive reweighting function. For example if $f(x) = e^x$, then this reweights the probability by an exponential function, where t is a hyper-parameter of choice and a larger value of t will lead to a more disproportional sampling of X for the second stage. For example if $f(x) = \exp(x)$, then this reweights the probability by an exponential function. We also scale the reweighting function by \sqrt{n} because the signal arm will contain signal that decreases as a function of \sqrt{n} as we describe now in the following section.

3.2 Theoretical Power Analysis Through Local Asymptotics

3.2.1 Setting

Although one could simulate the power for both the *iid* sampling scheme and the adaptive sampling scheme, we choose to theoretically characterize the power to allow for deeper insights and exploration of this setting across an entire grid of different signal strengths and dimension of X . For readers wishing to skip the theoretical details, they may choose to skip Section 3.2 with an understanding that we successfully characterized the asymptotic power of both the uniform *iid* sampling scheme and the two stage adaptive sampling scheme. To do this, we use key ideas from the classical local asymptotic theory Le Cam (1956). We remark that for our setting we apply the classical local asymptotic theory to characterize the power of different sampling schemes as opposed to characterizing the distribution of different test statistics of the data from a fixed sampling scheme. In our asymptotic setting, we keep p fixed and let $n \rightarrow \infty$. To avoid the power from approaching one, we scale our signal strength h proportional to the standard parametric rate $n^{-1/2}$, formally

$$h = \frac{h_0}{\sqrt{n}} > 0, \quad (8)$$

where h_0 is a positive constant.

As introduced in Definition 3.1, we first analyze the power under an *iid* sampling scheme with arbitrary weight vector $q = (q_1, q_2, \dots, q_p)$ such that q_i 's are all positive and $\sum_{i=1}^p q_i = 1$. Without loss of generality, we assume under H_1^{NMM} the signal is in the first arm, i.e., $j^* = 1$. Consequently, we have under H_1^{NMM} ,

$$\begin{aligned} \mathbf{X} &\sim \mathcal{M}(q) \\ Y_i | X_i = 1 &\stackrel{\text{i.i.d.}}{\sim} \mathcal{N}\left(\frac{h_0}{\sqrt{n}}, 1\right) \\ Y_i | X_i = j &\stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1), \text{ for } j \neq 1. \end{aligned}$$

Equivalently,

$$Y_i = S_i \left(W_i + \frac{h_0}{\sqrt{n}} \right) + (1 - S_i) G_i,$$

where W_i and G_i are standard normal random variables, $S_i := \mathbb{1}_{X_i=1} \sim \text{Bernoulli}(q_1)$ and all W_i 's, G_i 's and S_i 's are independent.

Following the CRT procedure in Section 1.3, since there is no Z to condition on, the fake resample copies, $\{\tilde{\mathbf{X}}^b\}_{b=1}^B$, are generated independently from exactly the same distribution as \mathbf{X} ,

$$\tilde{X}_i^b \stackrel{\text{i.i.d.}}{\sim} \mathcal{M}(q).$$

To finally compute the p -value as done in Equation 5, we need a reasonable test statistic. Therefore, we use maximum of all sample means for each arm as the main proposed test statistic,

$$T(\mathbf{X}, \mathbf{Y}) = \max_{j \in 1, 2, \dots, p} \bar{Y}_j := \max_{j \in 1, 2, \dots, p} \frac{\sum_{i=1}^n Y_i \mathbb{1}_{X_i=j}}{\sum_{i=1}^n \mathbb{1}_{X_i=j}}. \quad (9)$$

We remark that another natural testing statistic \bar{Y} is degenerate in our testing framework since it does not even depend on \mathbf{X} or $\tilde{\mathbf{X}}$. For the sake of notation simplicity, we define the following *resampled test statistic*

$$\tilde{T}(\tilde{\mathbf{X}}, \mathbf{Y}) = \max_{j \in 1, 2, \dots, p} \tilde{Y}_j := \max_{j \in 1, 2, \dots, p} \frac{\sum_{i=1}^n Y_i \mathbb{1}_{\tilde{X}_i=j}}{\sum_{i=1}^n \mathbb{1}_{\tilde{X}_i=j}},$$

in which, formally speaking, $\tilde{\mathbf{X}} = (\tilde{X}_1^1, \dots, \tilde{X}_n^1) := \tilde{\mathbf{X}}^1$ and readers should comprehend $\tilde{\mathbf{X}}$ as a generic copy of $\tilde{\mathbf{X}}^b$. Lastly, to deal with the Monte-Carlo parameter B , we show in Appendix B that as $B \rightarrow \infty$ the power of testing H_1 against H_0 is equal to

$$\mathbb{P} \left(\mathbb{P} \left[T(\mathbf{X}, \mathbf{Y}) > z_{1-\alpha}(\tilde{T}(\tilde{\mathbf{X}}, \mathbf{Y})) \mid \mathbf{Y} \right] \right). \quad (10)$$

where $z_{1-\alpha}(\tilde{T}(\tilde{\mathbf{X}}, \mathbf{Y}))$ is the $1 - \alpha$ quantile of the distribution of $\tilde{T}(\tilde{\mathbf{X}}, \mathbf{Y})$ conditioning on \mathbf{Y} . With the above setting, one can explicitly derive the joint asymptotic distributions of \bar{Y}_j 's, \tilde{Y}_j 's and \bar{Y} under the alternative H_1 . Consequently, we state the first main theorem of this section which characterizes the asymptotic power of the *iid* sampling schemes with test statistic T as defined in Equation 9.

3.2.2 Theoretical Results

All proofs presented in this section are in Appendix B.

Theorem 3.1 (Normal Means Model: Power of RT under *iid* sampling schemes). Upon taking $B \rightarrow \infty$, the asymptotic power of the *iid* sampling scheme with probability weight vector $q = (q_1, q_2, \dots, q_p)$, as defined in Definition 3.1, with respect to the RT with the “maximum” test statistic, is equal to

$$\text{Power}_{\text{iid}}(q) = \mathbb{P} \left(T_{\text{iid}} \geq z_{1-\alpha} \left(\tilde{T}_{\text{iid}} \right) \right),$$

where $z_{1-\alpha}$ is the $1 - \alpha$ quantile of the distribution of \tilde{T}_{iid} . T_{iid} and \tilde{T}_{iid} are defined/generated as a function of $G := (G_1, G_2, \dots, G_{p-1})$ and $H := (H_1, H_2, \dots, H_{p-1})$, both of which are independent and follow the same $(p - 1)$ dimensional multivariate Gaussian distribution $\mathcal{N}(0, \Sigma(q))$. T_{iid} and \tilde{T}_{iid} are then defined as

$$\begin{aligned} T_{\text{iid}} &= T_{\text{iid}}(q, G, H) \\ &:= \max \left(\left\{ H_1 + h_0 \right\} \cap \left\{ H_j, j = 2, \dots, p-1 \right\} \cap \left\{ -\frac{1}{q_p} \sum_{i=1}^{p-1} q_i H_i \right\} \right) \end{aligned} \quad (11)$$

and

$$\begin{aligned} \tilde{T}_{\text{iid}} &= \tilde{T}_{\text{iid}}(q, G, H) \\ &:= h_0 q_1 + \max \left(\left\{ G_j, j = 1, \dots, p-1 \right\} \cap \left\{ -\frac{1}{q_p} \sum_{j=1}^{p-1} q_j G_j \right\} \right). \end{aligned} \quad (12)$$

Matrices Σ_0 and D are defined as

$$\Sigma_0(q) := \begin{bmatrix} v(q_1) & -q_1 q_2 & -q_1 q_3 & \cdots & -q_1 q_{p-1} \\ -q_1 q_2 & v(q_2) & -q_2 q_3 & \cdots & -q_2 q_{p-1} \\ -q_1 q_3 & -q_2 q_3 & v(q_3) & \cdots & -q_3 q_{p-1} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ -q_1 q_{p-1} & -q_2 q_{p-1} & -q_3 q_{p-1} & \cdots & v(q_{p-1}) \end{bmatrix} \in \mathbb{R}^{(p-1) \times (p-1)},$$

with $v(x) = x(1 - x)$, and

$$D(q) := \text{diag}(q_1, q_2, \dots, q_{p-1}) \in \mathbb{R}^{(p-1) \times (p-1)}.$$

Finally,

$$\Sigma(q) := D(q)^{-1} \Sigma_0(q) D(q)^{-1}. \quad (13)$$

Although the Theorem 3.1 is stated for any general weight vector q , the default choice of weight vector q should be $(1/p, 1/p, \dots, 1/p)$ since the practitioner typically has no prior information about which arm is more important. We refer to this choice of q as the uniform *iid* sampling scheme. We also note that if we assume p to be “large” (in a generic sense) and our sampling probabilities $q_j = O(1/p)$ for all j , then the diagonal elements of $\Sigma(q)$ will be generally much larger than the off-diagonal elements. Consequently G and H in Theorem 3.1 will have approximately independent coordinates, thus both T_{iid} , \tilde{T}_{iid} are characterized by nearly independent Gaussian distribution. Before stating the theorem that characterizes the power of the adaptive sampling scheme, we make a few remarks that hint at surprising but interesting results we further explore in the subsequent sections.

Remark 2. Suppose an oracle that knows which arm is the signal. Then a naive, but natural idea, for the oracle would be to sample more from the arm with signal, i.e., choose large values of q_1 , to maximize power. As we will further demonstrate in the next section, choosing larger values of q_1 is not uniformly the dominant strategy. In other words, the optimizer $\hat{q}_1 := \arg \max_{q_1} \text{Power}_{\text{iid}}(q)$ is not necessarily larger than $1/p$, illustrating that it is actually better to sometimes sample less from the actual signal arm depending on the signal strength. This hints at the well known bias-variance trade-off between the mean difference of T and \tilde{T} and their variances, which can be hinted by comparing Equation 11 and Equation 12.

Remark 3. Following the previous remark, another naive but natural suggestion is to construct an adaptive procedure that up-weights or down-weights the signal arm according to the oracle q_1 . However, Section 3.3 shows this naive strategy is not always recommended as the adaptive procedure can do better than even the oracle *iid* sampling procedure.

By an argument similar to proof for Theorem 3.1, we can also derive the asymptotic power for our two-stage adaptive sampling schemes.

Theorem 3.2 (Normal Means Model: Power of the AdapRT under two-stage adaptive sampling schemes). Upon taking $B \rightarrow \infty$, the asymptotic power of a two-stage adaptive sampling schemes with *exploration parameter* ϵ , *reweighting function* f , *scaling parameter* t and test statistic T as defined in Definition 3.2, with respect to the AdapRT with “maximum” test statistic, is equal to

$$\text{Power}_{\text{adap}}(\epsilon, t, f) := \mathbb{P}_{R^F, G^F, R^S, H^F} \left(\mathbb{P} \left(T_{\text{adap}} \geq z_{1-\alpha}(\tilde{T}_{\text{adap}} \mid R^F, R^S, H^F, H^S) \mid R^F, R^S, H^F, H^S \right) \right) \quad (14)$$

where $z_{1-\alpha}(\tilde{T}_{\text{adap},j} \mid R^F, R^S, H^F, H^S)$ denotes the $1 - \alpha$ quantile of the conditional distribution of \tilde{T}_{adap} given R^F, R^S, G^F and G^S .

$$\begin{aligned} T_{\text{adap}} &= \max_{j \in \{1, 2, \dots, p\}} T_{\text{adap},j} \\ \tilde{T}_{\text{adap}} &= \max_{j \in \{1, 2, \dots, p\}} \tilde{T}_{\text{adap},j} \\ T_{\text{adap},j} &= \frac{q_j \sqrt{\epsilon} W_j + Q_j \sqrt{(1-\epsilon)} \left[H_j^S + R^S + \mathbb{1}_{j=1} \sqrt{1-\epsilon} h_0 \right]}{\epsilon q_j + (1-\epsilon) Q_j} \\ \tilde{T}_{\text{adap},j} &= \frac{q_j \sqrt{\epsilon} \tilde{W}_j + \tilde{Q}_j \sqrt{(1-\epsilon)} \left(G_j^S + R^S + \sqrt{1-\epsilon} h_0 Q_1 \right)}{\epsilon q_j + (1-\epsilon) \tilde{Q}_j} \end{aligned}$$

where $R^F, R^S, G^F, G^S, H^F, H^S, Q, \tilde{Q}, W$ and \tilde{W} are random quantities generated from the following procedure. First, generate $R^F \sim \mathcal{N}(0, 1)$, $G^F \sim \mathcal{N}(0, \Sigma(q))$, and $H^F \sim \mathcal{N}(0, \Sigma(q))$ independently, where $\Sigma(\cdot)$ is defined in Equation 13. Second, compute

$$\begin{aligned} W_j &= H_j^F + R^F + \mathbb{1}_{j=1} \sqrt{\epsilon} h_0, \text{ for } j \in \{1, 2, \dots, p-1\}, \\ \tilde{W}_j &= G_j^F + R^F + \sqrt{\epsilon} h_0 q_1, \text{ for } j \in \{1, 2, \dots, p-1\}, \\ W_p &= -\frac{1}{q_p} \sum_{j=1}^{p-1} q_j H_j^F + R^F + \sqrt{\epsilon} h_0 q_1 (1 - q_1), \\ \tilde{W}_p &= -\frac{1}{q_p} \sum_{j=1}^{p-1} q_j G_j^F + R^F + \sqrt{\epsilon} h_0 q_1. \end{aligned}$$

Third, compute

$$\begin{aligned} Q_j &= \frac{f(W_j / \sqrt{\epsilon})}{\sum_{j=1}^p f(W_j / \sqrt{\epsilon})}, \\ \tilde{Q}_j &= \frac{f(\tilde{W}_j / \sqrt{\epsilon})}{\sum_{j=1}^p f(\tilde{W}_j / \sqrt{\epsilon})}. \end{aligned}$$

We note that with a slight abuse of notation, the Q defined here is the asymptotic distributional characterization of that introduced in Equation 7. Lastly, generate $R^S \sim \mathcal{N}(0, 1)$, $H^S \sim \mathcal{N}(0, \Sigma(Q))$ and $G^S \sim \mathcal{N}(0, \Sigma(\tilde{Q}))$ independently.

Although Theorem 3.2 formally characterizes the asymptotic power for two-stage adaptive procedures, the final result for the asymptotic power, namely Equation 14, is not immediately insightful due to the complicated nature of both the “maximum” test statistic and the adaptive sampling scheme. Though Theorem 3.2 is not directly interpretable, the computational cost of evaluating it numerically is less than naively simulating the adaptive procedure for a large value of n by a factor of $O(n)$. Moreover, since the asymptotic power characterized in Theorem 3.1 and Theorem 3.2 does not depend on n , the conclusion is naturally more consistent and unified when compared to the empirical power obtained from simulating with different large n 's. Apart from the computational advantages the theorem provides, it is also of theoretical interest by itself, since local asymptotic power analysis is usually performed over different test statistics while our work leverages local asymptotic power analysis to characterize different sampling strategies. In addition, this theorem can also serve as a starting point and motivating example for theoretically analyzing future adaptive procedures.

3.3 Power Advantage of the AdapRT

Given the theory presented in the previous section, we now attempt to understand how the AdapRT may be more powerful than the *iid* sampling scheme. A natural starting point for devising a reasonable adaptive strategy is to leverage the “oracle” *iid* sampling scheme. The oracle *iid* sampling scheme can also serve as an important benchmark. As alluded in Remark 2, if a practitioner knows which arm contains the signal, then a naive but natural adaptive strategy is to up-weight or down-weight the known signal arm according to the oracle. We formally define the oracle in the following way, where we assume, without loss of generality, $j^* = 1$,

$$q_1^* := \arg \max_{0 \leq q_1 \leq 1} \text{Power}_{\text{iid}}(q(q_1)),$$

in which $q(q_1) := (q_1, (1 - q_1)/(p - 1), (1 - q_1)/(p - 1), \dots, (1 - q_1)/(p - 1)) \in \mathbb{R}^p$ denotes the sampling probabilities of all p arms, where the first signal arm has probability q_1 and the remaining arms (that have no signal) equally share the remaining sampling probability. Let $q^* = q(q_1^*)$, i.e., the oracle *iid* sampling scheme that samples the known treatment arm in an optimal way. We refer to the *iid* sampling with weight vector q^* as the “oracle *iid* sampling scheme”².

Next, we use numerical evaluations of Theorem 3.1 and Theorem 3.2 to compare the testing power of (two-stage) the AdapRT, uniform *iid* sampling and the oracle *iid* sampling scheme q^* across a grid of possible signal strengths h_0 and number of arms p . For the AdapRT procedure described in Definition 3.2, we choose the reweighting function f to be the exponential function, i.e., $f(x) = \exp(x)$.

The first figure, Figure 3, aims to show how the AdapRT's power is greater than both the uniform *iid* sampling scheme and even the oracle *iid* sampling scheme. To produce this figure, we first fix an arbitrary, but reasonable, combination of hyper-parameters for the AdapRT, i.e., we set exploration parameter $\epsilon = 0.5$ and reweighting parameters $t_0 = \log 2$ and $t = t_0/h_0$. We do this to demonstrate the AdapRT's (empirical) robustness as we present the preliminary power results without necessarily varying all the AdapRT adaptive parameters according to different values of h_0 and p . As a reminder, exploration parameter $\epsilon = 0.5$ implies the adaptive procedure spends half of the sampling budget on exploration and only adapts once by reweighting (see Definition 3.2) after the first half of *iid* samples are collected. The choice of $t_0 = \log 2$ allows the first arm (containing the real signal) to get roughly twice more sampling weight than the remaining arms in the second stage in expectation.

² q^* is not technically the optimal *iid* sampling scheme for all possible *iid* sampling scheme since we consider the maximum power when only varying q_1 while imposing the remaining arms to all have equal probabilities. However, we do not imagine any other reasonable *iid* sampling procedure to have a stronger power than q^* since the remaining $p - 1$ arms with no signals are not differentiable in any way, thus we lose no generality by setting them with equal probability.

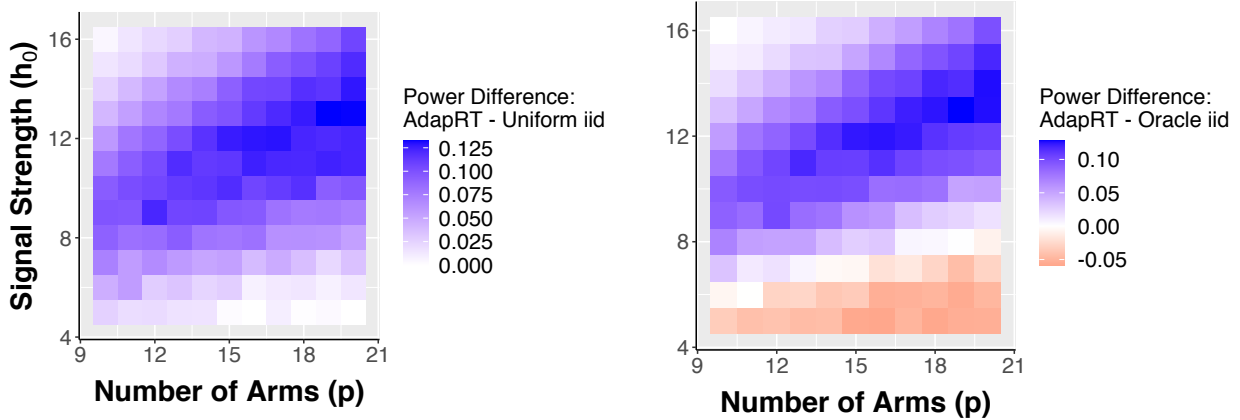


Figure 3: The figure shows the difference between the local asymptotic power of the AdapRT (with a fixed arbitrary choice of hyper-parameters $\epsilon = 0.5$ and $t = \log 2/h_0$) and the *iid* sampling scheme for different values of signal strength h_0 and number of arms p . The test statistic is the same "maximum of means" statistic as defined in Equation 9. The left plot showcases the fact that the power of the AdapRT is almost uniformly strictly higher than that of the default uniform *iid* sampling. The right plot shows that the power of the AdapRT is higher than that of even the oracle *iid* sampling procedure when the signal strength is relatively high. We note that values on the top left corners of both heatmaps are close to 0 only because the power of all three sampling schemes is almost degenerately one. The significance level is $\alpha = 0.05$.

The left panel of Figure 3 shows that the AdapRT is almost uniformly strictly better than the default uniform *iid* sampling. For example, in areas that have high number of arms and signal, the AdapRT can have close to 10% more power than the uniform *iid* sampling scheme. The right panel of Figure 3 surprisingly shows that the AdapRT can beat even the oracle *iid* sampling scheme when signal strength is relatively high. This power difference can be as large as 10% when the signal and number of arms are high. However, we note that the AdapRT's power can be lower than that of the oracle *iid* sampling scheme when the signal is low. We postulate further in Section 3.4 how and why the AdapRT may be helping in power. We note that for both panels in Figure 3, the top left corners of the heatmaps have zero difference between the two sampling schemes because this regime of strong signal and low p results in a degenerate power close to one, allowing no significant differences.

Figure 3 already shows how the AdapRT for an arbitrary choice of adaptive parameters can be uniformly more powerful than a typical *iid* sampling scheme. Additionally, Figure 3 already demonstrates the pipeline proposed in Algorithm 2 by testing one specific adaptive procedure against the *iid* sampling scheme for a variety of f_Q . Consequently, the practitioner can now be comfortable to use the proposed AdapRT with adaptive parameters chosen to $\epsilon = 0.5$ and $t = \log 2/h_0$ to run their experiment. However, to further optimize for multiple adaptive procedures A as shown in Algorithm 1, we additionally create Figure 4 to explore the different adaptive parameters ϵ and reweighting parameter t_0 that may lead to a more optimal adaptive procedure. Furthermore, since the practitioner will most likely know the number of arms he/she has for the respective problem, we fix $p = 15$ arms and vary the value of the signal.

Figure 4 shows that an adaptive procedure with exploration parameter $\epsilon = 0.7$ seems to be a favorable

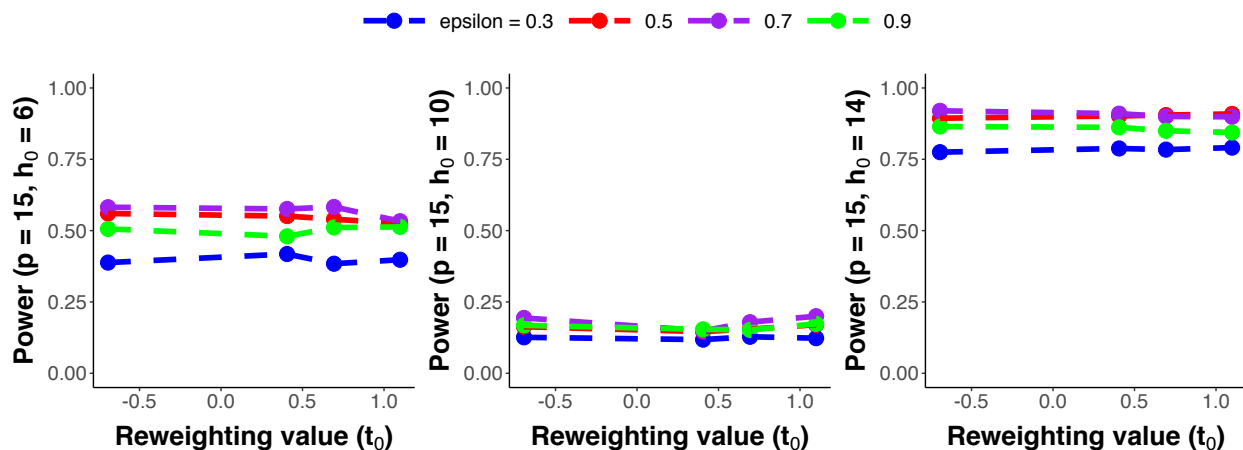


Figure 4: The figure above showcases the pipeline (see Section 2.5) of how to use pre-study simulations to choose among different possible adaptive schemes, or in this particular example, different adaptive hyper-parameters. Each panel showcases the power for different exploration parameter ϵ across different reweighting parameter t_0 , where $t = t_0/h_0$. The panels differ by different signal strengths $h_0 = 6, 10, 14$ while the number of arms are fixed at $p = 15$.

choice across different signal strengths. Additionally, we find that the optimal reweighting parameter t can be different across different scenarios but does not seem to matter largely across the different scenarios. Consequently, the practitioner should feel comfortable with employing the adaptive procedure with exploration parameter $\epsilon = 0.7$ and reweighting parameter $t_0 = \log(2)$.

3.4 Understanding why Adapting Helps

In this subsection, we summarize some of the insights we find from the above analysis of the normal means model. Our goal is to characterize why adapting is helpful so practitioners can use the same ideas to build their own successful adaptive scheme. We note that all statements here are respect to the specific normal-means model setting, but we believe that the main ideas should generalize to different applications and scenarios as shown in Section 4. Furthermore, we emphasize that all conclusion and insights presented here are speculations based on empirical evidence and intuition as opposed to strict theoretical characterizations. Unfortunately, it is difficult to precisely verify many of the presented insights because the power of the AdapRT and the CRT depends on the behavior of also the resampled test statistics. For example, even if we can empirically verify that the adaptive procedure is sampling arms without real signal with lower probability, it does not directly imply the power is greater because the resampled test statistic could similarly do the same thing. This would make both the observed and resampled test statistic approximately indistinguishable, leading to an insignificant p -value. Therefore, Figure 3 should serve as the main result that highlights how adapting can indeed help. Nevertheless, we attempt to show some empirical evidence of how adapting is helping but leave the precise theoretical understanding to future research.

As pointed out at the beginning of Section 3.3, a natural idea is to try to design adaptive strategies that mimic the oracle *iid* procedure, which indeed is a useful starting point. However, the power gain shown in Figure 3 can not be attributed to only mimicking the oracle *iid* sampling scheme because Figure 3 shows the AdapRT can beat even the oracle *iid* sampling as long as the signal strength is not too low. Additionally, it is not even clear if the oracle sampling scheme always samples the signal arm with higher probability like our adaptive sampling scheme does. Consequently, to understand the oracle sampling scheme's behavior further,

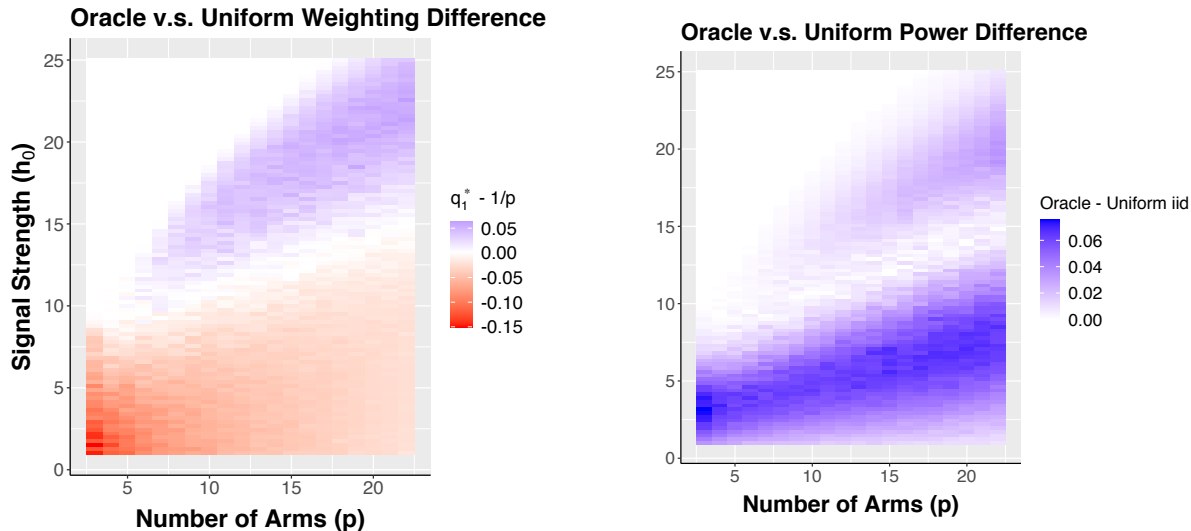


Figure 5: This figure compares the *iid* oracle sampling scheme with the uniform *iid* sampling scheme. The first panel on the left compares whether oracle q_1^* should down-weight (less than $1/p$) or up-weight (more than $1/p$) the signal arm. The second panel compares the power difference between the oracle and uniform sampling schemes.

we present Figure 5 that compares the oracle sampling scheme’s behavior with the *iid* uniform sampling scheme.

Figure 5 shows that whether the oracle should up-weight the signal arm or not, i.e., whether q_1^* is smaller or larger than $1/p$, actually depends on both h_0 and p . There are regions such as the red region plot on the left in Figure 5 where the oracle sampling scheme actually down-weights the signal arm to spend more sampling budget on other arms. Therefore, if mimicking the oracle sampling scheme is the ideal solution, one should similarly chosen an adaptive procedure that down-weights the signal arm in the red region. However, when comparing Figure 3 and the left plot in Figure 5, we see that the up-weighting (since $t > 0$) adaptive procedure can actually beat not only uniform *iid* sampling scheme but also oracle *iid* sampling scheme in parts of the region that we are supposed to down-weight.

Instead, as alluded previously, we believe the main intuition behind the success of the AdapRT is for the following three reasons. As expected, the first reason is that the AdapRT can, to some extent, mimic the oracle *iid* scheme and achieve closer-to-oracle sampling proportions on average (at least for the regimes that up-weight the signal arm). Additionally, and most importantly, when the AdapRT is sampling from the arms that look like signal it is not only sampling from the arms that is truly the real signal but also the arms that are “fake” signals due to chance. In other words, the AdapRT also samples more from these noisy “fake” signal arms to stabilize these arms to a correctly null state. Thirdly, the AdapRT also down-weights arms (with high probability) that contain no signal, allowing our remaining samples to focus on exploring the more relevant arms.

4 AdapRT in Conjoint Studies

In this section, we further demonstrate how the AdapRT can help in a popular factorial design - conjoint analysis. Conjoint analysis, introduced more than half a century ago (Luce and Tukey, 1964), is a factorial survey-based experiment designed to measure preferences on a multidimensional scale. Conjoint analysis has been extensively used by marketing firms to determine desirable product characteristics (e.g., Bodog and Florian, 2012; Green, Krieger and Wind, 2001). Recently, it has gained popularity among social scientists

(Hainmueller, Hopkins and Yamamoto, 2014; Raghavaram, Wiley and Chitturi, 2010) who are interested in studying individual preferences concerning elections (e.g., Ono and Burden, 2018), immigration (e.g., Hainmueller and Hopkins, 2015), employment (e.g., Popovic, Kuzmanovic and Martic, 2012), and other issues. Recently Ham, Imai and Janson introduced the CRT in the context of conjoint analysis to test whether a variable of interest X matters at all for a response Y given Z .

Following the guideline proposed in Algorithm 2, we first perform our power analysis through simulations in Section 4.1 to showcase how the proposed adaptive procedure can be helpful in a conjoint setting. Unlike the analysis performed above in Section 3, we do not theoretically characterize the power and in exchange consider a more realistic fully adaptive procedure and complicated test statistic. We then apply our proposed methodology on a recent conjoint study that studies whether a political candidate gender's matter in voting behavior given the candidate's age, experience, etc (Ono and Burden, 2018). We show how the proposed adaptive procedure in Section 4.1 leads to a greater power than that of the original *iid* sampling scheme by replicating the original experiment through "bootstrapping" the original sample.

4.1 Conjoint Analysis

In a typical conjoint design, respondents are forced to choose between two profiles presented to them - often known as a forced-choice conjoint design (Ham, Imai and Janson, 2022; Hainmueller, Hopkins and Yamamoto, 2014; Ono and Burden, 2018). We refer to the two profiles as the "left" (L) and "right" (R) profiles³. In this forced-choice design, the response Y is a binary variable that takes value 1 if the respondent chooses the left profile and zero otherwise. For simplicity, we consider the case when there are only two factors that are randomized. The first factor, X , is our factors of interest (for example the candidate's gender) and the second factor, Z , is a factor we additionally want to control for (for example the candidate's political party). Although both X and Z are single factors, both are two-dimensional because each X and Z consists of the left and right profile values. More formally, each respondent t observes $X_t = (X_t^L, X_t^R)$ and $Z_t = (Z_t^L, Z_t^R)$, where the superscripts L and R denote the left and right profiles respectively.

Before turning to the application, we first perform the power analysis described in Algorithm 2 via simulations. For our simulation setup, we allow both factors of X and Z to have up to four levels, i.e., all $X_t^L, X_t^R, Z_t^L, Z_t^R$ take values 1, 2, 3, 4. The response Y is then generated from the following logistic regression model, \hat{f}_Q , with main effects and interactions on only one specific combination,

$$\begin{aligned} \hat{f}_Q = \Pr(Y_t = 1 \mid X_t, Z_t) = \text{logit}^{-1} & \left[\beta_X \mathbb{1}\{X_t^L = 1, X_t^R \neq 1\} - \beta_X \mathbb{1}\{X_t^L \neq 1, X_t^R = 1\} \right. \\ & + \beta_Z \mathbb{1}\{Z_t^L = 1, Z_t^R \neq 1\} - \beta_Z \mathbb{1}\{Z_t^L \neq 1, Z_t^R = 1\} \\ & \left. + \beta_{XZ} \mathbb{1}\{X_t^L = 1, Z_t^L = 2, X_t^R \neq 1, Z_t^R \neq 2\} - \beta_{XZ} \mathbb{1}\{X_t^L \neq 1, Z_t^L \neq 2, X_t^R = 1, Z_t^R = 2\} \right], \end{aligned}$$

where the first four indicators force main effects β_X, β_Z of X and Z , respectively, to exist in only the first levels of each factor and the last two indicators force an interaction effect β_{XZ} in the first and second level of factor X, Z respectively. For example, $\mathbb{1}\{X_t^L = 1, X_t^R \neq 1\}$ is one if the left profile value of X takes value 1 but simultaneously the right profile value of X is not 1 (otherwise the two profiles have the same value of X). Similarly, $\mathbb{1}\{X_t^L = 1, Z_t^L = 2, X_t^R \neq 1, Z_t^R \neq 2\}$ is one if the left profile values of X, Z are 1, 2 but the right profile values of X, Z are not 1, 2 simultaneously. The indicator is still one if the $(X_t^L, Z_t^L) = (1, 2)$ and $(X_t^R, Z_t^R) = (1, 3)$ as long as both (X_t^R, Z_t^R) is not (1, 2). We purposefully choose the interaction to act on a different level of Z as to not "stack" up the interaction with the main effects. Lastly, our response model assumes "no profile order effect", which is commonly assumed in conjoint analysis (Hainmueller, Hopkins

³The profiles are not necessarily always presented side by side.

and Yamamoto, 2014; Ham, Imai and Janson, 2022). The “no profile order effect” assumption states that whether the left profile was on the right or vice-versa does not matter. We see this is explicitly written in the above response model as we repeat all main and interaction effects symmetrically for the right and left profile (except we shift the sign because $Y = 1$ refers to the left profile being selected). We later incorporate this information into the test statistic.

4.2 The Adaptive Procedure

To give intuition on why adapting may help, consider the typical uniform *iid* sampling scheme, where all levels for each factors are sampled with equal probability. If the sample size n is not sufficiently large enough, the data may have insufficient samples for levels of X that contain the true effect and by chance may have levels of X that look like “fake” effects due to noise. On the other hand, an adaptive sampling scheme can mitigate such issues by “screening out” levels that do not look like signal, thus allocating the remaining samples to explore the more noisy levels that may not be true signals. Therefore, we speculate the reasons presented in Section 3 for why adapting may be helpful also similarly applies for this setting.

To capture this intuition, we sample $X_t \sim \text{Multinomial}(p_{t,1}^X, p_{t,2}^X, \dots, p_{t,K^2}^X)$, where $p_{t,j}^X$ represents the probability of sampling the j th arm (arm refers to combination of left and right factor levels) out of K^2 possible arms and K is the total factor levels of X . For example, in our simulation setup $K = 4$ and there are 16 possible arms, (1, 1), (1, 2), etc., and $p_{t,j}^Z$ is defined similarly. Our goal is to come up with an adaptive procedure that assigns weights $p_{t,j}^X$ and $p_{t,j}^Z$ that may help increase power compared to the power from a uniform *iid* sampling scheme, where $p_{t,j}^X = \frac{1}{K^2}$, $p_{t,j}^Z = \frac{1}{L^2}$ for every j and L is the total number of factor levels for factor Z . We also note that conjoint applications do indeed default to the uniform *iid* sampling scheme (or a very minor variant from it) (Hainmueller and Hopkins, 2015; Ono and Burden, 2018). Although we present our adaptive procedure when the dimension of Z is only one (typical conjoint analysis have 8-10 other factors), our adaptive procedure loses no generality in higher dimensions of Z . We now propose the following adaptive procedure that adapts the sampling weights of $p_{t,j}^X, p_{t,j}^Z$ at each time step t in the following way,

$$p_{t,j}^X \propto |\bar{Y}_{j,t}^X - 0.5| + |N(0, 0.01^2)| \quad p_{t,j}^Z \propto |\bar{Y}_{j,t}^Z - 0.5| + |N(0, 0.01^2)|, \quad (15)$$

where $\bar{Y}_{j,t}^X$ denotes the sample mean of Y_1, Y_2, \dots, Y_{t-1} for arm j in variable X , $\bar{Y}_{j,t}^Z$ is defined similarly, and $N(0, 0.01^2)$ denotes a Gaussian random variable with mean zero and variance 0.01^2 (the two Gaussians in Equation 15 are drawn independently). To give intuition why Equation 15 may be a reasonable adaptive procedure, consider what we expect to observe when the j th arm is $X = (1, 1)$. This particular arm does not contain any signal so it is reasonable to expect that $\bar{Y}_{j,t}^X \approx 0.5$, i.e., $X = (1, 1)$ roughly produced an equal number of $Y = 1$ and $Y = 0$. Therefore, in expectation we do not expect to sample more from this arm in the future since $p_{t,j}^X \approx 0$. We add a slight perturbation in case $\bar{Y}_{j,t}^X$ is exactly equal to 0.5 to discourage an arm from having zero probability.

To further illustrate this point, consider the following four arms of X : (1,1), (1, 2), (1,3), (2,4). Suppose at time t the corresponding sample means for the four arms are 0.52, 0.60, 0.61, 0.59 respectively. Under our simulation setup, X has a main effect in the first level so obtaining an average of 0.60, 0.61 for the second and third arm is reasonable. Additionally the first and last arm are “useless” combinations with no real effect. However, by chance the last arm initially looks like a signal at time step t . After normalizing, our new adaptive probabilities will be roughly 0.063, 0.312, 0.343, 0.281. These new weights allow us to sample less from the first arm, which we are fairly certain has no effect. Consequently, this allows the sampling scheme to use more budget on sampling the signal arms and the fourth “fake” arm. This matches out previously stated intuition as the adaptive procedure allows the noisy “fake” signals to stabilize. We finally note that the adaptive weights chosen in Equation 15 is only one of many different ways to adapt. We choose one naive

Algorithm 3: Adaptive Procedure for Conjoint Studies

Given adaptive parameter ϵ **for** $t = 1, 2, \dots, [n\epsilon]$ **do**

- Sample $X_t \sim \text{Multinomial}(p_{t,1}^X, p_{t,2}^X, \dots, p_{t,K^2}^X)$, where $p_{t,j}^X = \frac{1}{K}$ for all $j = 1, 2, \dots, K^2$
- Sample $Z_t \sim \text{Multinomial}(p_{t,1}^Z, p_{t,2}^Z, \dots, p_{t,LL^2}^Z)$, where $p_{t,j}^Z = \frac{1}{L}$ for all $j = 1, 2, \dots, LL^2$

for $t = [n\epsilon] + 1, \dots, n$ **do**

- Sample $X_t \sim \text{Multinomial}(p_{t,1}^X, p_{t,2}^X, \dots, p_{t,K^2}^X)$, where $p_{t,j}^X$ is given in Equation 15
- Sample $Z_t \sim \text{Multinomial}(p_{t,1}^Z, p_{t,2}^Z, \dots, p_{t,LL^2}^Z)$, where $p_{t,j}^Z$ is given in Equation 15

and reasonable procedure for exposition and leave the theoretical and empirical characterization for optimal adaptive procedures under the conjoint setting to future research.

With this reweighting procedure, we build our adaptive procedure. Just like Definition 3.2, we also have an ϵ adaptive parameter that denotes the beginning $[n\epsilon]$ samples that are used for “exploration”. In this exploration stage, we sample from the typical uniform *iid* sampling scheme, i.e., $p_{t,j}^X = p_{t,j}^Z$ for all j and $t = 1, 2, \dots, [n\epsilon]$. This is necessary because if we adapt right away we may end up with high noisy estimates of $\bar{Y}_{j,t}^X$, leading to unreasonable adaptive schemes. In the remaining samples, we adapt by changing the weights according to Equation 15. We note that this adaptive sampling scheme immediately satisfies Assumption 1 and also Assumption 2 since each variable only looks at its own history and previous responses (not the other variables’ history). We summarize our adaptive procedure in Algorithm 3.

Lastly, in order for us to compute the p -value in Equation 5, we need a reasonable test statistic T . We emphasize that any test statistic leads to a valid finite-sample p -value. Although Ham, Imai and Janson consider a complicated Hierarchical Lasso model to capture all interactions, due to the simplicity of this setting we consider a simple cross-validated Lasso logistic test statistic that fits a Lasso logistic regression of \mathbf{Y} with main effects of \mathbf{X} and \mathbf{Z} and their interaction. Furthermore, to increase power we incorporate the common “no profile order effect” as done in (Hainmueller, Hopkins and Yamamoto, 2014; Ham, Imai and Janson, 2022), which states that the order of the pair of profiles do no matter, i.e., whether the left profile comes first or later. In other words, we do not expect the main effects corresponding to the left profile of X to be any different than the main effects corresponding to the right profile. To incorporate this symmetry constraint, we split our original $\mathbb{R}^{n \times (4+1)}$ data matrix $(\mathbf{X}, \mathbf{Z}, \mathbf{Y})$ into a new data matrix with dimension $\mathbb{R}^{2n \times (2+1)}$, where the first n rows contain the values for the left profile (and the corresponding Y) and the next n rows contain the values for the right profile with new response $1 - Y$ (see (Hainmueller, Hopkins and Yamamoto, 2014; Ham, Imai and Janson, 2022) for more details). This leads to the following test statistic

$$T^{\text{lasso}}(\mathbf{X}, \mathbf{Z}, \mathbf{Y}) = \sum_{k=1}^{K-1} |\hat{\beta}_k| + \sum_{k=1}^{K-1} \sum_{l=1}^{L-1} |\hat{\gamma}_{kl}|, \quad (16)$$

where $\hat{\beta}_k$ denotes the estimated main effects for level k out of K levels of X (one is held as baseline) and $\hat{\gamma}_{kl}$ denotes the estimated interaction effects for level k of X with level l of L levels of Z . Given this test statistic, we now present the simulation results.

4.3 Simulation Results

We first compare the power of our adaptive procedure stated in Algorithm 3 with the *iid* setting where each arm for X and Z are drawn uniformly at random, i.e., $p_{t,j}^X = p_{t,j}^Z = 1/16$ for all j under the simulation setting described in Section 4.1. We empirically compute the power as the proportion of $P = 1,000$ Monte-Carlo

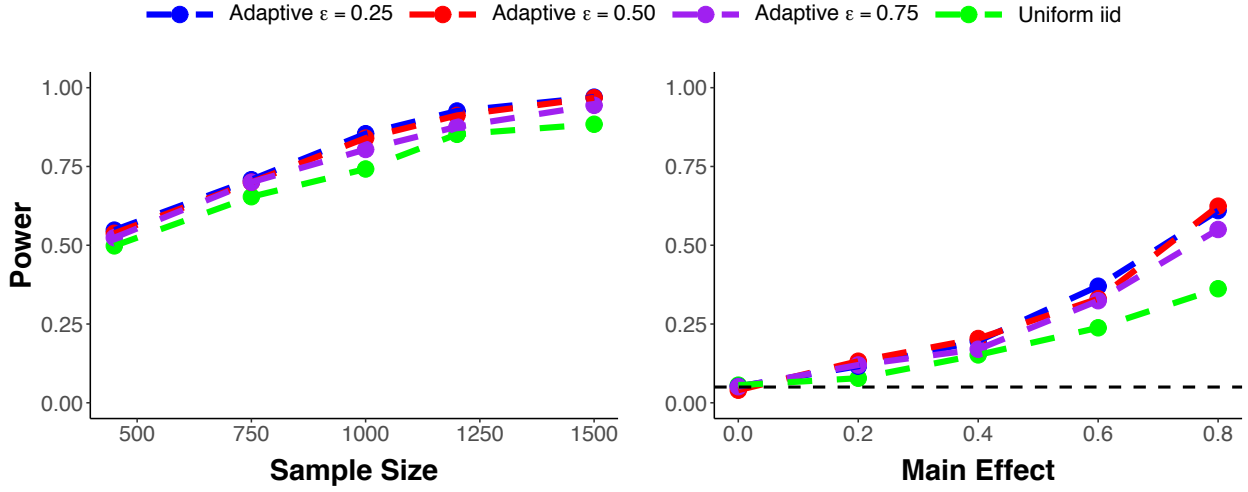


Figure 6: The figure shows how the power of the AdapRT and i.i.d based CRT tests varies as the sample size increases (left plot) or main effect increases (right plot). All power curves are calculated from 1,000 Monte-Carlo calculated p -values using Equation 5 with $B = 300$ and test statistic given in Equation 16. The blue, red, and purple power curves denote the power of the AdapRT using the adaptive procedure described in Algorithm 3 and $\epsilon = 0.25, 0.50, 0.75$, respectively. The green power curve denotes the power of the uniform *iid* sampling scheme. The black dotted line in the right panel shows the $\alpha = 0.05$ line. Finally, the standard errors are negligible with a maximum value of 0.016.

p -values less than $\alpha = 0.05$.

In accordance with the guideline presented in Algorithm 2, we simulate the power under different hypothesized \hat{f}_Q and different parameterizations of our proposed adaptive procedure. In the first scenario, we fix \hat{f}_Q but increase sample size when there exist both main effects and interaction effects of X in the left panel of Figure 6. More specifically, we vary our sample size $n = (450, 750, 1,000, 1200, 1500)$ and fix main effects $\beta_X = \beta_Z = 0.6$ and a stronger interaction effect at $\beta_{XZ} = 1.1$. For the next setting, we vary \hat{f}_Q by increasing main effects of X and Z but do not consider interaction effects ($\beta_{XZ} = 0$) in the right panel of Figure 6. In this setting, we fix sample size at $n = 1,000$ and increase main effects β_X and β_Z to $(0, 0.2, 0.4, 0.6, 0.8)$. To also test for various adaptive procedures, we vary the one natural adaptive sampling parameter ϵ in Algorithm 2 to $\epsilon = 0.25, 0.5, 0.75$.

Both panels of Figure 6 show that the adaptive power is uniformly dominating the uniform *iid* power (green) despite using the same test statistic and the same response model \hat{f}_Q . For example when $n = 1,000$ in the left panel, there is a difference in 10 percentage points (74% versus 84%) between the *iid* sampling scheme and the adaptive sampling scheme with $\epsilon = 0.5$ (red). When the main effect is as strong as 0.8 in the right panel, there is a difference in 26 percentage points (36% versus 62%) between the *iid* sampling scheme and the adaptive sampling scheme with $\epsilon = 0.5$. Additionally, when the main effect is 0 in the right panel, making H_0 true, the power of all methods, as expected, has type-1 error control as both powers are near $\alpha = 0.05$ (dotted black horizontal line). Lastly, we note that both $\epsilon = 0.25, 0.5$ are suitable choices for the adaptive procedure, uniformly dominating the power of the adaptive procedure with $\epsilon = 0.75$ (purple).

4.4 Application: Role of Gender in Political Candidate Evaluation

We now apply our proposed method to a recent conjoint study which examines whether voters prefer candidates of one gender over the other after controlling for other candidate characteristics (Ono and Burden, 2018). In this study, the authors conduct an experiment based on a sample of voting-eligible adults in the U.S.

collected in March 2016, where each of the 1,583 respondents were given 10 pairs of political candidates with uniformly sampled levels of: gender, age, race, family, experience in public office, salient personal characteristics, party affiliation, policy area of expertise, position on national security, position on immigrants, position on abortion, position on government deficit, and favorability among the public (see original article for details). The respondents were then forced to choose one of the two pair of candidate profiles to vote into office, which is our main binary response Y . The study consists of a total of 7,915 responses, where the primary objective was to test whether gender (X) matters in voting behavior (Y) while controlling for other variables such as age, race, etc. (Z)⁴.

Ono and Burden were able to find a statistically significant effect of candidate’s gender on voting behavior. We attempt to answer this important question of whether gender matters in voting behavior had the experimenter ran the same experiment for the first time but with a lower sample size or budget $n < 7,915$. To run this quasi-experiment, we assume the original data of size 7,915 is the population and we draw samples (without replacement) from the original dataset according to our experiment. Due to the similarity with the popular bootstrap procedure (Efron, 1979), we refer to this quasi-experiment scheme as “bootstrapping” the data. We remind the readers that our procedure differs from the original bootstrap procedure as it does not sample with replacement. Additionally, we allow the researchers to use an adaptive scheme to sample (X, Z) instead of a uniform *iid* scheme. As a reminder, the original experimental design independently and uniformly sampled all factor levels with equal probability. For example, the left and right profiles’ gender was either “Male” or “Female” with equal probability.

The “bootstrapping” procedure is as follows. For simplicity suppose X is gender and Z is only candidate party. Since each sample consists of a *pair* of profiles, one potential sample may be $X_1 = (\text{Male}, \text{Female})$ and $Z_1 = (\text{Democrat}, \text{Democrat})$, indicating the left profile was a Democratic male candidate and the right profile was Democratic female candidate. Given such a sample, we obtain the subsequent response Y from the original study of 7,915 samples from randomly drawing response Y with corresponding pair of profiles with a Democratic male candidate and a Democratic female candidate. Once we draw this response Y , we do not put it back into the population. Since Z in the original study contained 12 other factors, the probability of observing a unique sequence of a particular (X, Z) is close to zero due to the curse of dimensionality. For example, if Z contained only two more factors such as candidate age and experience in public office, then there may exist no samples in the original study that contain a specific profile that is a Democratic male with 20 years of experience in public office and 50 years of age. For this reason, we only “bootstrap” the available data up to one other Z , namely the candidate’s party affiliation (Democratic or Republican). We choose this variable because Ham, Imai and Janson suggest possible strong interactions of gender with the candidate’s party affiliation. Since our aim is to show that adapting can help achieve a greater power than that of the *iid* procedure, it is sensible to try to use other factors Z that may help in power as long as both experimental procedures (the adaptive sampling scheme and *iid* sampling scheme) use the same test statistic and variables for fair comparison.

Given a budget constraint $n < 7,915$, we obtain the power of the adaptive sampling scheme and the *iid* sampling scheme by computing 1,000 p -values using n bootstrapped sample of the original 7,915 sample. Each p -value is computed using Equation 5 and the appropriate resamples for the corresponding procedure. The 1,000 p -values are computed from 1,000 different possible bootstrapped samples of the original data. The power is empirically computed as the proportion of the 1,000 p -values less than $\alpha = 0.1$. Since the applied setting is the same as that of the simulation setting in Section 4.1, we use the same adaptive procedure in Algorithm 3 with $\epsilon = 0.5$ as suggested by Section 4.3 and the same test statistic in Equation 16. We also similarly impose “no profile order effect” in the test statistic as described in Section 4.2.

⁴The original study consists of 15,830 responses half of which were about Presidential candidates and the remaining half for Congressional candidates. Because the original study found a statistically significant result for only the Presidential candidates, we focus on the responses for Presidential candidates

	<i>iid</i> sampling scheme - CRT	Adaptive sampling scheme - AdapRT
$n = 500$	0.13	0.14
$n = 1,000$	0.14	0.17
$n = 2,000$	0.24	0.30
$n = 3,000$	0.31	0.40

Table 1: The two columns represent the power of the *iid* CRT and the AdapRT respectively for testing H_0 , where X is gender (Male or Female) in the gender political candidate study in (Ono and Burden, 2018) and Z is the candidate’s party affiliation (Democratic or Republican). Each row represents a different bootstrapped sample size n that aims to replicate the original experiment had the researchers re-ran the experiment with the respective sampling schemes. The power is calculated from the proportion of 1,000 p -values less than $\alpha = 0.1$. Each p -value is calculated using Equation 5 using the appropriate resamples for the corresponding procedure with test statistic in Equation 16. The AdapRT uses adaptive procedure in Algorithm 3 with $\epsilon = 0.5$.

Table 1 shows the power results using both the *iid* sampling scheme and the proposed AdapRT. Although the power difference is not as stark as that shown in the simulation in Figure 6, Table 1 still shows that the power of the AdapRT is consistently and non-trivially higher than that of the *iid* sampling scheme. For example, when $n = 3,000$ (approximately 37% of the original sample size), we observe a power difference of 9 percentage points with the *iid* sampling scheme only having 31% power, approximately a 30% increase of power.

5 Concluding Remarks

In this paper, we introduce the Adaptive Randomization Test (AdapRT) that allows the “Model-X” randomization inference approach for sequentially collected data. The AdapRT, like the CRT, tackles the fundamental independence testing problem in statistics. We showcase the AdapRT’s potential through various simulations and empirical examples that show how an adaptive sampling scheme can lead to a more powerful test compared to the typical *iid* sampling scheme. In particular, we demonstrate the AdapRT’s advantages in the normal-means model and conjoint settings. We believe that adaptively sampling can help for three main reasons. The first reason relates to how the AdapRT allows the adaptive procedure to automatically mimic the oracle *iid* procedure in terms of finding optimal sampling weight. Secondly, the up-weighting allows the AdapRT to not only sample more from arms that contain the true signal but also “fake” signal arms that may initially look like true signals. This is useful because sampling more from these “fake” signals stabilizes the signal. Thirdly, the AdapRT also down-weights arms (with high probability) that contain no signal, allowing our remaining samples to focus on exploring the more relevant arms.

Our work, however, is not comprehensive. While our work analyzes two common settings where the AdapRT is clearly helpful, there exist many future research that can further explore how to build efficient adaptive procedures with theoretical and empirical guarantees under many different scenarios for the respective application. Secondly, as briefly discussed in Section 2.3, the AdapRT can successfully give multiple valid p -values for each relevant hypothesis, but it is not clear if one could make theoretical or empirical guarantees about its properties in the context of multiple testing and variable selection such as controlling the false discovery rate. Thirdly, with the goal of extending our methodology beyond independence testing, it would be interesting to explore possible ways to combine adaptive sampling with other ideas from “Model-X” framework. For instance, Zhang and Janson recently proposed the Floodgate method that goes beyond independence testing by additionally characterizing the strength of the dependency. It would be interesting to extend our adaptive framework in this Floodgate setting. Lastly, the AdapRT is crucially reliant

on the natural adaptive resampling procedure (NARP) for the validity of the p -values in p_{AdapCRT} . As mentioned in Section 2.4, it may be possible to also have a feasible resampling procedure that does not require Assumption 1 but enjoys the same benefits of the AdapRT.

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Appendices

A Proof of Main Results Presented in Section 2

Proof of Theorem 2.1. By definition of our resampling procedure, under H_0 ,

$$\tilde{X}_1 | (Y_1, Z_1) \stackrel{d}{=} \tilde{X}_1 | Z_1 \stackrel{d}{=} X_1 | Z_1 \stackrel{d}{=} X_1 | (Y_1, Z_1)$$

where the last “ $\stackrel{d}{=}$ ” is by the null hypothesis of conditional independence, namely $X_1 \perp\!\!\!\perp Y_1 | Z_1$. Moreover, it also suggests

$$(\tilde{X}_1, Y_1, Z_1) \stackrel{d}{=} (X_1, Y_1, Z_1).$$

Then we will prove the following statement holds for any $k \in \{1, 2, \dots, n\}$ by induction,

$$(\tilde{X}_{1:k}, Y_{1:k}, Z_{1:k}) \stackrel{d}{=} (X_{1:k}, Y_{1:k}, Z_{1:k}). \quad (17)$$

Assuming Equation 17 holds for $k - 1$, we now prove it also holds for k . For simplicity, in the rest of this proof, we will use $P(\cdot)$ as a generic notation for *pdf* or *pmf*, though the proof holds for more general distributions without a *pdf* or *pmf*. First,

$$\begin{aligned} & P [(\tilde{X}_{1:(k-1)}, Y_{1:(k-1)}, Z_{1:k}) = (x_{1:(k-1)}, y_{1:(k-1)}, z_{1:k})] \\ \stackrel{(i)}{=} & P [Z_k | (\tilde{X}_{1:(k-1)}, Y_{1:(k-1)}, Z_{1:(k-1)}) = (x_{1:(k-1)}, y_{1:(k-1)}, z_{1:(k-1)})] \\ & \cdot P [(\tilde{X}_{1:(k-1)}, Y_{1:(k-1)}, Z_{1:(k-1)}) = (x_{1:(k-1)}, y_{1:(k-1)}, z_{1:(k-1)})] \\ \stackrel{(ii)}{=} & P [Z_k | (Y_{1:(k-1)}, Z_{1:(k-1)}) = (y_{1:(k-1)}, z_{1:(k-1)})] \\ & \cdot P [(\tilde{X}_{1:(k-1)}, Y_{1:(k-1)}, Z_{1:(k-1)}) = (x_{1:(k-1)}, y_{1:(k-1)}, z_{1:(k-1)})] \\ \stackrel{(iii)}{=} & P [Z_k | (Y_{1:(k-1)}, Z_{1:(k-1)}) = (y_{1:(k-1)}, z_{1:(k-1)})] \\ & \cdot P [(X_{1:(k-1)}, Y_{1:(k-1)}, Z_{1:(k-1)}) = (x_{1:(k-1)}, y_{1:(k-1)}, z_{1:(k-1)})] \\ \stackrel{(iv)}{=} & P [Z_k | (X_{1:(k-1)}, Y_{1:(k-1)}, Z_{1:(k-1)}) = (x_{1:(k-1)}, y_{1:(k-1)}, z_{1:(k-1)})] \\ & \cdot P [(X_{1:(k-1)}, Y_{1:(k-1)}, Z_{1:(k-1)}) = (x_{1:(k-1)}, y_{1:(k-1)}, z_{1:(k-1)})] \\ = & P [(X_{1:(k-1)}, Y_{1:(k-1)}, Z_{1:k}) = (x_{1:(k-1)}, y_{1:(k-1)}, z_{1:k})], \end{aligned} \quad (18)$$

where (i) is simply by Bayes rule; (ii) is because $Z_k \perp\!\!\!\perp \tilde{X}_{1:k-1} | (Y_{1:(k-1)}, Z_{1:(k-1)})$ since $\tilde{X}_{1:k-1}$ is a random function of only $Y_{1:(k-1)}$ and $Z_{1:(k-1)}$; and lastly, (iii) is by induction assumption; (iv) is by Assumption 1.

Moreover,

$$\begin{aligned}
& P [(\tilde{X}_{1:k}, Y_{1:k}, Z_{1:k}) = (x_{1:k}, y_{1:k}, z_{1:k})] \\
& \stackrel{(i)}{=} P [Y_k = y_k \mid (\tilde{X}_{1:k}, Y_{1:(k-1)}, Z_{1:k}) = (x_{1:k}, y_{1:(k-1)}, z_{1:k})] \cdot P [(\tilde{X}_{1:k}, Y_{1:(k-1)}, Z_{1:k}) = (x_{1:k}, y_{1:(k-1)}, z_{1:k})] \\
& \stackrel{(ii)}{=} P [Y_k = y_k \mid Z_k = z_k] \cdot P [(\tilde{X}_{1:k}, Y_{1:(k-1)}, Z_{1:k}) = (x_{1:k}, y_{1:(k-1)}, z_{1:k})] \\
& \stackrel{(iii)}{=} P [Y_k = y_k \mid Z_k = z_k] \cdot P [\tilde{X}_k = x_k \mid (\tilde{X}_{1:(k-1)}, Y_{1:(k-1)}, Z_{1:k}) = (x_{1:(k-1)}, y_{1:(k-1)}, z_{1:k})] \\
& \quad \cdot P [(\tilde{X}_{1:(k-1)}, Y_{1:(k-1)}, Z_{1:k}) = (x_{1:(k-1)}, y_{1:(k-1)}, z_{1:k})] \\
& \stackrel{(iv)}{=} P [Y_k = y_k \mid Z_k = z_k] \cdot P [X_k = x_k \mid (X_{1:(k-1)}, Y_{1:(k-1)}, Z_{1:k}) = (x_{1:(k-1)}, y_{1:(k-1)}, z_{1:k})] \\
& \quad \cdot P [(\tilde{X}_{1:(k-1)}, Y_{1:(k-1)}, Z_{1:k}) = (x_{1:(k-1)}, y_{1:(k-1)}, z_{1:k})] \\
& \stackrel{(v)}{=} P [Y_k = y_k \mid Z_k = z_k] \cdot P [X_k = x_k \mid (X_{1:(k-1)}, Y_{1:(k-1)}, Z_{1:k}) = (x_{1:(k-1)}, y_{1:(k-1)}, z_{1:k})] \\
& \quad \cdot P [(X_{1:(k-1)}, Y_{1:(k-1)}, Z_{1:k}) = (x_{1:(k-1)}, y_{1:(k-1)}, z_{1:k})] \\
& = P [(X_{1:k}, Y_{1:k}, Z_{1:k}) = (x_{1:k}, y_{1:k}, z_{1:k})],
\end{aligned}$$

where (i) is again simply by Bayes rule; (ii) is because Y_k is a random function of only Z_k (up to time k) under the null H_0 and thus is independent of anything with index smaller or equal to k conditioning on Z_k ; (iii) is again by Bayes rule; (iv) is by Definition 2.2; and finally (v) is by the previous equation above. Equation 17 is thus established by induction, as a corollary of which, we also get for any $k \leq n$,

$$\tilde{X}_{1:n} \mid (Y_{1:n}, Z_{1:n}) \stackrel{d}{=} X_{1:n} \mid (Y_{1:n}, Z_{1:n})$$

Finally, note that $\tilde{X} \perp\!\!\!\perp X \mid (Y, Z)$. So, conditioning on (Y, Z) , \tilde{X} and X are exchangeable, which means the p -value defined in Equation 5 is conditionally valid, conditioning on (Y, Z) . Since $\mathbb{P}(p < \alpha \mid Y, Z) \leq \alpha$ holds conditionally, it also holds marginally. \square

Proof of Theorem 2.2. Note that Assumption 1 was only utilized once in the proof of Theorem 2.1, namely (iv) of Equation 18. So upon assuming $(\tilde{X}_{1:k}, Y_{1:k}, Z_{1:k}) \stackrel{d}{=} (X_{1:k}, Y_{1:k}, Z_{1:k})$, we know immediately from Equation 18 that

$$\begin{aligned}
& P [Z_k = z_k \mid (Y_{1:(k-1)}, Z_{1:(k-1)}) = (y_{1:(k-1)}, z_{1:(k-1)})] \\
& = P [Z_k = z_k \mid (X_{1:(k-1)}, Y_{1:(k-1)}, Z_{1:(k-1)}) = (x_{1:(k-1)}, y_{1:(k-1)}, z_{1:(k-1)})]
\end{aligned}$$

which is exactly Assumption 1. \square

B Proof of Results Presented in Section 3

Before proving the main power results, we first state a self-explanatory lemma concerning the effect of taking B to go to infinity, which justifies assuming B to be large enough and ignoring the effect of discrete p -values like the one defined in Equation 5. Similar proof arguments are made in (Wu and Ding, 2021), thus we omit the proof of this lemma. The lemma states that as $B \rightarrow \infty$, conditioning on any given values of $(X, \mathbf{Y}, \mathbf{Z})$,

$$p\text{-value} := \frac{1}{B+1} \left[1 + \sum_{b=1}^B \mathbb{1}_{\{T(\tilde{\mathbf{X}}^b, \mathbf{Z}, \mathbf{Y}) \geq T(\mathbf{X}, \mathbf{Z}, \mathbf{Y})\}} \right] \xrightarrow{\text{a.s.}} \mathbb{P}(T(\tilde{\mathbf{X}}^b, \mathbf{Z}, \mathbf{Y}) \geq T(\mathbf{X}, \mathbf{Z}, \mathbf{Y}) \mid \mathbf{Y}, \mathbf{Z}).$$

Lemma .1 (Power of AdapRT under $B \rightarrow \infty$). For any adaptive sapling scheme A satisfies Definition 2.1 and any test statistic T , as we take $B \rightarrow \infty$, the asymptotic conditional power of AdapRT (with CRT being an degenerate special case) condition on (Y, Z) is equal to

$$\mathbb{P} \left(T(\mathbf{X}, \mathbf{Y}, \mathbf{Z}) \geq z_{1-\alpha}(T(\tilde{\mathbf{X}}, \mathbf{Y}, \mathbf{Z})) \mid \mathbf{Y}, \mathbf{Z} \right),$$

while the unconditional (marginal) power is equal to

$$\mathbb{P}_{\mathbf{X}, \tilde{\mathbf{X}}, \mathbf{Y}, \mathbf{Z}} \left(\mathbb{P} \left(T(\mathbf{X}, \mathbf{Y}, \mathbf{Z}) \geq z_{1-\alpha}(T(\tilde{\mathbf{X}}, \mathbf{Y}, \mathbf{Z})) \mid \mathbf{Y}, \mathbf{Z} \right) \right).$$

Note that the joint distribution of $(\mathbf{X}, \tilde{\mathbf{X}}, \mathbf{Y}, \mathbf{Z})$ is implicitly specified by the sampling procedure A .

Lemma .2 (Normal Means Model with *iid* sampling schemes: Joint Asymptotic Distributions of \tilde{Y}_j 's, \tilde{Y}_j 's and \bar{Y} Under the Alternative H_1). Define

$$T_{\text{all}} = \left(\tilde{Y}_1, \tilde{Y}_2, \dots, \tilde{Y}_{p-1}, \bar{Y}_1, \bar{Y}_2, \dots, \bar{Y}_{p-1}, \bar{Y} \right)^T \in \mathbb{R}^{2p-1}.$$

Upon assuming the normal means model introduced in Section 3, under the alternative H_1 with $h = h_0/\sqrt{n}$, as $n \rightarrow \infty$,

$$\sqrt{n} \cdot T_{\text{all}} \xrightarrow{d} T_{\text{all}}^\infty,$$

with

$$T_{\text{all}}^\infty = \begin{pmatrix} G_1 + R + h_0 q_1 \\ G_2 + R + h_0 q_1 \\ \dots \\ G_{p-1} + R + h_0 q_1 \\ H_1 + R + h_0 \\ H_2 + R \\ \dots \\ H_{p-1} + R \\ R \end{pmatrix} \in \mathbb{R}^{2p-1},$$

where $G := (G_1, G_2, \dots, G_{p-1})$ and $H := (H_1, H_2, \dots, H_{p-1})$ both follow the same $(p-1)$ dimensional multivariate Gaussian distribution $\mathcal{N}(0, \Sigma)$ and R is a standard normal random variable. Note that Σ was defined in the statement of Theorem 3.1. Moreover, G , H and R are independent.

Remark 4. Roughly speaking, after removing means, R captures the randomness of \mathbf{Y} being sampled from its marginal distribution; H captures the randomness of sampling \mathbf{X} conditioning on \mathbf{Y} ; lastly, G captures the randomness of resampling $\tilde{\mathbf{X}}$ given \mathbf{Y} .

Remark 5. We also note that we do not include characterizing the distribution of \tilde{Y}_p or \bar{Y}_p to avoid stating the convergence in terms of a degenerate multivariate Gaussian distribution since \bar{Y}_p is a deterministic function given \bar{Y} and the remaining $p-1$ means of the other arms.

Proof of Lemma .2. We first characterize the conditional distribution of \tilde{Y}_j . For any $j \in \{1, 2, \dots, p\}$,

$$\begin{aligned} \tilde{Y}_j &:= \frac{\sum_{i=1}^n Y_i \mathbb{1}_{\tilde{X}_i=j}}{\sum_{i=1}^n \mathbb{1}_{\tilde{X}_i=j}} \\ &= \frac{1}{\sqrt{n}} \left[\frac{1}{q_j} \frac{\sum_{i=1}^n Y_i (\mathbb{1}_{\tilde{X}_i=j} - q_j)}{\sqrt{n}} + \frac{\sum_{i=1}^n Y_i}{\sqrt{n}} \right] \frac{q_j n}{\sum_{i=1}^n \mathbb{1}_{\tilde{X}_i=j}}. \end{aligned}$$

By Central Limit Theorem, since $\text{Var}\left(Y_i(\mathbb{1}_{\tilde{X}_i=j} - q_j)\right) \rightarrow q_j(1 - q_j)$ as $n \rightarrow \infty$,

$$\frac{\sum_{i=1}^n Y_i \left(\mathbb{1}_{\tilde{X}_i=j} - q_j\right)}{\sqrt{q_j(1 - q_j)n}} \xrightarrow{d} \mathcal{N}(0, 1),$$

which together with Slutsky's Theorem and the fact that $q_j n / \sum_{i=1}^n \mathbb{1}_{\tilde{X}_i=j} \rightarrow 1$ almost surely gives,

$$J_{j,n} := \sqrt{n}\tilde{Y}_j - \frac{\sum_{i=1}^n Y_i}{\sqrt{n}} \xrightarrow{d} \mathcal{N}\left(0, \frac{v(q_j)}{q_j^2}\right),$$

where $v(q_j) = \text{Var}(\text{Bern}(q_j)) = \text{Var}(\mathbb{1}_{\tilde{X}_i=1}) = q_j(1 - q_j)$. Additional to these one dimensional asymptotic results, we can also derive their joint asymptotic distribution. Before moving forward, we define a few useful notations,

$$\begin{aligned} \mathbf{J}_{-p,n} &:= (J_{1,n}, J_{2,n}, \dots, J_{p-1,n}) \in \mathbb{R}^{p-1}, \\ V_i &:= \left(Y_i(\mathbb{1}_{\tilde{X}_i=1} - q_1), Y_i(\mathbb{1}_{\tilde{X}_i=2} - q_2), \dots, Y_i(\mathbb{1}_{\tilde{X}_i=p-1} - q_{p-1})\right) \in \mathbb{R}^{p-1}, \\ \bar{\Sigma}_n &:= \frac{1}{n} \sum_{i=1}^n \text{Var}(V_i), \end{aligned}$$

and

$$\Sigma_0 := \text{Var}\left(\left(\mathbb{1}_{\tilde{X}_i=1}, \mathbb{1}_{\tilde{X}_i=2}, \dots, \mathbb{1}_{\tilde{X}_i=p-1}\right)\right) = \begin{bmatrix} v(q_1) & -q_1 q_2 & -q_1 q_3 & \cdots & -q_1 q_{p-1} \\ -q_1 q_2 & v(q_2) & -q_2 q_3 & \cdots & -q_2 q_{p-1} \\ -q_1 q_3 & -q_2 q_3 & v(q_3) & \cdots & -q_3 q_{p-1} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ -q_1 q_{p-1} & -q_2 q_{p-1} & -q_3 q_{p-1} & \cdots & v(q_{p-1}) \end{bmatrix}. \quad (19)$$

By Multivariate Lindeberg-Feller CLT (see for instance Ash et al. (2000)),

$$\sqrt{n}\bar{\Sigma}_n^{-1/2} (\bar{V} - \mathbb{E}\bar{V}) \xrightarrow{d} \mathcal{N}(0, I_{p-1}). \quad (20)$$

which further gives

$$\sqrt{n}(\bar{V} - \mathbb{E}\bar{V}) \xrightarrow{d} \mathcal{N}(0, \Sigma_0)$$

because of

$$\lim_{n \rightarrow \infty} \bar{\Sigma}_n = \Sigma_0.$$

Therefore we have

$$\mathbf{J}_{-p,n} \xrightarrow{d} \mathcal{N}(0, \Sigma), \quad (21)$$

where

$$\Sigma = D^{-1} \Sigma_0 D^{-1}$$

with

$$D = \text{diag}(q_1, q_2, \dots, q_{p-1}) \in \mathbb{R}^{(p-1) \times (p-1)}. \quad (22)$$

Roughly speaking, this suggests that after removing the shared randomness induced by $\frac{\sum_{i=1}^n Y_i}{\sqrt{n}}$, all the $\sqrt{n}\tilde{Y}_j$'s are asymptotically independent and Gaussian distributed.

Next, we turn to \bar{Y}_j . Note that in this part we will view X_i as generated from $F_{X|Y}$ after the generation of Y_i according to its marginal distribution. The only difference in the observed test statistic and the above is that we have

$$X_i|Y_i \sim \mathcal{M}(q_i^*)$$

with $q_i^* = (q_{i,1}^*, q_{i,2}^*, \dots, q_{i,p}^*)$ and

$$q_{i,j}^* = \frac{q_j \mathcal{N}\left(Y_i; \frac{h_0}{\sqrt{n}} \mathbb{1}_{j=1}, 1\right)}{\sum_{k=1}^p q_k \mathcal{N}\left(Y_i; \frac{h_0}{\sqrt{n}} \mathbb{1}_{k=1}, 1\right)} = \frac{\exp\left[-\frac{1}{2}\left(Y_i - \frac{h_0}{\sqrt{n}} \mathbb{1}_{j=1}\right)^2\right]}{\sum_{k=1}^p q_k \exp\left[-\frac{1}{2}\left(Y_i - \frac{h_0}{\sqrt{n}} \mathbb{1}_{k=1}\right)^2\right]}$$

instead. Again, Multivariate Lindeberg-Feller CLT gives,

$$\sqrt{n}(\bar{\Sigma}_n^*)^{-1/2} (\bar{V}^* - \mathbb{E}\bar{V}^*) \xrightarrow{d} \mathcal{N}(0, I_{p-1}), \quad (23)$$

with

$$V_i^* := \left(Y_i(\mathbb{1}_{X_i=1} - q_{i,1}^*), Y_i(\mathbb{1}_{X_i=2} - q_{i,2}^*), \dots, Y_i(\mathbb{1}_{X_i=p-1} - q_{i,p-1}^*)\right) \in \mathbb{R}^{p-1},$$

$$\bar{\Sigma}_n^* = \frac{1}{n} \sum_{i=1}^n \text{Var}(V_i^*).$$

Note that, since $\lim_{n \rightarrow \infty} \text{Var}\left(Y_i(\mathbb{1}_{X_i=j} - q_{i,j}^*)\right) = q_j(1-q_j)$ and $\lim_{n \rightarrow \infty} \text{Cov}\left(Y_i(\mathbb{1}_{X_i=j_1} - q_{i,j_1}^*), Y_i(\mathbb{1}_{X_i=j_2} - q_{i,j_2}^*)\right) = -q_{j_1}q_{j_2}$,

$$\lim_{n \rightarrow \infty} \bar{\Sigma}_n^* = \Sigma_0,$$

which further gives

$$\sqrt{n}(\bar{V}^* - \mathbb{E}\bar{V}^*) \xrightarrow{d} \mathcal{N}(0, \Sigma_0). \quad (24)$$

Similar to \mathbf{J} 's, we define \mathbf{J}^* 's as well,

$$J_{j,n}^* := \sqrt{n}\bar{Y}_j - \frac{\sum_{i=1}^n q_{i,j}^* Y_i}{q_j \sqrt{n}} = \frac{\sum_{i=1}^n Y_i \mathbb{1}_{X_i=j}}{q_j \sqrt{n}} - \frac{\sum_{i=1}^n q_{i,j}^* Y_i}{q_j \sqrt{n}} + o_p(1) = \frac{\sqrt{n}(\bar{V}^*)_j}{q_j} + o_p(1).$$

and

$$\mathbf{J}_{-p,n}^* := (J_{1,n}^*, J_{2,n}^*, \dots, J_{p-1,n}^*) \in \mathbb{R}^{p-1},$$

which together with Equation 24 gives

$$\mathbf{J}_{-p,n}^* \xrightarrow{d} \mathcal{N}(0, \Sigma). \quad (25)$$

Note that though Equation 21 and Equation 25 are almost exactly the same, it does not suggest \bar{Y}_j 's and $\bar{\tilde{Y}}_j$'s have the same asymptotic distribution, since the ‘‘mean’’ parts that have been removed actually behave differently, namely $\frac{\sum_{i=1}^n Y_i}{\sqrt{n}}$ and $\frac{\sum_{i=1}^n q_{i,j}^* Y_i}{q_j \sqrt{n}}$, as demonstrated in Lemma .3, Lemma .4, Lemma .5 and Lemma .6. Roughly speaking, under this \sqrt{n} scaling, the randomness that leads to the Gaussian noise part in CLT is the same across them as demonstrated in Equation 21 and Equation 25, but the Gaussian distribution they are converging to have different means.

Finally, following exactly the same logic, we can further derive the following joint asymptotic distribution of $\mathbf{J}_{-p,n}$, $\mathbf{J}_{-p,n}^*$ and $\frac{\sum_{i=1}^n Y_i}{\sqrt{n}}$. Letting

$$\mathbf{J}_{\text{ALL}} = \left(\frac{\sum_{i=1}^n Y_i}{\sqrt{n}}, \mathbf{J}_{-p,n}, \mathbf{J}_{-p,n}^* \right) \in \mathbb{R}^{2p-1},$$

we have

$$\mathbf{J}_{\text{ALL}} \xrightarrow{d} \mathcal{N}(0, \Sigma_{\text{ALL}}) = \mathcal{N}\left(0, \begin{bmatrix} 1 & 0 & 0 \\ 0 & \Sigma & 0 \\ 0 & 0 & \Sigma \end{bmatrix}\right).$$

□

Lemma .3. As $n \rightarrow \infty$,

$$\frac{1}{n} \sum_{i=1}^n Y_i^2 \xrightarrow{\text{a.s.}} 1 \quad \text{and} \quad \frac{\sum_{i=1}^n Y_i}{\sqrt{n}} \xrightarrow{d} \mathcal{N}(h_0 q_1, 1).$$

Proof. By defining $E_i := S_i W_i + (1 - S_i) G_i \sim \mathcal{N}(0, 1)$, we have

$$Y_i = E_i + \frac{S_i h_0}{\sqrt{n}}$$

Note that E_i and S_i are not independent. Thus,

$$\begin{aligned} \frac{1}{n} \sum_{i=1}^n Y_i^2 &= \frac{1}{n} \sum_{i=1}^n \left(E_i + \frac{S_i h_0}{\sqrt{n}} \right)^2 \\ &= \frac{1}{n} \sum_{i=1}^n E_i^2 + \frac{1}{n^2} \sum_{i=1}^n S_i h_0 + \frac{1}{n^{3/2}} \sum_{i=1}^n 2h_0 E_i S_i \\ &\xrightarrow{\text{a.s.}} 1, \end{aligned}$$

since by Law of Large Numbers the last two terms will vanish asymptotically and the first term will converge to $\mathbb{E}(E_i^2) = 1$. Moreover,

$$\begin{aligned} \frac{\sum_{i=1}^n Y_i}{\sqrt{n}} &= \frac{\sum_{i=1}^n E_i}{\sqrt{n}} + h_0 \frac{\sum_{i=1}^n S_i}{n} \\ &\xrightarrow{d} \mathcal{N}(h_0 q_1, 1), \end{aligned}$$

where the last line is obtained by applying CLT to the first term and LLN to the second term. □

Lemma .4. As $n \rightarrow \infty$,

$$\frac{\sum_{i=1}^n q_{i,1}^* Y_i}{q_1 \sqrt{n}} \xrightarrow{d} \mathcal{N}(q_1 h_0, 1).$$

Proof. We first show

$$\lim_{n \rightarrow \infty} \mathbb{E} \left(\sqrt{n} q_{i,1}^* Y_i \right) = h_0. \quad (26)$$

Recall that Y_i can be seen as a mixture of two normal distributions $\mathcal{N}(0, 1)$ and $\mathcal{N}\left(\frac{h_0}{\sqrt{n}}, 1\right)$ with weights $1 - q_1$ and q_1 . Thus $\mathbb{E}\left(\sqrt{n}q_{i,1}^* Y_i\right)$ is equal to

$$\sqrt{n} \int_{\mathbb{R}} \frac{yq_1 e^{-(y-h_0/\sqrt{n})^2/2}}{q_1 e^{-(y-h_0/\sqrt{n})^2/2} + (1-q_1)e^{-y^2/2}} \left[(1-q_1) \frac{1}{\sqrt{2\pi}} e^{-y^2/2} + q_1 \frac{1}{\sqrt{2\pi}} e^{-(y-h_0/\sqrt{n})^2/2} \right] dy := A_0 + A_1.$$

Note that with a change of variable $h = h_0/\sqrt{n}$,

$$\begin{aligned} \lim_{n \rightarrow \infty} A_1 &= \frac{q_1^2 \sqrt{n}}{\sqrt{2\pi}} \int_{\mathbb{R}} \frac{y e^{-(y-h_0/\sqrt{n})^2/2}}{q_1 e^{-(y-h_0/\sqrt{n})^2/2} + (1-q_1)e^{-y^2/2}} e^{-(y-h_0/\sqrt{n})^2/2} dy \\ &= \lim_{h \rightarrow 0} \frac{q_1^2 h_0}{\sqrt{2\pi}} \left[\frac{1}{h} \int_{\mathbb{R}} \frac{y e^{-(y-h)^2/2}}{q_1 e^{-(y-h)^2/2} + (1-q_1)e^{-y^2/2}} e^{-(y-h)^2/2} dy \right] \\ &= \frac{q_1^2 h_0}{\sqrt{2\pi}} \left. \frac{d \left[\int_{\mathbb{R}} \frac{y e^{-(y-h)^2/2}}{q_1 e^{-(y-h)^2/2} + (1-q_1)e^{-y^2/2}} e^{-(y-h)^2/2} dy \right]}{dh} \right|_{h=0} \\ &= \frac{q_1^2 h_0}{\sqrt{2\pi}} \int_{\mathbb{R}} \left. \frac{d \left[\frac{y e^{-(y-h)^2/2}}{q_1 e^{-(y-h)^2/2} + (1-q_1)e^{-y^2/2}} e^{-(y-h)^2/2} \right]}{dh} \right|_{h=0} dy \\ &= \frac{q_1^2 h_0}{\sqrt{2\pi}} \int_{\mathbb{R}} (2 - q_1) y^2 e^{-y^2/2} dy \\ &= h_0 q_1^2 (2 - q_1). \end{aligned}$$

Similarly,

$$\lim_{n \rightarrow \infty} A_0 = h_0 q_1 (1 - q_1)^2.$$

Equation 26 is thereby established. Then we compute $\lim_{n \rightarrow \infty} \text{Var}(q_{i,1}^* Y_i)$ using the same strategy.

$$\begin{aligned} \lim_{n \rightarrow \infty} \text{Var}(q_{i,1}^* Y_i) &= \lim_{n \rightarrow \infty} \left\{ \mathbb{E} \left[(q_{i,1}^* Y_i)^2 \right] - \left[\mathbb{E}(q_{i,1}^* Y_i) \right]^2 \right\} \\ &= \lim_{n \rightarrow \infty} \mathbb{E} \left[(q_{i,1}^* Y_i)^2 \right] \\ &= \lim_{n \rightarrow \infty} \int_{\mathbb{R}} y^2 \left[\frac{q_1 e^{-(y-h_0/\sqrt{n})^2/2}}{q_1 e^{-(y-h_0/\sqrt{n})^2/2} + (1-q_1)e^{-y^2/2}} \right]^2 \left[(1-q_1) \frac{1}{\sqrt{2\pi}} e^{-y^2/2} + q_1 \frac{1}{\sqrt{2\pi}} e^{-(y-h_0/\sqrt{n})^2/2} \right] dy \\ &= \int_{\mathbb{R}} \lim_{h \rightarrow 0} \left\{ y^2 \left[\frac{q_1 e^{-(y-h)^2/2}}{q_1 e^{-(y-h)^2/2} + (1-q_1)e^{-y^2/2}} \right]^2 \left[(1-q_1) \frac{1}{\sqrt{2\pi}} e^{-y^2/2} + q_1 \frac{1}{\sqrt{2\pi}} e^{-(y-h)^2/2} \right] \right\} dy \\ &= \int_{\mathbb{R}} q_1^2 \frac{e^{-y^2/2}}{\sqrt{2\pi}} dy \\ &= q_1^2. \end{aligned} \tag{27}$$

Combining Equation 26 and Equation 27, the lemma is thus established by Central Limit Theorem. \square

Following exactly the same logic, we have the following parallel lemma for $j \neq 1$.

Lemma .5. For $j \neq 1$, as $n \rightarrow \infty$,

$$\frac{\sum_{i=1}^n q_{i,j}^* Y_i}{q_j \sqrt{n}} \xrightarrow{d} \mathcal{N}(0, 1)$$

Proof. We first show

$$\lim_{n \rightarrow \infty} \mathbb{E} \left(\sqrt{n} q_{i,j}^* Y_i \right) = 0.$$

Again, recall that Y_i can be seen as a mixture of two normal distributions $\mathcal{N}(0, 1)$ and $\mathcal{N}\left(\frac{h_0}{\sqrt{n}}, 1\right)$ with weights $1 - q_1$ and q_1 . Thus $\mathbb{E} \left(\sqrt{n} q_{i,j}^* Y_i \right)$ is equal to

$$\sqrt{n} \int_{\mathbb{R}} \frac{y q_j e^{-y^2/2}}{q_1 e^{-(y-h_0/\sqrt{n})^2/2} + (1-q_1) e^{-y^2/2}} \left[(1-q_1) \frac{1}{\sqrt{2\pi}} e^{-y^2/2} + q_1 \frac{1}{\sqrt{2\pi}} e^{-(y-h_0/\sqrt{n})^2/2} \right] dy := B_0 + B_1.$$

With a change of variable $h = h_0/\sqrt{n}$, we have

$$\begin{aligned} \lim_{n \rightarrow \infty} B_1 &= \frac{q_1 q_j \sqrt{n}}{\sqrt{2\pi}} \int_{\mathbb{R}} \frac{y e^{-y^2/2}}{q_1 e^{-(y-h_0/\sqrt{n})^2/2} + (1-q_1) e^{-y^2/2}} e^{-(y-h_0/\sqrt{n})^2/2} dy \\ &= \lim_{h \rightarrow 0} \frac{q_1 q_j h_0}{\sqrt{2\pi}} \left[\frac{1}{h} \int_{\mathbb{R}} \frac{y e^{-y^2/2}}{q_1 e^{-(y-h)^2/2} + (1-q_1) e^{-y^2/2}} e^{-(y-h)^2/2} dy \right] \\ &= \frac{q_1 q_j h_0}{\sqrt{2\pi}} \frac{d \left[\int_{\mathbb{R}} \frac{y e^{-y^2/2}}{q_1 e^{-(y-h)^2/2} + (1-q_1) e^{-y^2/2}} e^{-(y-h)^2/2} dy \right]}{dh} \Bigg|_{h=0} \\ &= \frac{q_1 q_j h_0}{\sqrt{2\pi}} \int_{\mathbb{R}} \frac{d \left[\frac{y e^{-y^2/2}}{q_1 e^{-(y-h)^2/2} + (1-q_1) e^{-y^2/2}} e^{-(y-h)^2/2} \right]}{dh} \Bigg|_{h=0} dy \\ &= \frac{q_1 q_j h_0}{\sqrt{2\pi}} \int_{\mathbb{R}} (1-q_1) y^2 e^{-y^2/2} dy \\ &= h_0 q_j q_1 (1-q_1). \end{aligned}$$

Similarly,

$$\lim_{n \rightarrow \infty} B_0 = -h_0 q_j q_1 (1-q_1).$$

Finally, we have $\lim_{n \rightarrow \infty} \text{Var}(q_{i,1}^* Y_i) = q_j^2$ as well, which by CLT finishes the proof. \square

We can further write down their asymptotic joint distribution. We note that $q_{i,j}^* = \frac{q_j}{q_2} q_{i,2}^*$ deterministically for $j > 2$, thus it suffices to only include $j = 1, 2$ in the joint asymptotic distribution.

Lemma .6. As $n \rightarrow \infty$,

$$\left(\frac{\sum_{i=1}^n Y_i}{\sqrt{n}}, \frac{\sum_{i=1}^n q_{i,1}^* Y_i}{q_1 \sqrt{n}}, \frac{\sum_{i=1}^n q_{i,2}^* Y_i}{q_2 \sqrt{n}} \right) \xrightarrow{d} \mathcal{N}(\mu_3, \Sigma_3),$$

where

$$\mu_3 = (h_0 q_1, h_0 q_1 (2 - q_1), h_0 q_1 (1 - q_1))^T \in \mathbb{R}^3,$$

and $\Sigma_3 \in \mathbb{R}^{3 \times 3}$ is equal to

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}.$$

In other words, asymptotically these three random variables are completely linearly correlated.

Proof. By Lemma .4, it suffices to show

$$\lim_{n \rightarrow \infty} \text{Cor} \left(\frac{\sum_{i=1}^n Y_i}{\sqrt{n}}, \frac{\sum_{i=1}^n q_{i,1}^* Y_i}{q_1 \sqrt{n}} \right) = \lim_{n \rightarrow \infty} \text{Cor} \left(\frac{\sum_{i=1}^n Y_i}{\sqrt{n}}, \frac{\sum_{i=1}^n q_{i,2}^* Y_i}{q_2 \sqrt{n}} \right) = \lim_{n \rightarrow \infty} \text{Cor} \left(\frac{\sum_{i=1}^n q_{i,1}^* Y_i}{q_1 \sqrt{n}}, \frac{\sum_{i=1}^n q_{i,2}^* Y_i}{q_2 \sqrt{n}} \right) = 1,$$

which can be established by the following three computations,

$$\begin{aligned} \lim_{n \rightarrow \infty} \text{Cov} (Y_i, q_{i,1}^* Y_i) &= \lim_{n \rightarrow \infty} \mathbb{E} (Y_i \cdot q_{i,1}^* Y_i) \\ &= \lim_{n \rightarrow \infty} \int_{\mathbb{R}} \frac{y^2 q_1 e^{-(y-h_0/\sqrt{n})^2/2}}{q_1 e^{-(y-h_0/\sqrt{n})^2/2} + (1-q_1)e^{-y^2/2}} \left[(1-q_1) \frac{1}{\sqrt{2\pi}} e^{-y^2/2} + q_1 \frac{1}{\sqrt{2\pi}} e^{-(y-h_0/\sqrt{n})^2/2} \right] dy \\ &= \lim_{h \rightarrow 0} \int_{\mathbb{R}} \frac{y^2 q_1 e^{-(y-h)^2/2}}{q_1 e^{-(y-h)^2/2} + (1-q_1)e^{-y^2/2}} \left[(1-q_1) \frac{1}{\sqrt{2\pi}} e^{-y^2/2} + q_1 \frac{1}{\sqrt{2\pi}} e^{-(y-h)^2/2} \right] dy \\ &= \int_{\mathbb{R}} \lim_{h \rightarrow 0} \left\{ \frac{y^2 q_1 e^{-(y-h)^2/2}}{q_1 e^{-(y-h)^2/2} + (1-q_1)e^{-y^2/2}} \left[(1-q_1) \frac{1}{\sqrt{2\pi}} e^{-y^2/2} + q_1 \frac{1}{\sqrt{2\pi}} e^{-(y-h)^2/2} \right] \right\} dy \\ &= q_1 \int_{\mathbb{R}} y^2 \frac{e^{-y^2/2}}{\sqrt{2\pi}} dy \\ &= q_1; \end{aligned}$$

$$\begin{aligned} \lim_{n \rightarrow \infty} \text{Cov} (Y_i, q_{i,2}^* Y_i) &= \lim_{n \rightarrow \infty} \mathbb{E} (Y_i \cdot q_{i,2}^* Y_i) \\ &= \lim_{n \rightarrow \infty} \int_{\mathbb{R}} \frac{y^2 q_2 e^{-y^2/2}}{q_1 e^{-(y-h_0/\sqrt{n})^2/2} + (1-q_1)e^{-y^2/2}} \left[(1-q_1) \frac{1}{\sqrt{2\pi}} e^{-y^2/2} + q_1 \frac{1}{\sqrt{2\pi}} e^{-(y-h_0/\sqrt{n})^2/2} \right] dy \\ &= \lim_{h \rightarrow 0} \int_{\mathbb{R}} \frac{y^2 q_2 e^{-y^2/2}}{q_1 e^{-(y-h)^2/2} + (1-q_1)e^{-y^2/2}} \left[(1-q_1) \frac{1}{\sqrt{2\pi}} e^{-y^2/2} + q_1 \frac{1}{\sqrt{2\pi}} e^{-(y-h)^2/2} \right] dy \\ &= \int_{\mathbb{R}} \lim_{h \rightarrow 0} \left\{ \frac{y^2 q_2 e^{-y^2/2}}{q_1 e^{-(y-h)^2/2} + (1-q_1)e^{-y^2/2}} \left[(1-q_1) \frac{1}{\sqrt{2\pi}} e^{-y^2/2} + q_1 \frac{1}{\sqrt{2\pi}} e^{-(y-h)^2/2} \right] \right\} dy \\ &= q_2 \int_{\mathbb{R}} y^2 \frac{e^{-y^2/2}}{\sqrt{2\pi}} dy \\ &= q_2; \end{aligned}$$

$$\begin{aligned}
\lim_{n \rightarrow \infty} \text{Cov} \left(q_{i,1}^* Y_i, q_{i,2}^* Y_i \right) &= \lim_{n \rightarrow \infty} \mathbb{E} \left(q_{i,1}^* q_{i,2}^* Y_i^2 \right) \\
&= \lim_{n \rightarrow \infty} \int_{\mathbb{R}} \frac{y^2 q_1 q_2 e^{-(y-h_0/\sqrt{n})^2/2} e^{-y^2/2}}{\left[q_1 e^{-(y-h_0/\sqrt{n})^2/2} + (1-q_1) e^{-y^2/2} \right]^2} \left[(1-q_1) \frac{1}{\sqrt{2\pi}} e^{-y^2/2} + q_1 \frac{1}{\sqrt{2\pi}} e^{-(y-h_0/\sqrt{n})^2/2} \right] dy \\
&= \lim_{h \rightarrow 0} \int_{\mathbb{R}} \frac{y^2 q_1 q_2 e^{-(y-h)^2/2} e^{-y^2/2}}{\left[q_1 e^{-(y-h)^2/2} + (1-q_1) e^{-y^2/2} \right]^2} \left[(1-q_1) \frac{1}{\sqrt{2\pi}} e^{-y^2/2} + q_1 \frac{1}{\sqrt{2\pi}} e^{-(y-h)^2/2} \right] dy \\
&= \int_{\mathbb{R}} \lim_{h \rightarrow 0} \left\{ \frac{y^2 q_1 q_2 e^{-(y-h)^2/2} e^{-y^2/2}}{\left[q_1 e^{-(y-h)^2/2} + (1-q_1) e^{-y^2/2} \right]^2} \left[(1-q_1) \frac{1}{\sqrt{2\pi}} e^{-y^2/2} + q_1 \frac{1}{\sqrt{2\pi}} e^{-(y-h)^2/2} \right] \right\} dy \\
&= q_1 q_2 \int_{\mathbb{R}} y^2 \frac{e^{-y^2/2}}{\sqrt{2\pi}} dy \\
&= q_1 q_2.
\end{aligned}$$

□