Efficient Adaptive Experimental Design for Average Treatment Effect Estimation

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Abstract

We study how to efficiently estimate average treatment effects (ATEs) using adaptive experiments. In adaptive experiments, experimenters sequentially assign treatments to experimental units while updating treatment assignment probabilities based on past data. We start by defining the efficient treatment-assignment probability, which minimizes the semiparametric efficiency bound for ATE estimation. Our proposed experimental design estimates and uses the efficient treatment-assignment probability to assign treatments. At the end of the proposed design, the experimenter estimates the ATE using a newly proposed Adaptive Augmented Inverse Probability Weighting (A2IPW) estimator. We show that the asymptotic variance of the A2IPW estimator using data from the proposed design achieves the minimized semiparametric efficiency bound. We also analyze the estimator’s finite-sample properties and develop nonparametric and nonasymptotic confidence intervals that are valid at any round of the proposed design. These anytime valid confidence intervals allow us to conduct rate-optimal sequential hypothesis testing, allowing for early stopping and reducing necessary sample size. 1

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1 Introduction

Adaptive experiments are increasingly common in the social sciences, the tech industry, and medicine. In adaptive experiments, experimenters sequentially assign treatments to experimental units while updating treatment assignment probabilities based on past data. Compared to the non-adaptive randomized control trial (RCT), adaptive designs often allow experimenters to more efficiently or quickly detect causal effects, thus exposing fewer experimental units to costly or harmful treatments. This merit has led organizations such as the US Food and Drug Administration to recommend adaptive designs (FDA, 2019).

Adaptive experiments also produce social and economic applications and spark theoretical interest.

This paper studies how to design an adaptive experiment for efficient estimation of the average effects of treatment (ATE) and hypothesis testing. Let \( Y(1), Y(0) \in Y \) be potential outcomes of treatment \( 1 \) and control \( 0 \), respectively, where \( Y \subset \mathbb{R} \) is a bounded outcome space (see Assumption 1). Let \( X \in \mathcal{X} \) be covariates, where \( \mathcal{X} \) represents a space of covariates. The random variables \( (X, Y(1), Y(0)) \) jointly follow an unknown distribution \( P_0 \in \mathcal{P} \), where \( \mathcal{P} \) is the set of the distributions over \( (X, Y(1), Y(0)) \). We are interested in the estimation of average treatment effect (ATE), defined as

\[
\theta_0 := \mathbb{E}[Y(1)] - \mathbb{E}[Y(0)],
\]

where \( \mathbb{E}[Y(a)] \) denotes the mean potential outcome for each treatment \( a \in \{1, 0\} \). The experiment involves \( T \in \mathbb{N} \) experimental units, who are assigned to the treatment \( (1) \) or the control \( (0) \). For each \( t \in [T] \), let \((X_t, Y_t(1), Y_t(0))\) be an i.i.d. draw of \((X, Y(1), Y(0))\) following the distribution \( P_0 \).

We propose the following adaptive experiment consisting of (1) a treatment-assignment phase and (2) an ATE-estimation phase using a novel estimator. :

- **Step 1.** Treatment-assignment phase:
  - In each round \( t \in [T] = 1, 2, \ldots, T \), an experimental unit with covariate \( X_t \in \mathcal{X} \) visits the experimenter;
  - The experimenter assigns treatment \( A_t \in \{1, 0\} \) with probability \( \pi_t(a \mid X_t, \mathcal{H}_{t-1}) \), based on the covariate \( X_t \) and past observations
    \[
    \mathcal{H}_{t-1} := \{X_1, A_1, Y_1, X_2, \ldots, Y_{t-2}, X_{t-1}, A_{t-1}, Y_{t-1}\},
    \]
    where \( Y_t = \mathbb{1}[A_t = 1]Y_t(1) + \mathbb{1}[A_t = 0]Y_t(0) \) is the observed outcome;
  - After treatment assignment, the experimenter observes the outcome \( Y_t \in \mathbb{R} \);

- **Step 2.** ATE-estimation phase:
  - We estimate ATE \( \theta_0 \) using observations
    \[
    \mathcal{H}_T = \{(X_i, A_i, Y_i)\}_{i=1}^T.
    \]
The treatment-assignment probability can be updated after each round based on the observations collected up to that point. Our method is also applicable to batch settings, where updates occur only in specified rounds. The treatment-assignment probability $\pi_t$ is usually called a propensity score in observational studies.

Note that from our assumption that $(X_t, Y_t(1), Y_t(0))$ is i.i.d. over $t \in [T]$, the Stable Unit Treatment Value Assumption (SUTVA) holds (Imbens and Rubin, 2015). Furthermore, unconfoundedness also holds from the construction of the treatment assignment probability $\pi_t(a | X_t, \mathcal{H}_{t-1})$; that is, outcomes $(Y_t(1), Y_t(0))$ and treatment $A_t$ are conditionally independent given $X_t$ and $\mathcal{H}_{t-1}$.

In addition to ATE estimation, we also analyze hypothesis testing about $\theta_0$ with null and alternative hypotheses defined for some $\mu \in \mathbb{R}$ as

$$H_0 : \theta_0 = \mu, \quad H_1 : \theta_0 \neq \mu. \quad (1)$$

We begin by investigating the semiparametric efficiency bound for ATE estimators. Following the approach of Hahn et al. (2011), we minimize the semiparametric efficiency bound with respect to treatment-assignment probabilities and define the minimizer as the efficient treatment-assignment probability. This efficient treatment-assignment probability is expressed as the ratio of the covariate-conditional standard deviations of the potential outcomes. This treatment-assignment probability is a variant of the one proposed in Neyman (1934), which recently has been called the Neyman allocation.

Step (1) of our adaptive experiment sequentially estimates these conditional standard deviations, calculates the efficient treatment-assignment probability, and assigns treatment based on this estimate. To implement Step (2) of efficient ATE estimation, we introduce and use an ATE estimator, which we call the Adaptive Augmented Inverse Probability Weighting (A2IPW) estimator, which is a variant of the Augmented Inverse Probability Weighting (AIPW) estimator designed for adaptive experiments (Bang and Robins, 2005).

We analyze both the infinite-sample and finite-sample properties of the A2IPW estimator. In the infinite-sample analysis, we demonstrate its consistency and asymptotic normality, showing that its asymptotic variance reaches the minimized semiparametric efficiency bound. We then study hypothesis testing under two frameworks: single-stage testing and sequential testing. In the single-stage approach, we perform standard hypothesis testing by constructing confidence intervals with a fixed sample size to decide whether to reject the null hypothesis. In the sequential testing approach, the sample size is not fixed; instead, we continue collecting data until a decision can be made with a predetermined Type I error probability. Sequential testing has the potential to reduce the sample size by stopping the adaptive experiment early.

We propose a sequential testing procedure based on the finite-sample analysis of our estimator. Specifically, we derive a confidence interval that is nonparametric and non-asymptotic; it does not rely on a distributional assumption and an asymptotic approximation. We derive our confidence interval based on the Law of the Iterated Logarithm (LIL, Balsubramani and Ramdas, 2016; Howard et al., 2021). In addition, our confidence intervals are Bernstein-type and use information about the variance of potential outcomes. As a result, our sequential testing with LIL-type anytime valid confidence intervals is rate-optimal for stopping time and effectively reduces the sample size (Jamieson et al., 2014). In particular, our confidence intervals are narrower than other confidence intervals, such as those based on Hoeffding’s inequality, which rely solely on the boundedness of outcomes.
1.1 Related Work

This study contributes to the growing work on adaptive experimental design for efficient estimation and inference of treatment effects. Important problems include how to design treatment assignment probabilities (Hahn et al., 2011) and how to make statistical decisions (Manski, 2000). This paper addresses those problems by designing an adaptive experiment for efficiently estimating the ATE with associated hypothesis testing and decision-making methods.

Compared to existing studies such as Hahn et al. (2011), our adaptive experiment offers the following advantages:

**Flexible sample size computation:** Our proposed design does not require dividing experimental units into discrete prespecified batches (though our design can also be used in such batch settings). Without prefixing the sample size for batches, our approach allows for the sequential construction of the optimal treatment assignment.

**Semiparametric inference without the Donsker condition:** Our experiment does not require the Donsker condition for the estimators of the nuisance parameters (i.e., the conditional expected outcome and the efficient treatment-assignment probability). Instead, we impose convergence rate conditions for the estimators, similar to double machine learning in Chernozhukov et al. (2018). This flexibility allows us to use a variety of machine learning estimators for estimating nuisance parameters.

**Weaker assumptions on the covariate distribution:** We do not require specific assumptions (such as discrete support) on the covariate distribution as long as the convergence rate conditions are satisfied.

Furthermore, our study examines the finite sample properties of ATE estimation and the sequential testing method.

Kato et al. (2021) complements this work by highlighting that the proposed A2IPW estimator is a variant of double machine learning. They generalize the A2IPW estimator into the Adaptive Doubly Robust (ADR) estimator, which enables the estimation of the treatment-assignment probability. Their findings indicate that empirical performance can be improved by replacing the treatment-assignment probability with its estimator, even when the true value of the treatment-assignment probability is known. For a detailed discussion of double machine learning in adaptive experiments, see their paper. Kato (2021) further extends the ADR estimator for the case where the average of the treatment-assignment probability converges to a constant, even if the probability itself does not converge.

Our method and the framework for adaptive experimental design for ATE estimation have been extended in various directions. Some works have relaxed our assumptions (Cook et al., 2024; Waudby-Smith et al., 2024a), and others have adapted our proposed estimator for cases with unknown treatment-assignment probabilities (Kato et al., 2021; Li and Owen, 2024). Deep et al. (2024) refines the asymptotic optimality in this problem. Gupta et al. (2021) and Chandak et al. (2024) address endogeneity problems with instrumental variables, while Li et al. (2024) explore privacy-preserving aspects. Simchi-Levi et al. (2023) investigates the setting under nonstationarity. Zrnic and Candes (2024), Kato et al. (2024a) and Ao et al. (2024) introduce the idea of active learning for this problem setting.
The framework of Hahn et al. (2011) is called a stratified experiment, where experimental units are divided into several strata based on their covariates (Bugni et al., 2018, 2019). Concurrently with our work, Tabord-Meehan (2022) proposes a stratification method based on a tree-based algorithm within a two-stage experimental framework to relax the assumption of discrete support in Hahn et al. (2011). In contrast, our algorithm does not depend on specific models or algorithms for determining treatment-assignment probabilities or for estimating the ATE. Instead, our method incorporates double machine learning techniques into our experimental design (Chernozhukov et al., 2018), allowing for a wide range of traditional and modern machine learning estimators. Furthermore, our method is applicable to various settings of adaptive experimental design, including two-stage, multi-stage, and sequential experiments.

Furthermore, after the initial public draft of this paper (Kato et al., 2020), several related studies have emerged. Kallus et al. (2021), Bai et al. (2025), and Rafi (2023) discuss efficiency bounds or efficient experiments under the stratification setting. Armstrong (2022) and Hirano and Porter (2023) investigate asymptotically optimal treatment rules in adaptive experiments. Furthermore, Cai and Rafi (2024) and Zhao (2023) investigate the Neyman allocation from perspectives different from ours.

We derive the asymptotic distribution of our A2IPW estimator using martingale theory. Notably, our asymptotic normality result does not require the Donsker condition for the nuisance parameter estimator. This approach is similar in spirit to sample-splitting methods used in the semiparametric analysis, such as double machine learning (Klaassen, 1987; Zheng and van der Laan, 2011; Chernozhukov et al., 2018). Hadad et al. (2021) also independently proposes a closely related estimator, including ATE estimation, for bandit problems, focusing on cases where the treatment-assignment probability approaches zero at a certain rate with respect to $t$.

Efficient estimation with adaptive experiments is closely related to the Best Arm Identification (BAI) problem in multi-armed bandit (MAB) settings (Bubeck et al., 2009; Kasy and Sautmann, 2021). Neyman allocation is known to be optimal in BAI problems under certain conditions, such as Gaussian outcomes when variances are known (Chen et al., 2000; Glynn and Juneja, 2004; Kaufmann et al., 2016). When variances are unknown, our proposed A2IPW strategy is still optimal in BAI as the ATE approaches zero (Adusumilli, 2022; Kato, 2025). Adusumilli (2022) proves that the Neyman allocation is minimax optimal for the BAI problem. Armstrong (2022) and Adusumilli (2023) study asymptotic treatment rules in adaptive experiments. In the setting of BAI, Kato (2025) generalizes the Neyman allocation for the multi-armed case. In BAI problems with covariates, researchers investigate identifying the best treatment arm based on expected outcomes marginalized over the covariate distribution or the conditional on covariates (Russac et al., 2021; Kato and Ariu, 2021; Simchi-Levi et al., 2024; Kato et al., 2024b). Simchi-Levi and Wang (2023) and Caria et al. (2023) integrate the statistical inference problem with the regret minimization problem in MAB.

This study investigates the finite-sample property of the AIPW estimator in adaptive experiments. Our non-asymptotic error analysis is based on the law of the iterated logarithm (LIL, Darling and Robbins, 1967; Howard et al., 2021). The LIL plays an important role in finite-sample analysis and sequential testing since it is known to return tighter confidence intervals. Balsubramani and Randas (2016) propose nonparametric sequential testing using the LIL, and we apply their results to adaptive ATE estimation with the A2IPW estimator.
Waudby-Smith et al. (2024b) and Cai and Rafi (2024) also address the finite-sample analysis.

1.2 Organization

This study is organized as follows. In Section 2, we introduce the data-generating process and discuss the semiparametric efficiency bound. In Section 3, we design an adaptive experiment for efficient ATE estimation and powerful hypothesis testing, and we also propose the A2IPW estimator. Next, in Section 4, we present the theoretical properties of our A2IPW estimator, focusing on its asymptotic normality, efficiency, and non-asymptotic results. Notably, its asymptotic variance aligns with the semiparametric efficiency bound. In Section 5, we examine hypothesis testing under our adaptive experimental framework. Finally, in Section 6, we assess the empirical performance of the proposed method using both synthetic and semi-synthetic data. All Appendices are provided in the online supplementary materials.

2 Semiparametric Efficiency Bound and Efficient Assignment Probability

2.1 Semiparametric Efficiency Bound in Adaptive Experimental Design

This section provides a lower bound for the asymptotic variance of regular estimators of the ATE in adaptive experiments, following the arguments in Hahn et al. (2011). Specifically, we focus on the semiparametric lower bound, which establishes a theoretical limit for the asymptotic variances of regular ATE estimators under semiparametric models.

Consider i.i.d. observations \
{(X_i, A_i, Y_i)}_{i=1}^n generated from a distribution \(P_0\) with a treatment-assignment probability \(\pi_0(a \mid X_i)\). This treatment-assignment probability can be optimized for ATE estimation; thus, we refer to an algorithm with such a treatment-assignment probability as an oracle algorithm. In this case, from Theorem 1 of Hahn (1998), the semiparametric efficiency bound is given as follows:

\[
\text{Proposition 1 (Semiparametric efficiency bound of ATE estimators. Based on Theorem 1 of Hahn (1998).)}
\]

Suppose that the same regularity conditions assumed in Theorem 1 of Hahn (1998) hold. Under an oracle algorithm with treatment-assignment probability \(\pi_0\), the asymptotic variance of regular ATE estimators is lower bounded by

\[
V(\pi_0) := \mathbb{E}_{P_0} \left[ \frac{\sigma_0^2(1, X)}{\pi_0(1 \mid X)} + \frac{\sigma_0^2(0, X)}{\pi_0(0 \mid X)} + \left( \theta_0(X) - \theta_0 \right)^2 \right], \tag{2}
\]

where \(\sigma_0^2(a, X)\) is the conditional variance of \(Y(a)\) given \(X\) for \(a \in \{1, 0\}\).
This proposition corresponds to the case where the oracle treatment-assignment probability \( \pi_0 \) is known in advance, eliminating the need for estimation during the adaptive experiment. In such a scenario, treatments are assigned directly using the oracle treatment-assignment probability. This static oracle algorithm serves as a benchmark in the study of adaptive experimental designs (Hahn et al., 2011).

If we restrict the algorithm to those where \( \pi_t \overset{p}{\to} \pi_0 \) as \( t \to \infty \), the result can be extended to non-i.i.d. observations using the martingale central limit theorem, as demonstrated in the derivation of asymptotic normality. Various extensions of lower bounds also have been proposed (Li and Owen, 2024; Rafi, 2023).

### 2.2 Efficient Treatment-assignment Probability

In the semiparametric efficiency bound (2), decision-makers can select \( \pi_0 \) to minimize the asymptotic variance. Denote the efficient treatment-assignment probability by

\[
\pi^* = \arg \min_{\pi_0 \in \Pi} V(\pi_0).
\]

The minimization problem has a closed-form solution, as shown below:

**Proposition 2 (Efficient treatment-assignment probability).** The efficient treatment-assignment probability \( \pi^* \) is:

\[
\pi^*(a \mid x) = \frac{\sqrt{\sigma_0^2(a, x)}}{\sqrt{\sigma_0^2(1, x) + \sqrt{\sigma_0^2(0, x)}}}, \quad \forall a \in \{1, 0\}, \quad \forall x \in X.
\]

The proof is presented in Appendix C.

Intuitively, conditional on \( x \), the asymptotic variance can be minimized by assigning the treatment with a higher variance of the potential outcome. This treatment-assignment probability is recently referred to as the Neyman allocation (Neyman, 1934) and has been investigated in various studies on experimental design (Chen et al., 2000; Glynn and Juneja, 2004; van der Laan, 2008; Hahn et al., 2011; Kaufmann et al., 2016; Tabord-Meehan, 2022).

### 3 Semiparametric Efficient Adaptive Experiment

In this section, we design an adaptive experiment that minimizes the semiparametric efficiency bound and an ATE estimator whose asymptotic variance hits the minimized semiparametric efficiency bound. As explained in the Introduction, our experiment consists of two steps:

- **Step (1). Treatment-assignment phase:** In each round \( t \in [T] \), we estimate the efficient treatment-assignment probability \( \pi^*(a \mid x) \) and assign a treatment based on the estimated efficient treatment-assignment probability.

- **Step (2). ATE-estimation phase:** At the end of the experiment, we estimate the ATE using our proposed A2IPW estimator.

The pseudo-code is provided in Algorithm 1. In the following subsections, we explain the details of our experimental design.
3.1 Step (1): Treatment-Assignment Phase

We assign treatments in each round \( t \in [T] \) to gather data. Although assigning treatments with probability \( \pi^* \) minimizes the semiparametric efficiency bound, it is infeasible since we do not know the conditional variance \( \sigma_0^2(a, x) \). To overcome this challenge, in each round \( t \), we estimate the conditional variance \( \sigma_0^2(a, x) \), estimate the efficient treatment-assignment probability \( \pi^* \) using the estimator of \( \sigma_0^2(a, x) \), and assign a treatment based on the estimated efficient treatment-assignment probability.

Let \( T_0 \) (\( 2 \leq T_0 \leq T \)) be the number of initialization rounds, which is a constant independent of \( T \). In the initialization rounds \( t = 1, 2, \ldots, T_0 \), we assign treatment \( A_t = 1 \) if \( t \) is odd and \( A_t = 0 \) if \( t \) is even; for example, if \( T_0 = 6 \), \((A_1, A_2, A_3, A_4, A_5, A_6) = (1, 0, 1, 0, 1, 0)\). We set \( \pi_t(1 \mid X_t, \mathcal{H}_{t-1}) = 1/2 \) for all \( t = 1, 2, \ldots, T_0 \).

In each round \( t \in \{T_0 + 1, T_0 + 2, \ldots, T\} \), we construct a consistent estimator \( \hat{\sigma}_t^2(a, x) \) of \( \sigma_0^2(a, x) \) such that \( \hat{\sigma}_t^2(a, x) \in (0, \infty) \) for all \( a \in \{1, 0\} \) and \( x \in \mathcal{X} \), and \( \hat{\sigma}_t^2(a, x) \) is constructed only by using \( \mathcal{H}_{t-1} \). The reason we use only \( \mathcal{H}_{t-1} \) is to construct an ATE estimator whose scores consist of a martingale difference sequence, as shown in the next subsection. Under this property, we can apply the martingale central limit theorem and martingale concentration inequality to analyze the asymptotic and non-asymptotic behaviors of the ATE estimator.

To estimate \( \sigma_0^2(a, X_t) \), we propose estimating \( f_0(a, X_t) = \mathbb{E}[Y_t(a) \mid X_t] \) and \( e_0(a, X_t) = \mathbb{E}[Y_t^2(a) \mid X_t] \) using nonparametric models based on observations \( \mathcal{H}_{t-1} \) up to round \( t \). Let \( \hat{f}_t(a, X_t) \) and \( \hat{e}_t(a, X_t) \) denote such estimators. In MAB problems, several nonparametric estimators, such as \( K \)-nearest neighbor regression and Nadaraya–Watson kernel regression, have been shown to be consistent (Yang and Zhu, 2002; Qian and Yang, 2016). For example, given a bandwidth \( h_T > 0 \) and a kernel function \( K : \mathcal{X} \to \mathbb{R} \), a Nadaraya–Watson estimator of \( f_0(a, X_t) \) is defined as

\[
\hat{f}_t(a, X_t) = \frac{1}{t} \sum_{s=1}^{t} 1[A_s=a]K((X_s-X_t)/h_t) Y_t \quad \forall a \in \{1,0\}.
\]

We can also estimate \( e_0(a, X_t) \). By appropriately obtaining samples, we can also employ random forests (Wager and Athey, 2018) and neural networks as nonparametric estimators (Schmidt-Hieber, 2020; Farrell et al., 2021).

We then estimate \( \sigma_t^2(a, X_t) \) as follows:

\[
\hat{\sigma}_t^2 = \begin{cases} 
\hat{e}_t(a, X_t) - \hat{f}_t^2(a, X_t) & \text{if } \hat{e}_t(a, X_t) - \hat{f}_t^2(a, X_t) > 0, \\
\varepsilon & \text{otherwise,}
\end{cases}
\]

where \( \varepsilon > 0 \) is a small positive constant introduced to ensure that \( \hat{\sigma}_t^2 \) remains non-negative. Note that when \( \sigma_0^2(a, X_t) > 0 \), the term \( \varepsilon \) becomes unnecessary as \( t \) grows large.

We assign treatment \( A_t \) with probability \( \pi_t(A_t \mid X_t, \mathcal{H}_{t-1}) \), defined as

\[
\pi_t(a \mid X_t, \mathcal{H}_{t-1}) = \frac{\sqrt{\hat{\sigma}_t^2(a, X_t)}}{\sqrt{\hat{\sigma}_t^2(1, X_t) + \hat{\sigma}_t^2(0, X_t)}} \quad \forall a \in \{1, 0\},
\]

Note that our experiment can be used in a batch setting, where we update \( \pi_t(a \mid x, \mathcal{H}_{t-1}) \) only at certain rounds \( T_1, T_2, \ldots \in \{1, \ldots, T\} \). We require that \( \pi_t(a \mid x, \mathcal{H}_{t-1}) \to \pi^*(a \mid x) \) for each \( x \in \mathcal{X} \) as \( t \to \infty \).\(^3\)

\(^3\)As long as this condition is satisfied, we do not need to sequentially update \( \pi_t(a \mid x, \mathcal{H}_{t-1}) \). This implies
3.2 Step (2): ATE-Estimation Phase

At the end of the experiment, we construct an ATE estimator that is asymptotically normal with an asymptotic variance, achieving the semiparametric lower bound \( (2) \). In adaptive experiments, due to the changing assignment probabilities, dependencies among samples can complicate the estimation process. To address this dependency problem, we propose the A2IPW estimator:

\[
\hat{\theta}_T^{\text{A2IPW}} = \frac{1}{T} \sum_{t=1}^{T} \Psi_t,
\]

where

\[
\Psi_t = \left( \frac{[A_t = 1](Y_t - \hat{f}_{t-1}(1, X_t))}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} - \frac{[A_t = 0](Y_t - \hat{f}_{t-1}(0, X_t))}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} + \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) \right).
\]

and \( \hat{f}_t(a, x) \) is an estimator of \( f_0(a, x) \), constructed from \( \mathcal{H}_t \). As stated in Theorem 1, the asymptotic optimality of our proposed ATE estimator holds with any consistent estimator for \( f_0(a, x) \), due to the unbiasedness of \( \hat{\theta}_T^{\text{A2IPW}} \) for \( \theta_0 \). This point is also discussed in Section 4 of Kato et al. (2021), our follow-up study. Additionally, consistency holds even if the estimator of \( f_0(a, x) \) is inconsistent, as stated in Corollary 1. Here, \( \Psi_t \) is the semiparametric efficient score for ATE estimators. Regular estimators with scores \( \Psi_t \) achieve the smallest asymptotic variance within the class of such estimators.

For \( z_t = \Psi_t - \theta_0 \), the sequence \( \{z_t\}_{t=1}^T \) forms a martingale difference sequence, which means that \( \mathbb{E}[z_t \mid \mathcal{H}_{t-1}] = 0 \). Using this property, we will derive the theoretical results for \( \hat{\theta}_T^{\text{A2IPW}} \). This construction shares a similar motivation to sample-splitting techniques in semiparametric inference (Klaassen, 1987), including double machine learning (Chernozhukov et al., 2018).

3.3 Stabilizations and Extensions

While not required to obtain the asymptotic properties, here we introduce stabilization techniques that contribute to the finite-sample stabilization of the designed experiment. The above sections show that our designed experiment is asymptotically efficient in the sense that the asymptotic variance of the ATE estimator aligns with the semiparametric efficiency bound. However, such asymptotic optimality does not necessarily guarantee accurate ATE estimation in finite samples.

that we can keep \( \pi_t(a \mid x, \mathcal{H}_{t-1}) \) constant for several rounds and update \( \pi_t(a \mid x, \mathcal{H}_{t-1}) \) in specific rounds. For example, we can consider a two-stage design similar to Hahn et al. (2011). In this case, we update \( \pi_t(a \mid x, \mathcal{H}_{t-1}) \) only at \( T_1 \). Assume that \( T_1 = rT \), where \( r \in (0, 1) \) is a constant independent of \( T \). In rounds \( 1, 2, \ldots, T_1 \), we assign treatment \( a \in \{1, 0\} \) with probability \( 1/2 \), where \( \pi_t(a \mid x, \mathcal{H}_{t-1}) = 1/2 \) for all \( x \in \mathcal{X} \). Afterward, we update \( \pi_t(a \mid x, \mathcal{H}_{t-1}) \) by estimating \( \pi^*(a \mid x) \). If \( \pi_t(a \mid x, \mathcal{H}_{t-1}) \to \pi^*(a \mid x) \) as \( t \to \infty \) holds for all \( x \in \mathcal{X} \), we can prove the same asymptotic optimality of our experimental design. To verify that \( \pi_t(a \mid x, \mathcal{H}_{t-1}) \to \pi^*(a \mid x) \) as \( t \to \infty \), it is sufficient to check \( \pi_{T_1}(a \mid x, \mathcal{H}_{t-1}) \to \pi^*(a \mid x) \) as \( T_1 \to \infty \) (\( T \to \infty \)).
The ADR estimator. Kato et al. (2021) reports that replacing the true \( \pi_t \) with its estimate can paradoxically improve performance. This is because the original \( \pi_t \) may take values close to zero, causing the inverse of \( \pi_t \) to become large and making the A2IPW estimator unstable. By replacing \( \pi_t \) with its estimate, even when the true value of \( \pi_t \) is known, the A2IPW estimator can be stabilized.\(^4\)

The ADR estimator is defined as follows:

\[
\hat{\theta}_T^{ADR} = \frac{1}{T} \sum_{t=1}^T \left( \frac{1[A_t = 1](Y_t - \hat{f}_{t-1}(1, X_t))}{\hat{g}_t(1 \mid X_t)} - \frac{1[A_t = 0](Y_t - \hat{f}_{t-1}(0, X_t))}{\hat{g}_t(0 \mid X_t)} + \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) \right),
\]

where \( \hat{g}_t(a \mid X_t) \) is an estimator of \( \pi_t(a \mid X_t, \mathcal{H}_{t-1}) \) constructed from the past observations \( \{(X_s, A_s, Y_s)\}_{s=1}^{t-1} \). Although this estimator is no longer unbiased, asymptotic normality holds under convergence rate conditions for \( \hat{f}_t \) and \( \hat{\pi}_t \), as well as double machine learning techniques. The theorem regarding its asymptotic normality is introduced in Proposition 3.

Kato et al. (2021) refer to the sample splitting used in both the A2IPW and ADR estimators as adaptive fitting, where only past observations up to time \( t \) are used to obtain the plug-in estimators for each \( t \). Figure 1 illustrates the difference between cross-fitting as described in Chernozhukov et al. (2018) and our adaptive fitting approach.

Stabilization techniques. To stabilize the finite-sample behavior, we can further introduce certain elements into our experiment. These elements are designed not to affect the asymptotic behavior, meaning their influence vanishes as \( t \to \infty \).

(a) We define the treatment-assignment probability as

\[
\pi_t(1 \mid x, \mathcal{H}_{t-1}) = \gamma_t \frac{1}{2} + (1 - \gamma_t) \frac{\sqrt{\sigma_{t-1}^2(1, x)}}{\sqrt{\sigma_{t-1}^2(1, x)} + \sqrt{\sigma_{t-1}^2(0, x)}},
\]

\(^4\)Note that, unlike the classical problem regarding the use of an estimated propensity score in the IPW estimators, the asymptotic properties remain unchanged between the cases where the true \( \pi_t \) is used and where \( \pi_t \) is estimated when we use the AIPW estimator (Hirano et al., 2003; Henmi and Eguchi, 2004).
π_t(0 \mid x, \mathcal{H}_{t-1}) = 1 - π_t(1 \mid x, \mathcal{H}_{t-1}),

where \( γ_t = O(1/\sqrt{t}) \);

(b) As an alternative estimator, we propose the mixed A2IPW (MA2IPW) estimator, defined as
\[
\hat{\theta}_t^{MA2IPW} = \zeta_t \hat{\theta}_t^{IPW} + (1 - \zeta_t) \hat{\theta}_t^{A2IPW},
\]
where \( \hat{\theta}_t^{IPW} \) is the IPW estimator defined as
\[
\hat{\theta}_t^{IPW} = \frac{1}{T} \sum_{t=1}^{T} \left( \frac{1(\pi_t = 1 | X_t, \mathcal{H}_{t-1})}{\pi_t(1 | X_t, \mathcal{H}_{t-1})} - \frac{1(\pi_t = 0 | X_t, \mathcal{H}_{t-1})}{\pi_t(0 | X_t, \mathcal{H}_{t-1})} \right)
\]
and \( \zeta_t = o(1/\sqrt{T}) \).

Note that the IPW estimator is a special case of the A2IPW estimator with \( f_{t-1}(x) = 0 \).

Technique (a) aims to stabilize the treatment assignment probability. If \( π_t \) fluctuates significantly, it may unstabilize the A2IPW estimator for the ATE. Furthermore, when the value of \( π_t \) is too close to zero, its inverse is included in the elements averaged by A2IPW, potentially causing those elements to become extremely large. Technique (a) prevents such cases.\(^5\)

Technique (b) controls the estimator’s behavior by avoiding situations where \( \hat{f}_{t-1} \) takes unpredictable values in the early stages. Since the nonparametric convergence rate is generally slower than \( 1/\sqrt{t} \), the convergence rate of \( π_t \) to \( π^* \) does not exceed \( O(1/\sqrt{t}) \). Therefore, \( γ_t = O(1/\sqrt{t}) \) does not asymptotically affect the convergence rate of the treatment-assignment probability. Similarly, the asymptotic distribution of \( \hat{\theta}_t^{MA2IPW} \) is asymptotically equivalent to \( \hat{\theta}_t^{A2IPW} \) because it holds that \( \sqrt{T} \hat{\theta}_t^{MA2IPW} = \sqrt{T} (\zeta_t \hat{\theta}_t^{IPW} + (1 - \zeta_t) \hat{\theta}_t^{A2IPW}) = \sqrt{T} \hat{\theta}_t^{A2IPW} + o(1) \) as \( T \to \infty \).

There are additional stabilization techniques. For example, Cook et al. (2024) also develops stabilization techniques based on Waudby-Smith et al. (2024a).

4 Theoretical Results about Treatment Effect Estimation

This section provides theoretical results on the A2IPW estimator. We present its asymptotic distribution, a regret bound, and a non-asymptotic confidence bound for the A2IPW estimator.

4.1 Consistency and Asymptotic Normality of the A2IPW Estimator

We first show the asymptotic normality of the A2IPW estimator \( \hat{\theta}_t^{A2IPW} \). Before showing the asymptotic normality, we make the following assumption.

**Assumption 1** (Boundedness). There exists an absolute constant \( C \) such that \( |Y_t(a)| \leq C \) holds for \( a \in \{1, 0\} \).

\(^5\)Performance can be further improved by replacing \( π_t \) with its estimator constructed from past observations \( \{(X_s, A_s, Y_s)\}_{s=1}^{t-1} \) and \( X_t \), as noted by Kato et al. (2021), a subsequent study to our study. Kato et al. (2021) observes that the A2IPW estimator with the true \( π_t \) incurs a larger mean squared error than when using an estimated \( π_t \). This is because when the true \( π_t \) fluctuates significantly, the A2IPW estimator also becomes unstable. However, Kato et al. (2021) finds that replacing the volatile \( π_t \) with a more stable estimator helps stabilize the behavior of the A2IPW estimator. The A2IPW estimator with an estimated \( π_t \) is referred to as the Adaptive Doubly Robust (ADR) estimator. Although we do not focus on this type of stabilization in this study, it is a promising approach. We compare our estimator with the ADR estimator in our simulation studies. Cook et al. (2024) also develops stabilization techniques based on Waudby-Smith et al. (2024a).
Algorithm 1 Adaptive experiment for efficient ATE estimation.

**Parameter:** The number of initialization rounds, $T_0$. The lower bound of the variance $\nu$, $\nu > 0$. The stabilization parameter $\gamma_t, \zeta_T \in (0,1)$, such that $\gamma_t = O(1/\sqrt{t})$ and $\zeta_T = o(1/\sqrt{T})$.

**Initialization:**
At $t = 1, 2, \ldots, T_0$, assign treatment $A_t = 1$ if $t$ is odd and assign treatment $A_t = 2$ if $t$ is even. Set $\pi_t(a \mid X_t, H_{t-1}) = 1/2$ for all $a \in \{1,0\}$.

for $t = T_0 + 1$ to $T$ do
  if $t < \rho$ then
    Set $\pi_t(1 \mid X_t, \Omega_{t-1}) = 0.5$.
  else
    Construct estimators $\hat{f}_{t-1}$ and $\hat{\pi}_{t-1}$ using a nonparametric method.
    Construct $\hat{\pi}_{t-1}$ from $\hat{f}_{t-1}$ and $\hat{\pi}_{t-1}$.
    Using $\hat{\pi}_{t-1}$, construct an estimator of $\pi^*(k \mid X_t)$ and set it as $\pi_t(k \mid X_t, \Omega_{t-1})$.
  end if
  Draw $\xi_t$ from the uniform distribution on $[0,1]$.
  $A_t = \mathbb{1} [\xi_t \leq \pi_t(1 \mid X_t, \Omega_{t-1})]$.
end for

Estimate the ATE by using the A2IPW estimator $\hat{\theta}_T^{A2IPW}$.

The following theorem states the asymptotic normality.

**Theorem 1** (Asymptotic distribution of the A2IPW estimator). Suppose that Assumption 1 holds, and

(i) point convergence in probability of $\hat{f}_{t-1}$ and $\pi_t$, i.e., for all $x \in X$ and $a \in \{0,1\}$,

\[
\hat{f}_{t-1}(a,x) - f_0(a,x) \xrightarrow{p} 0 \quad \text{and} \quad \pi_t(a \mid x, H_{t-1}) - \bar{\pi}(a \mid x) \xrightarrow{p} 0,
\]

where $\bar{\pi} \in \Pi$;

(ii) there exists a constant $C_f$ such that $|\hat{f}_{t-1}| \leq C_f$.

Then, the A2IPW estimator is asymptotically normal:

\[
\sqrt{T} \left( \frac{\hat{\theta}_T^{A2IPW}}{\theta_0} - \theta_0 \right) \xrightarrow{d} \mathcal{N}(0, V),
\]

where

\[
V := E \left[ \frac{\tilde{\sigma}^2(1, X_t)}{\bar{\pi}(1 \mid X_t)} + \frac{\tilde{\sigma}^2(0, X_t)}{\bar{\pi}(0 \mid X_t)} + \left( f_0(1, X_t) - f_0(0, X_t) - \theta_0 \right)^2 \right].
\]

The asymptotic variance aligns with the semiparametric efficiency bound derived under the treatment-assignment probability $\bar{\pi}$. Note that we do not have to impose the Donsker condition, similar to cross-fitting (Klaassen, 1987; Zheng and van der Laan, 2011; Chernozhukov et al., 2018). Here, we do not impose the convergence rate of $\hat{f}_{t-1}$ owing to the unbiasedness of the A2IPW estimator $\hat{\theta}_T^{A2IPW}$ for the ATE $\theta_0$. 

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Consistency holds under a weaker assumption, i.e., even if the treatment-assignment probability $\pi_t$ does not converge. We omit the proof because it follows from the boundedness of $z_t$ and the weak law of large numbers for a martingale difference sequence (Proposition 6 in Appendix B).

**Corollary 1** (Consistency of the A2IPW estimator). Suppose that there exists a constant $C_f$ such that $|\hat{f}_{t-1}| \leq C_f$. Then, under Assumption 1, $\hat{\theta}_T^{A2IPW} \overset{p}{\to} \theta_0$ holds as $T \to \infty$.

Note that Corollary 1 holds even if $\hat{f}_t$ is inconsistent. Therefore, compared to Theorem 1, Corollary 1 holds with a weaker assumption.

We also present the theorem about the asymptotic normality of the ADR estimator from Kato et al. (2021), which is a follow-up study that investigates the A2IPW estimator and generalizes it as the ADR estimator.

**Proposition 3** (Asymptotic distribution of the ADR estimator. From Theorem 1 in Kato et al. (2021)). Suppose that Assumption 1 holds, and

(i) For all $x \in X$ and $a \in \{0, 1\}$, there exist $p, q > 0$ such that $p + q = 1/2$, it holds that $|\hat{g}_{t-1}(a \mid x) - \hat{\pi}(a \mid x)| = o_p(t^{-p})$, and $|\hat{f}_{t-1}(a, x) - f_0(a, x)| = o_p(t^{-q})$ where $\hat{\pi} \in \Pi$;

(ii) There exists a constant $C_f$ such that $|\hat{f}_t| \leq C_f$.

Then, the ADR estimator is consistent and asymptotically normal:

$$\sqrt{T} \left( \hat{\theta}_T^{ADR} - \theta_0 \right) \overset{d}{\to} \mathcal{N}(0, V).$$

### 4.2 Regret Bound of the A2IPW Estimator

In addition to the above asymptotic analysis, we introduce the finite-sample regret framework often used in the literature on the MAB problem. We define regret based on the MSE. We define the optimal experiment $\Pi^{OPT}$ as an experiment that chooses a treatment with the probability $\pi^*$ defined in Proposition 2, and an estimator $\hat{\theta}_T^{OPT}$ with oracle $f_0$ as

$$\hat{\theta}_T^{OPT} = \frac{1}{T} \sum_{t=1}^{T} \left( \frac{1[A_t = 1](Y_t - f_0(1, X_t))}{\pi^*(1 \mid X_t)} - \frac{1[A_t = 0](Y_t - f_0(0, X_t))}{1 - \pi^*(1 \mid X_t)} \right).$$

For any experiment $\Pi$ adapted by the experimenter, we define the regret of $\Pi$ as

$$\text{regret} = \mathbb{E}_\Pi \left[ \left( \theta_0 - \hat{\theta}_T^{A2IPW} \right)^2 \right] - \mathbb{E}_\Pi^{OPT} \left[ \left( \theta_0 - \hat{\theta}_T^{OPT} \right)^2 \right],$$

where the expectations are taken over each experiment. The following theorem provides an upper bound on the regret.
Theorem 2 (Regret Bound of A2IPW). Suppose that there exists a constant $C_f$ such that $|\hat{f}_{t-1}| \leq C_f$. Then, under Assumption 1, there exist constants $C > 0$ and $T_0$ such that for all $T > T_0$, it holds that

$$\text{regret} \leq \frac{C}{T^2} \sum_{a \in \{1,0\}} \sum_{t=1}^{T} \left( \mathbb{E} \left[ \left| \sqrt{\pi^*(a \mid X_t)} - \sqrt{\pi_t(a \mid X_t, H_{t-1})} \right| \right] ight. $$

$$+ \left. \mathbb{E} \left[ |f_0(a, X_t) - \hat{f}_{t-1}(a, X_t)| \right] \right),$$

where the expectation is taken over the random variables including $H_{t-1}$.

The proof is shown in Appendix E. This result tells us that regret is bounded by $o(1/T)$ under the consistencies of $\pi_t$ and $\hat{f}_t$, since under the consistencies and uniform integrability, as $T \to \infty$, it holds that

$$\sum_{a \in \{1,0\}} \sum_{t=1}^{T} \left( \mathbb{E} \left[ \left| \sqrt{\pi^*(a \mid X_t)} - \sqrt{\pi_t(a \mid X_t, H_{t-1})} \right| \right] ight. $$

$$+ \left. \mathbb{E} \left[ |f_0(a, X_t) - \hat{f}_{t-1}(a, X_t)| \right] \right) = o(T).$$

By contrast, if we use a constant value for $\pi_t$, regret is $O(1/T)$. The regret bound for finite samples can also be obtained by substituting the finite sample bounds of

$$\mathbb{E} \left[ \left| \sqrt{\pi^*(a \mid X_t)} - \sqrt{\pi_t(a \mid X_t, H_{t-1})} \right| \right]$$

and $\mathbb{E} \left[ |f_0(a, X_t) - \hat{f}_{t-1}(a, X_t)| \right]$. We can bound $\hat{f}_{t-1}(a, X_t)$ and $\sqrt{\pi_t(a \mid X_t, H_{t-1})}$ by the same argument as existing work on the MAB problem such as Yang and Zhu (2002).

4.3 Any Time Confidence Interval

The asymptotic normality shown in the previous section holds for large fixed $T$. In this section, we consider a confidence interval that is valid for any $t \in [T]$. This type of anytime confidence interval guarantees a finite sample estimation error and plays an important role in sequential hypothesis testing.

Among the various candidates for constructing confidence intervals, we employ concentration inequalities based on the LIL. The LIL is originally derived as an asymptotic property of independent random variables by Khintchine (1924) and Kolmogoroff (1929). Following their methods, several works have derived an asymptotic LIL for a martingale difference sequence under some regularity conditions (Stout, 1970; Fisher, 1992). Balsubramani and Ramdas (2016) derived a non-asymptotic LIL-based concentration inequality for sequential testing. The reason for using the LIL-based concentration inequality is that sequential testing with the LIL-based confidence sequence requires a smaller sample size needed to identify the parameter of interest since the confidence intervals depend on the distributional
information and are said to be tight (Jamieson et al., 2014), as explained later. Due to the tightness of the inequality, LIL-based concentration inequalities have been widely accepted in sequential testing (Balsubramani and Ramdas, 2016) and in the best arm identification in the Multi-Armed Bandit (MAB) problem (Jamieson et al., 2014; Jamieson and Jain, 2018).

We construct the confidence sequence \( \{q_t\} \) based on the LIL-based concentration inequality for the A2IPW estimator as follows.

**Theorem 3 (Concentration Inequality of the A2IPW Estimator).** Suppose that the null hypothesis is correct; that is, \( \mu = \theta_0 \) and \( z_t = \Psi_t - \theta_0 \). Let \( C > 0 \) and \( C_z > 0 \) be constants independent of \( t \) and \( T \) such that \( \left| z_t \right| \leq C \) and \( \left| (z_t - z_{t-1})^2 - \mathbb{E}[(z_t - z_{t-1})^2 | \mathcal{H}_{t-1}] \right| \leq C_z \) hold. For any \( \delta \), with probability \( \geq 1 - \delta \), for all \( t \geq T_0 \) simultaneously,

\[
\left| \sum_{i=1}^{t} z_i \right| = t \left| \hat{\theta}_t^{A2IPW} - \theta_0 \right| \leq \frac{2C}{e^2} \left( C_0(\delta) + \sqrt{2C_1 \hat{V}_t^* \left( \log \log \hat{V}_t^* + \log \left( \frac{4}{\delta} \right) \right)} \right),
\]

where \( \hat{V}_t^* = C_f \left( \frac{e^4}{4e^2} \sum_{i=1}^{t} z_i^2 + \frac{2C_0(\delta)C_z}{e^2} \right) \), \( C_0(\delta) = 3(e - 2) + 2 \sqrt{\frac{173}{2(e - 2)}} \log \left( \frac{1}{\delta} \right) \), \( C_1 = 6(e - 2) \) and \( C_f \) is an absolute constant.

The proof is provided in Appendix E.1. This result, derived by applying the findings of Balsubramani (2014), not only shows an anytime confidence interval but also establishes a finite-sample estimation error bound in estimating \( \theta_0 \).

We obtain confidence sequences, \( \{q_t\}_t \), with the Type I error at \( \alpha \) from the results of Theorem 3 and Balsubramani and Ramdas (2016) as

\[
q_t \propto \log \left( \frac{1}{\alpha} \right) + \sqrt{2 \sum_{i=1}^{t} z_i^2 \left( \log \frac{\log \sum_{i=1}^{t} z_i^2}{\alpha} \right)}.
\]

Balsubramani and Ramdas (2016) proposes using constant 1.1 to specify \( q_t \), namely,

\[
q_t = 1.1 \left( \log \left( \frac{1}{\alpha} \right) + \sqrt{2 \sum_{i=1}^{t} z_i^2 \left( \log \frac{\log \sum_{i=1}^{t} z_i^2}{\alpha} \right)} \right).
\]

This choice is motivated by the asymptotic property of the LIL such that

\[
\limsup_{t \to \infty} \frac{\left| t \hat{\theta}_t^{A2IPW} - t \theta_0 \right|}{\sqrt{2 \hat{V}_t^* \left( \log \log \hat{V}_t^* \right)}} = 1
\]

with probability 1 for sufficiently large samples (Stout, 1970; Balsubramani and Ramdas, 2016), where \( \hat{V}_t^2 = \sum_{i=1}^{t} \mathbb{E}[z_i^2 | \mathcal{H}_{i-1}] \), as well as the empirical results of Balsubramani and Ramdas (2016).

The confidence interval tightly depends on the underlying distribution through the variances, in contrast to confidence intervals that rely on less information, such as those based on Hoeffding’s inequality, which only uses the boundedness of the outcomes. Additionally,
the tightness of the confidence intervals is also guaranteed by the lower bounds for sequential testing, as discussed in Jamieson et al. (2014). It is known that the \(O(\sqrt{t^{-1}\log\log t})\) asymptotic rate of the confidence intervals aligns with the lower bound implied by the LIL (Farrell, 1964). Non-asymptotic bounds of this form are referred to as finite LIL bounds (Howard et al., 2021).

5 Hypothesis Testing

This section studies hypothesis testing about the ATE. We begin by formulating the hypothesis testing framework, introduce the testing procedures, and conclude by presenting the theoretical properties. We demonstrate how to compute the required sample size for hypothesis testing. The pseudo-code for our experimental design incorporating hypothesis testing is provided in Algorithm 2, which encompasses Algorithm 1.

5.1 Hypothesis Testing in Adaptive Experiments

The experimenter aims to decide whether to reject the null hypothesis \(H_0\) in (1) while maximizing the power and controlling the Type I error. In adaptive experiments, hypothesis testing can be framed in two ways: single-stage testing and sequential hypothesis testing. In single-stage testing, the test is performed only at the end of the experiment \((t = T)\). In sequential hypothesis testing, the test is conducted sequentially at each stage of the experiment, where the sample size is treated as a stopping time (a random variable). Sequential testing is expected to reduce the required sample size by allowing the experiment to stop earlier.

For each \(t \in [T]\), let \(\hat{\theta}_T\) be an ATE estimator constructed using \(H_T\). In single-stage testing, we fix a threshold \(p_T \in \mathbb{R}^+\) before gathering data via the experiment. At the end of the experiment, we reject the null hypothesis if:

\[ T \left| \hat{\theta}_T - \mu \right| > p_T. \]

We can conduct the most powerful test in single-stage testing by using the \(t\)-test with our efficient ATE estimator, which is asymptotically normal.

In sequential testing, we define thresholds \(q_t \in \mathbb{R}^+\) for each \(t \in [T]\). At each time \(t \in [T]\), we reject the null hypothesis if:

\[ t \left| \hat{\theta}_t - \mu \right| \geq q_t. \]

The difference between single-stage and sequential testing is illustrated in Figure 2.

In single-stage testing, it is natural to analyze the power of the test. In contrast, in sequential testing, we focus on the expected sample size (stopping time). Both are related to the minimum required sample size under Type I error control.

**Controlling the Type I and Type II errors.** Recall that our null and alternative hypotheses are \(H_0 : \theta_0 = \mu\) and \(H_1 : \theta_0 \neq \mu\), respectively. Let \(\mathbb{P}_{H_0}\) and \(\mathbb{P}_{H_1}\) represent the probabilities when the null and alternative hypotheses are correct, respectively. When \(\mathbb{P}_{H_0}(\text{reject } H_0) \leq \alpha\), we say that we control the Type I error at level \(\alpha\). Similarly, when \(\mathbb{P}_{H_1}(\text{reject } H_0) \geq 1 - \beta\), we say that we control the Type II error, where \(\beta\) is also referred to as the power of the test.
1: Fix $T$ and compute $p_T$.
2: if $T \mid \hat{\theta}_T^{\text{A2IPW}} - \mu > p_T$ then
3: Reject $H_0$.
4: else
5: Fail to reject $H_0$.
6: end if

1: Fix $T$.
2: for $t = 1$ to $T$ do
3: Compute $q_t$.
4: if $t \mid \hat{\theta}_t - \mu > q_t$ then
5: Reject $H_0$.
6: end if
7: end for
8: Fail to reject $H_0$.

Figure 2: Single-stage (left) and sequential (right) hypothesis testing (from Figure 1 in Balsubramani and Ramdas (2016)).

We set $p_T$ and $q_t$ to control both the Type I and Type II errors. We use asymptotic normality to construct $p_T$ and the LIL-based concentration inequality to construct $\{q_t\}_{t=1}^T$. Controlling errors in sequential testing is more complex than in single-stage testing. If we naively apply standard single-stage testing at each $t$ sequentially, the probability of a Type I error increases due to the multiple testing problem (Balsubramani and Ramdas, 2016). A common approach to this problem is to apply multiple testing corrections, such as the Bonferroni (BF) or Benjamini–Hochberg procedures. However, these methods tend to be overly conservative, resulting in suboptimal outcomes when conducting many tests. To avoid this issue in sequential hypothesis testing, we employ the non-asymptotic anytime confidence interval derived in Section 4.3, which holds for any time $t$ (Johari et al., 2015; Howard et al., 2021).

**Sample size and stopping time.** We are interested in determining the sample size required to reject the null hypothesis while controlling the Type II error at level $\beta$, assuming the alternative hypothesis $H_1$ is true.

To control the Type II error, we introduce a parameter $\Delta > 0$, commonly referred to as the *effect size* in hypothesis testing literature. We redefine the alternative hypothesis as $H_1(\Delta) : |\theta_0 - \mu| > \Delta$, where $\mathbb{P}_{H_1(\Delta)}$ represents the probability when the alternative hypothesis $H_1(\Delta)$ is correct. Let $R_n$ denote the rejection region for controlling the Type II error at level $\beta$ given $n$ observations. In other words, when $\hat{\theta}_n^{\text{A2IPW}} \in R_n$ and the alternative hypothesis $H_1$ is true, the null hypothesis is rejected with a probability of at least $1 - \beta$. For $\Delta$ and $\beta$, the minimum sample size required to control the Type II error at $\beta$ is defined as:

$$n_\beta^*(\Delta) = \min \left\{ n : \mathbb{P}_{H_1(\Delta)}\left(\hat{\theta}_n^{\text{A2IPW}} \in R_n \right) \geq 1 - \beta \right\}.$$ 

In single-stage testing, we can compute the sample size $n_\beta^*$ by using the asymptotic distribution of $\hat{\theta}_T^{\text{A2IPW}}$. See Section 5.3.1. Note that to compute $n_\beta^*(\Delta)$, we need to know the conditional variance $\sigma^2(a, x)$ to calculate $V$ in Theorem 1. In practice, conjectured values or upper bounds of the conditional variance or $V$ can be used. It is important to note that as the conditional variance or $V$ increases, the required sample size also increases.

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6By contrast, the probability of a Type II error does not increase in sequential testing (Balsubramani and Ramdas, 2016), though there are methods to control the Type II error more precisely (Jamieson and Jain, 2018).
In sequential testing, the sample size corresponds to the stopping time when the algorithm stops after rejecting the null hypothesis. Letting $\tau$ denote the stopping time, we evaluate the expected value of $\tau$, which is also referred to as the sample complexity. In Theorem 4, we show that the sequential test is essentially as powerful as a batch test with a sample size of $T$.

5.2 Implementation

Let $\alpha \in (0, 1)$ be the target Type-I error, and the experimenter aims to perform hypothesis testing without a Type-I error exceeding $\alpha$.

**Single-stage testing.** When our interest lies in single-stage testing (at the end of the experiment), we utilize the asymptotic normality of $\hat{\theta}_T^{A^\text{IPW}}$ in Theorem 1:

$$\sqrt{T} (\hat{\theta}_T^{A^\text{IPW}} - \theta_0) \xrightarrow{d} \mathcal{N}(0, V).$$

In this case, we apply the (asymptotic) Student’s $t$-test using the $t$-statistic $\frac{\hat{\theta}_T^{A^\text{IPW}} - \mu}{\hat{V}^{1/2}/T}$, where $\hat{V}$ is a consistent estimator of $V$.

If the null hypothesis (i.e., $\theta_0 = 0$) is true, the $t$-statistic asymptotically follows the standard normal distribution. Based on these results, the test rejects the null hypothesis when

$$T | \hat{\theta}_T^{A^\text{IPW}} - \mu | > \sqrt{T} \hat{V} z_{1-\alpha/2} := p_T,$$

where $z_\alpha$ is the $\alpha$ quantile of the standard normal distribution. When the sample size $T$ is large, the Type I error is controlled as

$$\mathbb{P}_{H_0} \left( T | \hat{\theta}_T^{A^\text{IPW}} - \mu | > p_T \right) \leq \alpha.$$

**Sequential testing.** In sequential testing, we construct a confidence interval using a LIL-based concentration inequality, as shown in Theorem 3. Based on this result, we define the confidence sequences $\{q_t\}_{t \in \mathbb{T}}$ as

$$q_t := 1.1 \left( \log \left( \frac{1}{\alpha} \right) + \sqrt{2 \sum_{i=1}^t z_i^2 \left( \log \frac{\log \sum_{i=1}^t z_i^2}{\alpha} \right)} \right),$$

where $z_t := z_t(\mu) := \Psi_t - \mu$.

5.3 Sample Size Computation

In this subsection, we compute the sample size needed to control the Type I error at $\alpha$ while achieving power $\beta$. In single-stage testing, we calculate the required minimum sample size $T$. In sequential testing, we compute the expected stopping time $\mathbb{E}[\tau]$, where $\tau$ is the stopping time when the null hypothesis is rejected.
5.3.1 Minimum Sample Size under the Optimal Experiment

First, we derive the required minimum sample size for single-stage testing. Theorem 1 shows that
\[ \sqrt{T} \left( \hat{\theta}_T - \theta_0 \right) \overset{d}{\rightarrow} N(0, V). \]
When the null hypothesis is true (\( \theta_0 = \mu \)),
\[ \frac{\sqrt{T} \left( \hat{\theta}_T^{A2IPW} - \mu \right)}{\sqrt{V}} \overset{d}{\rightarrow} H_0 N(0, 1). \]
Based on these results, with sufficient samples and knowledge of \( \sigma^2_0 \), we reject the null hypothesis when
\[ \sqrt{T} \left( \hat{\theta}_T^{A2IPW} - \mu \right) > \sqrt{V z_{1-\alpha/2}}, \]
where \( z_{1-\alpha/2} \) is the \( 1 - \alpha/2 \) quantile of the standard normal distribution. As explained in Section 5.1, the Type I error is controlled at \( \alpha \).

We now compute the smallest sample size \( n^{\text{OPT}*}_\beta(\Delta) \) required to achieve power \( \beta \). The asymptotic power is given as
\[ \mathbb{P}_{H_1} \left( \sqrt{T} \left( \hat{\theta}_T^{A2IPW} - \mu \right) \right) > \sqrt{V z_{1-\alpha/2}}. \]
For \( T \geq \frac{\sigma^2_0 (z_{1-\alpha/2} - z_\beta)^2}{\Delta^2} \), the asymptotic power becomes at least \( \beta \). Therefore, to achieve power \( \beta \), the required sample size is:
\[ n^{\text{OPT}*}_\beta(\Delta) = \frac{\mathbb{E} \left[ \sigma^2_0(\mu, X_1) + \sigma^2_0(0, X_1) + (f_0(1, X_t) - f_0(0, X_t) - \theta_0)^2 \right]}{\Delta^2} \left( z_{1-\alpha/2} - z_\beta \right)^2. \]

5.3.2 Expected Sample Size in Sequential Testing

In this section, we calculate the upper bound of the expected stopping time \( \tau \). In sequential testing using an LIL-based concentration inequality, we propose an algorithm that rejects the null hypothesis when
\[ \left| \hat{\theta}_t^{A2IPW} - t\mu \right| > 1.1 \left( \log \left( \frac{1}{\alpha} \right) + \sqrt{2 \sum_{i=1}^{t} z_{i}^2 \left( \log \frac{\log \sum_{i=1}^{t} z_{i}^2}{\alpha} \right)} \right) = q_t. \]
Let \( \tau \) be the stopping time of the sequential test, i.e., \( \tau = \min \left\{ t : \left| \hat{\theta}_t^{A2IPW} - t\mu \right| > q_t \right\} \).
When \( t = \tau \), the null hypothesis is rejected.

We show that as time progresses, the probability that the sequential test does not reject the hypothesis becomes small. We bound \( \mathbb{P}_{H_1}(\tau > \tilde{t}) \) for sufficiently large \( \tilde{t} \) such that
\[ \tilde{t} \Delta \gg 1.1 \left( \log \left( \frac{1}{\alpha} \right) + \sqrt{2C^2 \tilde{t} \left( \log \frac{\log C^2\tilde{t}}{\alpha} \right)} \right). \]
First, we consider the probability of \( \tau \geq \tilde{t} \) for a stopping time \( \tau \). The proof is shown in Appendix F.1.
Lemma 1. When the alternative hypothesis is true, $\tau > \tilde{t}$ occurs with probability

$$\mathbb{P}_{H_1}(\tau > \tilde{t}) = O \left( \exp \left( -\frac{\tilde{t} \Delta^2}{8C^2} \right) \right).$$

With this lemma, we prove the following theorem. The proof is in Appendix F.2.

Theorem 4 (Expected sample size in sequential testing). When the alternative hypothesis is true, if

$$n_{\beta}^{\text{OPT}*}(\Delta) \gg 1.1 \left( \log \left( \frac{1}{\alpha} \right) + \sqrt{2C^2 n_{\beta}^{\text{OPT}*}(\Delta) \left( \log \frac{\log C^2 n_{\beta}^{\text{OPT}*}(\Delta)}{\alpha} \right)} \right),$$

then the expected sample size in sequential testing satisfies

$$\mathbb{E}_{H_1}[\tau] = \left( 1 + \frac{8C^2}{V(z_{1-\alpha/2} - z_\beta)^2 \mathbb{P}_{H_1}(\tau > n_{\beta}^{\text{OPT}*}(\Delta))} \right) n_{\beta}^{\text{OPT}*}(\Delta).$$

This result implies that given $\alpha$ and $\beta$, $\mathbb{E}_{H_1}[\tau]$ is approximately equal to $n_{\beta}^{\text{OPT}*}(\Delta)$, multiplied by a constant term independent of $\Delta$. As $\Delta$ approaches zero, both $\mathbb{E}_{H_1}[\tau]$ and $n_{\beta}^{\text{OPT}*}(\Delta)$ approach infinity. From this result, we find that the expected stopping time $\mathbb{E}_{H_1}[\tau]$ in sequential testing grows proportionally to the sample size $n_{\beta}^{\text{OPT}*}(\Delta)$ in single-stage testing ($\mathbb{E}_{H_1}[\tau] = (1 + O(1))n_{\beta}^{\text{OPT}*}(\Delta)$ as $\Delta \to 0$). Hence, for sufficiently small $\Delta$, we can consider that $\mathbb{E}_{H_1}[\tau]$ becomes close to $n_{\beta}^{\text{OPT}*}(\Delta)$.

This result suggests that sequential testing has the potential to stop an experiment earlier than single-stage testing since the expected sample size is nearly identical to the (non-random) oracle sample size of single-stage testing, even though we do not know $n_{\beta}^{\text{OPT}*}(\Delta)$ in advance of the experiment. That is, our sequential testing only uses the (unknown) minimum sample size in expectation.

Here, we emphasize that the oracle sample size $n_{\beta}^{\text{OPT}*}(\Delta)$ is unknown because computing it requires the efficiency bound, which depends on the true expected conditional outcomes and the conditional variances. In single-stage testing, we cannot change the sample size during an experiment, as doing so is considered a violation of standard experimental design principles. Sequential testing, on the other hand, allows us to conduct a nearly optimal adaptive experiment without knowing $n_{\beta}^{\text{OPT}*}(\Delta)$. Thus, sequential testing effectively reduces the sample size.

Note that the condition

$$n_{\beta}^{\text{OPT}*}(\Delta) \Delta \gg 1.1 \left( \log \left( \frac{1}{\alpha} \right) + \sqrt{2C^2 n_{\beta}^{\text{OPT}*}(\Delta) \left( \log \frac{\log C^2 n_{\beta}^{\text{OPT}*}(\Delta)}{\alpha} \right)} \right)$$

holds when $\beta$ is sufficiently close to 0. This theorem leads to the following corollary.

Corollary 2. Suppose that

$$n_{\beta}^{\text{OPT}*}(\Delta) \Delta \gg 1.1 \left( \log \left( \frac{1}{\alpha} \right) + \sqrt{2C^2 n_{\beta}^{\text{OPT}*}(\Delta) \left( \log \frac{\log C^2 n_{\beta}^{\text{OPT}*}(\Delta)}{\alpha} \right)} \right)$$
and \( \pi_t = \pi^* \). Under \( H_1 \), for a sufficiently large sample size, the expected stopping time for the sequential test using \( q_t \) is proportional to \( n_{\beta}^{OPT*}(\Delta) \).

### 5.3.3 Minimum Sample Size and Early Stopping

For a user-defined treatment assignment probability \( \pi_t \), if \( \pi_t(a \mid x) \xrightarrow{p} \pi^*(a \mid x) \) holds for all \( a, x \), the asymptotic variance is the same as \( \tilde{\sigma}_x^2 \) from Theorem 1. Therefore, when \( \pi_t(a \mid x) \xrightarrow{p} \pi^*(a \mid x) \) holds for all \( a, x \), the minimum sample size required for hypothesis testing is also \( n_{\beta}^{OPT*}(\Delta) \). By applying the same method as in the previous section, we can verify that the expected stopping time for sequential testing under a user-defined treatment assignment probability \( \pi_t \) using \( q_t \) is proportional to \( n_{\beta}^{OPT*}(\Delta) \).

### 5.4 Summary

We introduced two approaches for hypothesis testing: single-stage testing and sequential testing. Single-stage testing employs a fixed, non-random sample size determined prior to the experiment, while sequential testing continues the experiment until a predefined stopping criterion is satisfied. Single-stage testing is justified by the asymptotic normality of the A2IPW estimator, which allows us to compute both the statistical power and the required sample size. Sequential testing, in contrast, is designed for finite-sample analysis and allows early stopping.

In contrast to single-stage testing with a fixed sample size, sequential testing has the potential to reduce sample size by terminating the experiment early. For example, if the null hypothesis assumes zero ATE but the actual ATE is significantly large, sequential testing may be able to reject the null and finish the experiment in an early round. On the other hand, in cases where the null hypothesis is not easily rejected, sequential testing may require larger sample sizes. Even in such cases, if the true ATE is sufficiently small and the sample size required for single-stage testing is large, the expected sample size for sequential testing is approximately equal to the fixed sample size used in single-stage testing.

### 6 Simulation Studies

In this section, we evaluate the effectiveness of the proposed algorithm through experimental comparisons. The proposed method using the A2IPW estimator is compared against several alternative approaches, including the MA2IPW estimator, the IPW estimator, a randomized controlled trial (RCT) with a fixed treatment assignment probability of \( \pi_t(1 \mid X_t, \mathcal{H}_{t-1}) = \pi_t(0 \mid X_t, \mathcal{H}_{t-1}) = 0.5 \) for all \( t \), an oracle estimator \( \theta_T^{OPT} \) that operates under the optimal treatment-assignment probability, and a direct method (DM) estimator defined as \( \frac{1}{T} \sum_{t=1}^{T} \left( \hat{f}_t(1, X_t) - \hat{f}_t(0, X_t) \right) \).

To estimate the treatment-assignment probability and expected outcomes, we consider two cases using different nonparametric estimators: the Nadaraya–Watson (NW) estimator and the \( K \)-nearest neighbor (K-nn) estimator. For the MA2IPW estimator, we set the parameter as \( \zeta = t^{-1/1.5} \).
Table 1: Experimental results using Dataset 1.

|            | $T = 150$ | $T = 300$ | ST | MSE  | STD  | Testing | MSE  | STD  | Testing | LIL  | BF  |
|------------|-----------|-----------|----|------|------|---------|------|------|---------|------|-----|
| RCT        | 0.145     | 0.178     | 25.0% | 0.073 | 0.100 | 46.0%   | 455.4 | 370.4 |
| A2IPW (K-nn) | 0.085     | 0.116     | 38.4% | 0.038 | 0.054 | 67.9%   | 389.5 | 302.8 |
| A2IPW (NW)   | 0.064     | 0.092     | 51.4% | 0.025 | 0.035 | 88.1%   | 303.8 | 239.8 |
| MA2IPW (K-nn) | 0.092     | 0.126     | 38.5% | 0.044 | 0.058 | 66.2%   | 387.5 | 303.4 |
| MA2IPW (NW)  | 0.062     | 0.085     | 52.7% | 0.023 | 0.033 | 90.2%   | 303.3 | 236.6 |
| IPW (K-nn)   | 0.151     | 0.208     | 26.1% | 0.075 | 0.103 | 43.6%   | 446.3 | 367.0 |
| IPW (NW)     | 0.161     | 0.232     | 23.4% | 0.081 | 0.115 | 41.1%   | 446.6 | 375.0 |
| DM (K-nn)    | 0.175     | 0.252     | 88.7% | 0.086 | 0.126 | 96.1%   | 59.9  | 164.6 |
| DM (NW)      | 0.111     | 0.167     | 82.1% | 0.045 | 0.066 | 95.6%   | 119.6 | 176.2 |
| OPT         | 0.008     | 0.011     | 100.0%| 0.004 | 0.005 | 100.0%  | 63.9  | 150.0 |

Table 2: Experimental results using Dataset 2.

|            | $T = 150$ | $T = 300$ | ST | MSE  | STD  | Testing | MSE  | STD  | Testing | LIL  | BF  |
|------------|-----------|-----------|----|------|------|---------|------|------|---------|------|-----|
| RCT        | 0.084     | 0.129     | 4.7% | 0.044 | 0.062 | 4.9%    | 497.2 | 481.8 |
| A2IPW (K-nn) | 0.050     | 0.071     | 5.6% | 0.026 | 0.037 | 5.6%    | 497.2 | 477.3 |
| A2IPW (NW)  | 0.029     | 0.045     | 4.4% | 0.012 | 0.018 | 4.7%    | 496.2 | 480.6 |
| MA2IPW (K-nn) | 0.052     | 0.073     | 5.4% | 0.025 | 0.034 | 4.7%    | 497.9 | 477.0 |
| MA2IPW (NW) | 0.032     | 0.047     | 6.3% | 0.012 | 0.018 | 4.4%    | 496.6 | 475.3 |
| IPW (K-nn)  | 0.088     | 0.126     | 5.6% | 0.043 | 0.062 | 5.2%    | 495.8 | 478.1 |
| IPW (NW)    | 0.094     | 0.140     | 5.8% | 0.045 | 0.064 | 5.3%    | 495.6 | 471.6 |
| DM (K-nn)   | 0.096     | 0.129     | 85.3%| 0.046 | 0.063 | 89.5%   | 97.3  | 188.3 |
| DM (NW)     | 0.054     | 0.075     | 53.7%| 0.023 | 0.032 | 55.4%   | 312.8 | 305.3 |
| OPT         | 0.005     | 0.007     | 4.4% | 0.002 | 0.003 | 4.4%    | 498.4 | 483.0 |

In Appendix G, we show simulation studies in which we compare our method using the A2IPW and the ADR estimator with the stratification tree method proposed in Tabord-Meehan (2022).

6.1 Setting

We conduct simulation studies using synthetic and semi-synthetic datasets. In each dataset, we perform the following three types of hypothesis testing:

- Single-stage testing using a $T$-test.
- Sequential testing with Bonferroni (BF) correction.
Table 3: Experimental results using Datasets 3.

| Method       | $T = 150$ MSE | $T = 150$ STD | Testing MSE | Testing STD | $T = 300$ MSE | $T = 300$ STD | LIL | BF  |
|--------------|---------------|---------------|-------------|-------------|---------------|---------------|-----|-----|
| RCT          | 0.139         | 0.191         | 24.2%       | 0.069       | 0.102         | 44.8%         | 450.1| 371.7|
| A2IPW (K-nn) | 0.089         | 0.127         | 39.0%       | 0.042       | 0.064         | 69.8%         | 385.8| 296.6|
| A2IPW (NW)   | 0.061         | 0.089         | 53.8%       | 0.024       | 0.033         | 90.3%         | 290.5| 230.4|
| MA2IPW (K-nn)| 0.087         | 0.121         | 42.6%       | 0.040       | 0.054         | 70.2%         | 378.1| 291.4|
| MA2IPW (NW)  | 0.060         | 0.083         | 53.1%       | 0.025       | 0.035         | 90.8%         | 292.6| 233.6|
| IPW (K-nn)   | 0.158         | 0.214         | 26.3%       | 0.076       | 0.110         | 46.0%         | 443.2| 365.6|
| IPW (NW)     | 0.147         | 0.202         | 25.1%       | 0.080       | 0.112         | 46.1%         | 440.0| 367.6|
| DM (K-nn)    | 0.167         | 0.237         | 90.3%       | 0.084       | 0.120         | 96.0%         | 57.3 | 162.6|
| DM (NW)      | 0.109         | 0.156         | 83.2%       | 0.044       | 0.065         | 96.8%         | 116.8| 173.0|
| OPT          | 0.007         | 0.010         | 100.0%      | 0.003       | 0.005         | 100.0%        | 55.8 | 150.0|

Table 4: Experimental results using Datasets 4.

| Method       | $T = 150$ MSE | $T = 150$ STD | Testing MSE | Testing STD | $T = 300$ MSE | $T = 300$ STD | LIL | BF  |
|--------------|---------------|---------------|-------------|-------------|---------------|---------------|-----|-----|
| RCT          | 0.081         | 0.117         | 4.5%        | 0.041       | 0.056         | 3.5%          | 496.3| 484.0|
| A2IPW (K-nn) | 0.053         | 0.073         | 6.2%        | 0.024       | 0.035         | 5.1%          | 496.8| 474.1|
| A2IPW (NW)   | 0.031         | 0.044         | 5.2%        | 0.012       | 0.017         | 6.1%          | 495.6| 477.0|
| MA2IPW (K-nn)| 0.048         | 0.065         | 5.1%        | 0.024       | 0.035         | 4.9%          | 495.8| 477.5|
| MA2IPW (NW)  | 0.029         | 0.042         | 4.3%        | 0.011       | 0.015         | 4.4%          | 498.1| 477.6|
| IPW (K-nn)   | 0.091         | 0.120         | 4.7%        | 0.048       | 0.067         | 6.1%          | 496.0| 475.2|
| IPW (NW)     | 0.098         | 0.132         | 5.1%        | 0.049       | 0.066         | 5.9%          | 497.2| 474.6|
| DM (K-nn)    | 0.101         | 0.155         | 84.1%       | 0.049       | 0.075         | 87.2%         | 102.9| 190.4|
| DM (NW)      | 0.057         | 0.086         | 53.6%       | 0.023       | 0.034         | 57.6%         | 299.9| 306.1|
| OPT          | 0.004         | 0.005         | 4.5%        | 0.002       | 0.003         | 4.5%          | 497.4| 482.3|
Table 5: Experimental results using IHDP dataset with surface A.

| Method               | $T = 150$ | $T = 300$ | ST         |
|----------------------|-----------|-----------|------------|
|                      | MSE   | STD  | Testing  | MSE   | STD  | Testing  | LIL | BF  |
| RCT                  | 0.674 | 1.066 | 60.4%    | 0.333 | 0.562 | 93.4%    | 355.4 | 228.0 |
| A2IPW (K-nn)         | 0.606 | 0.891 | 99.6%    | 0.310 | 0.500 | 100.0%   | 86.3 | 150.5 |
| A2IPW (NW)           | 0.485 | 0.740 | 99.8%    | 0.202 | 0.311 | 100.0%   | 76.2 | 150.2 |
| DM (K-nn)            | 1.138 | 1.745 | 99.9%    | 0.578 | 0.892 | 100.0%   | 15.1 | 150.1 |
| DM (NW)              | 0.999 | 1.427 | 100.0%   | 0.454 | 0.623 | 100.0%   | 26.4 | 150.0 |

Table 6: Experimental results using IHDP dataset with surface B.

| Method               | $T = 150$ | $T = 300$ | ST         |
|----------------------|-----------|-----------|------------|
|                      | MSE   | STD  | Testing  | MSE   | STD  | Testing  | LIL | BF  |
| RCT                  | 4.522 | 19.635 | 53.9%    | 2.492 | 9.903 | 72.7%    | 355.3 | 274.4 |
| A2IPW (K-nn)         | 5.153 | 33.698 | 84.5%    | 2.683 | 13.545 | 90.6%    | 147.7 | 186.2 |
| A2IPW (NW)           | 4.379 | 23.713 | 84.3%    | 2.198 | 11.874 | 91.0%    | 142.9 | 185.0 |
| DM (K-nn)            | 7.065 | 23.954 | 98.1%    | 3.892 | 14.737 | 98.8%    | 18.7 | 152.1 |
| DM (NW)              | 7.410 | 30.313 | 94.1%    | 3.821 | 16.227 | 96.5%    | 53.0 | 162.6 |

- Sequential testing based on an adaptive confidence sequence derived from the LIL-based concentration inequality.

For all settings, the null and alternative hypotheses are given by

$$H_0 : \theta_0 = 0, \quad H_1 : \theta_0 \neq 0.$$  

For the standard hypothesis testing, we construct confidence intervals using $T$-statistics derived from the asymptotic distribution in Theorem 1. The sequential testing with BF correction is conducted at $t = 150, 250, 350, 450$. For the LIL-based sequential testing, confidence intervals are constructed using $q_t$ as shown in Theorem 3.

### 6.2 Simulation Studies with Synthetic Dataset

We first conduct experiments using synthetic datasets to evaluate the proposed method. At each round $t$, a covariate vector $X_t \in \mathbb{R}^5$ is generated as

$$X_t = (X_{t1}, X_{t2}, X_{t3}, X_{t4}, X_{t5})^\top, \quad X_{tk} \sim \mathcal{N}(0, 1) \text{ for } k = 1, 2, 3, 4, 5.$$  

The potential outcome model is given by

$$Y_t(d) = \mu_d + \sum_{k=1}^{5} X_{tk} + \epsilon_{td},$$  

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where \( \mu_d \) is a constant and \( e_{td} \) follows a normal distribution with standard deviation \( \sigma_d \). The expectation of the potential outcome is \( \mathbb{E}[Y_t(d)] = \mu_d \).

We generate four datasets, each containing 500 units, under different settings for \( \mu_d \) and \( \sigma_d \):

- **Dataset 1**: \( \mu_1 = 0.8, \mu_0 = 0.3, \sigma_1 = 0.8, \sigma_0 = 0.3 \).
- **Dataset 2**: \( \mu_1 = 0.5, \mu_0 = 0.5, \sigma_1 = 0.8, \sigma_0 = 0.3 \).
- **Dataset 3**: \( \mu_1 = 0.8, \mu_0 = 0.3, \sigma_1 = 0.6, \sigma_0 = 0.4 \).
- **Dataset 4**: \( \mu_1 = 0.5, \mu_0 = 0.5, \sigma_1 = 0.6, \sigma_0 = 0.4 \).

For each setting, we conduct 1000 independent trials. The results are summarized in Tables 1, 3, and 4. We report the mean squared error (MSE) between \( \theta \) and \( \hat{\theta} \), the standard deviation of the MSE (STD), and the rejection rates of hypothesis testing based on \( T \)-statistics at the 150th (mid) and 300th (final) rounds. Additionally, we present the stopping times for the LIL-based algorithm and the multiple testing with BF correction. If the null hypothesis is not rejected in sequential testing, the stopping time is set to 500.

Across various datasets, the proposed algorithm achieved lower MSE compared to other methods. The DM estimator tends to reject the null hypothesis with small samples in Dataset 1 but exhibited high Type II error in Dataset 2.

### 6.3 Simulation Studies with Semi-Synthetic Data

We also evaluated the proposed algorithm using semi-synthetic datasets constructed from the Infant Health and Development Program (IHDP). The IHDP dataset consists of simulated outcomes and covariates based on a real study, following the simulation setting proposed by Hill (2011). The dataset contains 747 units with 6 continuous and 19 binary covariates, with outcomes generated artificially.

Hill (2011) considers two response surfaces:

- **Response Surface A**:
  
  \[
  Y_t(0) \sim \mathcal{N}(X_t^\top \beta_A, 1),
  \]
  \[
  Y_t(1) \sim \mathcal{N}(X_t^\top \beta_A + 4, 1),
  \]

  where elements of \( \beta_A \in \mathbb{R}^{25} \) are randomly sampled from \( \{0, 1, 2, 3, 4\} \) with probabilities \( (0.5, 0.2, 0.15, 0.1, 0.05) \).

- **Response Surface B**:

  \[
  Y_t(0) \sim \mathcal{N}(\exp((X_t + W)^\top \beta_B), 1),
  \]
  \[
  Y_t(1) \sim \mathcal{N}(X_t^\top \beta_B - q, 1),
  \]

  where \( W \) is an offset matrix with all elements equal to 0.5, \( q \) is a constant ensuring an average treatment effect of 4, and elements of \( \beta_B \) are randomly sampled from \( \{0, 0.1, 0.2, 0.3, 0.4\} \) with probabilities \( (0.6, 0.1, 0.1, 0.1, 0.1) \).
For experiments, we randomly select 500 units from the dataset. The results, summarized in Tables 5 and 6, include MSE, the standard deviation of MSE (STD), rejection rates at the 150th and 300th periods, and stopping times for the LIL-based and BF correction-based sequential testing. If the hypothesis is not rejected in sequential testing, the stopping time is set to 500.

6.4 Results

The experimental results in Tables 1–4 (synthetic data) and Tables 5–6 (semi-synthetic IHDP data) reveal several notable patterns. In all datasets, the proposed adaptive algorithm using the A2IPW estimator, particularly with the Nadaraya–Watson kernel, consistently yields lower mean squared error than the baseline RCT and DM estimators. This performance gap becomes more pronounced at larger sample sizes, indicating that adaptively refining treatment-assignment probabilities based on accumulated data improves estimation accuracy.

Another observation concerns the DM estimator, which sometimes rejects the null hypothesis more readily when the true effect is clearly different from zero (as in Dataset 1). However, in scenarios where the true effect is close to zero (Dataset 2), it can fail to reject the null and thus exhibit higher Type II error. This pattern underscores that DM methods are sensitive to both sample size and the true effect magnitude and may be less robust when the treatment effect is marginal.

Standard RCT designs with constant assignment probabilities maintain unbiasedness but often show higher mean squared error relative to A2IPW. The adaptive nature of A2IPW allows it to focus allocations more efficiently, leading to more precise estimates of the treatment effect. The oracle (optimal) estimator, which knows the true assignment probabilities in advance, outperforms all other methods in terms of mean squared error and is included only to demonstrate the theoretical upper bound of performance.

The sequential testing procedures exhibit distinct behaviors. The LIL-based approach is typically conservative in practice and requires larger sample sizes before rejecting the null hypothesis, while the Bonferroni-based correction often stops earlier but can inflate Type I error. For instance, Tables 1 and 4 show cases where the Bonferroni-based method rejects the null more frequently, even when the underlying effect is subtle. Standard hypothesis testing (using a fixed sample size and T-statistics) avoids the complexity of sequential testing but does not allow the possibility of early termination.

Overall, the results suggest that the A2IPW-based adaptive design achieves lower estimation error and maintains favorable operating characteristics in both standard and sequential testing frameworks. Whether to use a sequential testing procedure depends on factors such as how rapidly decisions must be reached, the acceptable risk of false positives, and whether the total sample size can be determined in advance.

7 Conclusion

In this study, we designed an adaptive experimental framework to efficiently estimate the ATE and conduct hypothesis testing. We began by reviewing the semiparametric efficiency bound, which characterizes the fundamental limits of estimation efficiency as a function of
the treatment-assignment probability. We then defined the efficient treatment-assignment probability as the minimizer of the semiparametric efficiency bound and leveraged this result to develop an optimal adaptive experimental design.

Our proposed method consists of two key phases: the treatment-assignment phase and the ATE-estimation phase. In the treatment-assignment phase, treatments are adaptively assigned based on an estimate of the efficient treatment-assignment probability. In the ATE estimation phase, we estimate the ATE using the proposed A2IPW estimator, which is constructed from the data collected in the treatment-assignment phase. We demonstrated that this estimator achieves asymptotic optimality by proving that its asymptotic variance matches the semiparametric efficiency bound. This optimality also ensures smaller sample sizes in hypothesis testing, improving the efficiency of experimental design.

In addition to establishing asymptotic optimality, we derived both asymptotic and non-asymptotic confidence intervals for the A2IPW estimator. The non-asymptotic bounds provide finite-sample guarantees, which are particularly useful in practical applications where sample sizes are limited. These confidence intervals enable rigorous inference while maintaining a tight dependence on the underlying data distribution.

Furthermore, we developed a hypothesis-testing framework tailored to our adaptive experimental design. We introduced two approaches: single-stage testing, which relies on a fixed sample size and asymptotic normality, and sequential testing, which dynamically determines sample size based on intermediate test results. We analyzed the theoretical properties of both approaches and highlighted scenarios where sequential testing can substantially reduce the required sample size while maintaining statistical rigor.

Our study contributes to the broader literature on adaptive experimental design by providing a theoretically grounded and practically implementable methodology for efficient ATE estimation and inference. Future research directions include extending our framework to accommodate more complex settings, such as network interference (Viviano, 2022), clustered experimental designs (Viviano et al., 2025), and heterogeneous treatment effects (Kato et al., 2024b). Further exploration of optimality guarantees in finite-sample regimes and their connections to best-arm identification remains an important avenue for research (Kasy and Sautmann, 2021; Kock et al., 2023). Additionally, incorporating reinforcement learning techniques into the treatment-assignment phase may enhance adaptability and extend the applicability of our approach to more dynamic experimental settings (Kallus and Uehara, 2020; Adusumilli et al., 2024; Sakaguchi, 2024).

In summary, this study provides a comprehensive methodological framework for designing and analyzing adaptive experiments, ensuring both statistical efficiency and practical applicability in treatment-effect estimation and hypothesis testing.

References

Adusumilli, K. (2022), “Neyman allocation is minimax optimal for best arm identification with two arms,” arXiv:2204.05527.

— (2023), “Risk and optimal policies in bandit experiments,” arXiv:2112.06363.
Adusumilli, K., Geiecke, F., and Schilter, C. (2024), “Dynamically Optimal Treatment Allocation,” arXiv:1904.01047.

Ao, R., Chen, H., and Simchi-Levi, D. (2024), “Prediction-Guided Active Experiments,” arXiv: 2411.12036.

Armstrong, T. B. (2022), “Asymptotic Efficiency Bounds for a Class of Experimental Designs,” arXiv:2205.02726.

Athey, S. and Imbens, G. (2016), “Recursive partitioning for heterogeneous causal effects,” Proceedings of the National Academy of Sciences, 113, 7353–7360.

Azuma, K. (1967), “Weighted sums of certain dependent random variables,” Tohoku Math. J. (2), 19, 357–367.

Bai, Y., Liu, J., Shaikh, A. M., and Tabord-Meehan, M. (2025), “On the Efficiency of Finely Stratified Experiments,” arXiv:2307.15181.

Balsubramani, A. (2014), “Sharp Finite-Time Iterated-Logarithm Martingale Concentration,” arXiv preprint arXiv:1405.2639.

Balsubramani, A. and Ramdas, A. (2016), “Sequential Nonparametric Testing with the Law of the Iterated Logarithm,” in UAI, AUAI Press, p. 42–51.

Bang, H. and Robins, J. M. (2005), “Doubly Robust Estimation in Missing Data and Causal Inference Models,” Biometrics, 61, 962–973.

Bubeck, S., Munos, R., and Stoltz, G. (2009), “Pure Exploration in Multi-armed Bandits Problems,” in Algorithmic Learning Theory, Springer Berlin Heidelberg, pp. 23–37.

Bugni, F. A., Canay, I. A., and Shaikh, A. M. (2018), “Inference Under Covariate-Adaptive Randomization,” Journal of the American Statistical Association, 113, 1784–1796.

— (2019), “Inference under covariate-adaptive randomization with multiple treatments,” Quantitative Economics, 10, 1747–1785.

Cai, Y. and Rafi, A. (2024), “On the performance of the Neyman Allocation with small pilots,” Journal of Econometrics, 242.

Caria, A. S., Gordon, G., Kasy, M., Quinn, S., Shami, S. O., and Teytelboym, A. (2023), “An Adaptive Targeted Field Experiment: Job Search Assistance for Refugees in Jordan,” Journal of the European Economic Association, 22.

Chandak, Y., Shankar, S., Syrgkanis, V., and Brunskill, E. (2024), “Adaptive Instrument Design for Indirect Experiments,” in International Conference on Learning Representations (ICLR).

Chen, C.-H., Lin, J., Yücesan, E., and Chick, S. E. (2000), “Simulation Budget Allocation for Further Enhancing The Efficiency of Ordinal Optimization,” Discrete Event Dynamic Systems, 10, 251–270.
Chernozhukov, V., Chetverikov, D., Demirer, M., Duflo, E., Hansen, C., Newey, W., and Robins, J. (2018), “Double/debiased machine learning for treatment and structural parameters,” *Econometrics Journal*, 21, C1–C68.

Cook, T., Mishler, A., and Ramdas, A. (2024), “Semiparametric Efficient Inference in Adaptive Experiments,” in *Proceedings of the Third Conference on Causal Learning and Reasoning*, pp. 1033–1064.

Darling, D. A. and Robbins, H. (1967), “Confidence sequences for mean, variance, and median,” *Proceedings of the National Academy of Sciences of the United States of America*, 58, 66–68.

Deep, V., Bassamboo, A., and Juneja, S. K. (2024), “Asymptotically Optimal and Computationally Efficient Average Treatment Effect Estimation in A/B testing,” in *International Conference on Machine Learning (ICML)*, PMLR, vol. 235 of *Proceedings of Machine Learning Research*, pp. 10317–10367.

Durrett, R. (2010), *Probability: Theory and Examples*, USA: Cambridge University Press, 4th ed.

Farrell, M. H., Liang, T., and Misra, S. (2021), “Deep Neural Networks for Estimation and Inference,” *Econometrica*, 89, 181–213.

Farrell, R. H. (1964), “Asymptotic Behavior of Expected Sample Size in Certain One Sided Tests,” *The Annals of Mathematical Statistics*, 35, 36 – 72.

FDA (2019), “Adaptive Designs for Clinical Trials of Drugs and Biologics: Guidance for Industry,” Tech. rep., U.S. Department of Health and Human Services Food and Drug Administration (FDA), Center for Drug Evaluation and Research (CDER), Center for Biologics Evaluation and Research (CBER).

Fisher, E. (1992), “On the Law of the Iterated Logarithm for Martingales,” *The Annals of Probability*, 20, 675–680.

Glynn, P. and Juneja, S. (2004), “A large deviations perspective on ordinal optimization,” in *Proceedings of the 2004 Winter Simulation Conference*, IEEE, vol. 1.

Gupta, S., Lipton, Z. C., and Childers, D. (2021), “Efficient Online Estimation of Causal Effects by Deciding What to Observe,” in *Advances in Neural Information Processing Systems*.

Hadad, V., Hirshberg, D. A., Zhan, R., Wager, S., and Athey, S. (2021), “Confidence intervals for policy evaluation in adaptive experiments,” *Proceedings of the National Academy of Sciences (PNAS)*, 118.

Hahn, J. (1998), “On the Role of the Propensity Score in Efficient Semiparametric Estimation of Average Treatment Effects,” *Econometrica*, 66, 315–331.
Hahn, J., Hirano, K., and Karlan, D. (2011), “Adaptive experimental design using the propensity score,” *Journal of Business and Economic Statistics*, 29, 96–108.

Hall, P. and Hayde, C. (1980), *Martingale Limit Theory and Its Application*, Probability and mathematical statistics, Academic Press.

Hall, P., Heyde, C., Birnbaum, Z., and Lukacs, E. (2014), *Martingale Limit Theory and Its Application*, Communication and Behavior, Elsevier Science.

Hamilton, J. (1994), *Time series analysis* Princeton, NJ: Princeton Univ. Press.

Henni, M. and Eguchi, S. (2004), “A paradox concerning nuisance parameters and projected estimating functions,” *Biometrika*.

Hill, J. L. (2011), “Bayesian Nonparametric Modeling for Causal Inference,” *Journal of Computational and Graphical Statistics*, 20, 217–240.

Hirano, K., Imbens, G., and Ridder, G. (2003), “Efficient estimation of average treatment effects using the estimated propensity score,” *Econometrica*, 71, 1161–1189.

Hirano, K. and Porter, J. R. (2023), “Asymptotic Representations for Sequential Decisions, Adaptive Experiments, and Batched Bandits,” arXiv:2302.03117.

Hoeffding, W. (1963), “Probability inequalities for sums of bounded random variables,” *Journal of the American statistical association*, 58, 13–30.

Howard, S. R., Ramdas, A., McAuliffe, J. D., and Sekhon, J. S. (2021), “Time-uniform, nonparametric, nonasymptotic confidence sequences,” *Annals of Statistics*.

Imbens, G. W. and Rubin, D. B. (2015), *Causal Inference for Statistics, Social, and Biomedical Sciences: An Introduction*, Cambridge University Press.

Jamieson, K., Malloy, M., Nowak, R., and Bubeck, S. (2014), “lil’ UCB : An Optimal Exploration Algorithm for Multi-Armed Bandits,” in *COLT*, vol. 35.

Jamieson, K. G. and Jain, L. (2018), “A Bandit Approach to Sequential Experimental Design with False Discovery Control,” in *NeurIPS*, Curran Associates, Inc., pp. 3664–3674.

Johari, R., Pekelis, L., and Walsh, D. J. (2015), “Always Valid Inference: Bringing Sequential Analysis to A/B Testing,” arXiv preprint arXiv:1512.04922.

Kallus, N., Saito, Y., and Uehara, M. (2021), “Optimal Off-Policy Evaluation from Multiple Logging Policies,” in *International Conference on Machine Learning (ICML)*, PMLR, vol. 139 of *Proceedings of Machine Learning Research*, pp. 5247–5256.

Kallus, N. and Uehara, M. (2020), “Double reinforcement learning for efficient off-policy evaluation in Markov decision processes,” *Journal of Machine Learning Research*, 21.

Kasy, M. and Sautmann, A. (2021), “Adaptive Treatment Assignment in Experiments for Policy Choice,” *Econometrica*, 89, 113–132.
Kato, M. (2021), “Adaptive Doubly Robust Estimator from Non-stationary Logging Policy under a Convergence of Average Probability,” arXiv:2102.08975.

— (2025), “Generalized Neyman Allocation for Locally Minimax Optimal Best-Arm Identification,” arXiv:2405.19317.

Kato, M. and Ariu, K. (2021), “The Role of Contextual Information in Best Arm Identification,” arXiv:2106.14077v1.

Kato, M., Ishihara, T., Honda, J., and Narita, Y. (2020), “Efficient Adaptive Experimental Design for Average Treatment Effect Estimation,” arXiv:2002.05308.

Kato, M., McAlinn, K., and Yasui, S. (2021), “The Adaptive Doubly Robust Estimator and a Paradox Concerning Logging Policy,” in Advances in Neural Information Processing Systems.

Kato, M., Oga, A., Komatsubara, W., and Inokuchi, R. (2024a), “Active Adaptive Experimental Design for Treatment Effect Estimation with Covariate Choices,” in International Conference on Machine Learning (ICML).

Kato, M., Okumura, K., Ishihara, T., and Kitagawa, T. (2024b), “Adaptive Experimental Design for Policy Learning,” arXiv:2401.03756.

Kaufmann, E., Cappé, O., and Garivier, A. (2016), “On the Complexity of Best-Arm Identification in Multi-Armed Bandit Models,” Journal of Machine Learning Research, 17, 1–42.

Khintchine, A. (1924), “Über einen Satz der Wahrscheinlichkeitsrechnung,” Fundamenta Mathematicae, 6, 9–20.

Klaassen, C. A. J. (1987), “Consistent Estimation of the Influence Function of Locally Asymptotically Linear Estimators,” Ann. Statist.

Kock, A. B., Preinerstorfer, D., and Veliyev, B. (2023), “Treatment recommendation with distributional targets,” Journal of Econometrics, 234, 624–646.

Kolmogoroff, A. (1929), “Über das Gesetz des iterierten Logarithmus,” Mathematische Annalen, 101, 126–135.

Li, H. H. and Owen, A. B. (2024), “Double machine learning and design in batch adaptive experiments,” Journal of Causal Inference, 12, 20230068.

Li, J., Shi, K., and Simchi-Levi, D. (2024), “Privacy Preserving Adaptive Experiment Design,”

Loeve, M. (1977), Probability Theory, Graduate Texts in Mathematics, Springer.

Manski, C. (2000), “Identification problems and decisions under ambiguity: Empirical analysis of treatment response and normative analysis of treatment choice,” Journal of Econometrics, 95, 415–442.
Neyman, J. (1934), “On the Two Different Aspects of the Representative Method: the Method of Stratified Sampling and the Method of Purposive Selection,” *Journal of the Royal Statistical Society*, 97, 123–150.

Qian, W. and Yang, Y. (2016), “Kernel Estimation and Model Combination in A Bandit Problem with Covariates,” *Journal of Machine Learning Research*, 17, 1–37.

Rafi, A. (2023), “Efficient Semiparametric Estimation of Average Treatment Effects Under Covariate Adaptive Randomization,” arXiv:2305.08340.

Russac, Y., Katsimerou, C., Bohle, D., Cappé, O., Garivier, A., and Koolen, W. M. (2021), “A/B/n Testing with Control in the Presence of Subpopulations,” in *NeurIPS*.

Sakaguchi, S. (2024), “Policy Learning for Optimal Dynamic Treatment Regimes with Observational Data,” arXiv: 2404.00221.

Schmidt-Hieber, J. (2020), “Nonparametric regression using deep neural networks with ReLU activation function,” *The Annals of Statistics*, 48.

Simchi-Levi, D. and Wang, C. (2023), “Multi-armed Bandit Experimental Design: Online Decision-making and Adaptive Inference,” in *International Conference on Artificial Intelligence and Statistics (AISTATS)*, PMLR, Proceedings of Machine Learning Research.

Simchi-Levi, D., Wang, C., and Xu, J. (2024), “On Experimentation With Heterogeneous Subgroups: An Asymptotic Optimal δ-Weighted-PAC Design,” SSRN:4721755.

Simchi-Levi, D., Wang, C., and Zheng, Z. (2023), “Non-stationary Experimental Design under Linear Trends,” in *Advances in Neural Information Processing Systems (NeurIPS)*, pp. 32102–32116.

Stout, W. F. (1970), “A martingale analogue of Kolmogorov’s law of the iterated logarithm,” *Zeitschrift für Wahrscheinlichkeitstheorie und Verwandte Gebiete*, 15, 279–290.

Tabord-Meehan, M. (2022), “Stratification Trees for Adaptive Randomisation in Randomised Controlled Trials,” *The Review of Economic Studies*, 90, 2646–2673.

van der Laan, M. J. (2008), “The Construction and Analysis of Adaptive Group Sequential Designs.”

Viviano, D. (2022), “Experimental Design under Network Interference,” arXiv:arXiv.

Viviano, D., Lei, L., Imbens, G., Karrer, B., Schrijvers, O., and Shi, L. (2025), “Causal clustering: design of cluster experiments under network interference,” arXiv:2310.14983.

Wager, S. and Athey, S. (2018), “Estimation and Inference of Heterogeneous Treatment Effects using Random Forests,” *Journal of the American Statistical Association*, 113, 1228–1242.

Waudby-Smith, I., Wu, L., Ramdas, A., Karampatziakis, N., and Mineiro, P. (2024a), “Anytime-valid off-policy inference for contextual bandits,” *ACM / IMS J. Data Sci.*
— (2024b), “Anytime-valid off-policy Inference for Contextual Bandits,” *ACM / IMS Journal of Data Science*, 1.

Yang, Y. and Zhu, D. (2002), “Randomized Allocation with nonparametric estimation for a multi-armed bandit problem with covariates,” *Ann. Statist.*, 30, 100–121.

Zhao, J. (2023), “Adaptive Neyman Allocation,” arXiv:2309.08808.

Zheng, W. and van der Laan, M. J. (2011), “Cross-Validated Targeted Minimum-Loss-Based Estimation,” in *Targeted Learning: Causal Inference for Observational and Experimental Data*, Springer, New York, NY.

Zrnic, T. and Candes, E. (2024), “Active Statistical Inference,” in *International Conference on Machine Learning (ICML)*.
Algorithm 2 Adaptive experiment for efficient ATE estimation with hypothesis testing.

**Parameter:** The number of initialization rounds, $T_0$. The lower bound of the variance $\nu$, $\nu > 0$. The stabilization parameter $\gamma_t, \zeta_t \in (0, 1)$, such that $\gamma_t = O(1/\sqrt{t})$ and $\zeta_t = o(1/\sqrt{t})$. Type I error $\alpha$. Set $\rho \geq 0$, which is the number of samples that we assign treatments with equal probability.

**Initialization:**
At $t = 1, 2$, select $A_t = t - 1$. Set $\pi_t(1 \mid X_t, \Omega_{t-1}) = 1/2$.

for $t = 3$ to $T$ do
  if $t < \rho$ then
    Set $\pi_t(1 \mid X_t, \Omega_{t-1}) = 0.5$.
  else
    Construct estimators $\hat{f}_{t-1}$ and $\hat{e}_{t-1}$ using a nonparametric method.
    Construct $\hat{\nu}_{t-1}$ from $\hat{f}_{t-1}$ and $\hat{e}_{t-1}$.
    Using $\hat{\nu}_{t-1}$, construct an estimator of $\pi^*(k \mid X_t)$ and set it as $\pi_t(k \mid X_t, \Omega_{t-1})$.
  end if
  Draw $\xi_t$ from the uniform distribution on $[0, 1]$. $A_t = 1[\xi_t \leq \pi_t(1 \mid X_t, \Omega_{t-1})]$.
  if Sequential testing based on LIL then
    Construct $\hat{\theta}_t^{A2IPW}$.
    Construct $q_t$ based on (4.3) with $\alpha$.
    if $t \hat{\theta}_t^{A2IPW} > q_t$ then
      Reject the null hypothesis.
    end if
  end if
  if Sequential testing based on BF correction then
    Construct $\hat{\theta}_t^{A2IPW}$.
    Construct p-value from $\hat{\theta}_t^{A2IPW}$ under BF correction.
    if If the p-value is less than $\alpha$ then
      Reject the null hypothesis.
    end if
  end if
end for
if Standard hypothesis testing then
  Construct $\hat{\theta}_T^{A2IPW}$.
  Construct p-value from $\hat{\theta}_T^{A2IPW}$.
  if If the p-value is less than $\alpha$ then
    Reject the null hypothesis.
  end if
A Estimation of $\mathbb{E}[Y_t(a) \mid x]$ and $\mathbb{E}[Y_t^2(a) \mid x]$

First, we consider how to estimate $f_0(a, x) = \mathbb{E}[Y_t(a) \mid x]$ and $e_0(a, x) = \mathbb{E}[Y_t^2(a) \mid x]$. When estimating $f_0(a, x)$ and $e_0(a, x)$, we need to construct consistent estimators from dependent samples obtained from an adaptive experiment. In a MAB problem, several non-parametric estimators are proved to be consistent, such as the $K$-nearest neighbor regression estimator and the Nadaraya-Watson kernel regression estimator (Yang and Zhu, 2002; Qian and Yang, 2016). As an example, we show the theoretical properties of the $K$-nearest neighbor regression estimator when using samples with bandit feedback in the following part.

**$K$-nearest neighbor regression:** We introduce nonparametric estimation of $f_0$ based on $K$-nearest neighbor regression using samples with bandit feedback (Yang and Zhu, 2002). For simplicity, we restrict $\mathcal{X}$ as $\mathcal{X} = [0, 1]^d$, which can be relaxed for each application.

First, we fix $x^* \in \mathcal{X}$. Let $k_n > 0$ be a value depending on the sample size $n$. Let $N_{t,k}$ be $\sum_{s=1}^t 1[A_s = k]$. At $t$-th round, we gather $N_{t,k}$ samples from the case of $A_t = k$ and reindex the samples as $\{(X_{t'}, Y_{t'})\}_{t'=1}^{N_{t,k}}$. We construct estimators using the $k_{N_{t,k}}$-NN regression estimator and $\{(X_{t'}, Y_{t'})\}_{t'=1}^{N_{t,k}}$ as

$$
\hat{f}_t(a, x^*) = \frac{1}{k_{N_{t,k}}} \sum_{i=1}^{k_{N_{t,k}}} Y_{\pi(x^*, i)}, \quad \text{and} \quad \hat{e}_t(a, x^*) = \frac{1}{k_{N_{t,k}}} \sum_{i=1}^{k_{N_{t,k}}} Y_{\pi(x^*, i)}^2,
$$

where $\pi$ is the permutation of $\{1, 2, \ldots, N_{t,k}\}$ such that

$$
\|X_{\pi(x^*, 1)} - x^*\| \leq \|X_{\pi(x^*, 2)} - x^*\| \leq \cdots \leq \|X_{\pi(x^*, N_{t,k})} - x^*\|.
$$

For $\hat{f}_{t-1}(a, x)$, Yang and Zhu (2002) showed the following theoretical results. For simplicity, assume $\mathcal{X} = [0, 1]^d$ for an integer $d > 0$. First, they make the following assumption.

**Assumption 2** (Yang and Zhu (2002), Eq. (5)). The function $f_0(a, x)$ be continuous in $x \in \mathcal{X}$ for all $k \in \{1, 0\}$.

Let $\psi(z; f_0(a, \cdot))$ be a modulus of continuity defined by

$$
\psi(z; f_0(a, \cdot)) = \sup \{|f_0(a, x') - f_0(a, x'')| : |x' - x''|_{\infty} \leq z\}.
$$

The term $\psi$ represents the smoothness of the function $\nu_d$.

**Assumption 3** (Yang and Zhu (2002), Assumption 2). The probability $\mu(x)$ is uniformly bounded above and away from 0 on $\mathcal{X} = [0, 1]^d$, i.e., $c \leq \mu(x) \leq \bar{c}$.

Assume $Y_t(a) = f_0(a, X_t) + \epsilon_{t,k}$, where $\epsilon_{t,k}$ is a random variable with mean 0 and finite variance.

**Assumption 4** (Yang and Zhu (2002), Assumption 3). The error term $\epsilon_{t,k}$ also satisfies the moment condition such that there exist positive constants $\nu$ and $w$ satisfying, for all $m \geq 2$,

$$
\mathbb{E}[|\epsilon_{t,k}|^m] \leq \frac{m!}{2} \nu^2 w^{m-2}.
$$
Under these assumptions, we can show the following lemma from the result of Yang and Zhu (2002).

**Lemma 2** (Yang and Zhu (2002), Eq. (4)). For $\kappa > 0$, let $\eta_\kappa = \sup\{z : \psi(z; f_0(a, \cdot)) \leq \kappa\}$. There exists a constant $M > 0$ such that, for $\kappa > 0$, $h < \eta_\kappa / 4$, and $k_{N_{t,k}} \leq c t h^{k}/2$,

\[
\mathbb{P} \left( \left| f_t(a, x^*) - f_0(a, x^*) \right| \geq \kappa \right) \\
\leq M \exp \left( - \frac{3k_{N_{t,k}}}{14} \right) + (t^{d+2} + 1) \left( \exp \left( - \frac{3k_{t}\varepsilon}{28} \right) + \exp \left( - \frac{k_{N_{t,k}} \varepsilon^2 \kappa^2}{16(v^2 + w\varepsilon K/4)} \right) \right).
\]

According to Yang and Zhu (2002), for $k_t$ such that $k_t \varepsilon^2 / \log t \to \infty$ and $k_{N_{t,k}} = o(t)$, we can choose $h \to 0$ that satisfies $h \geq (2k_{N_{t,k}}/(ct))^{1/d}$. From this discussion and the Borel-Cantelli lemma, we can show the following corollary (Yang and Zhu, 2002).

**Corollary 3** (Yang and Zhu (2002)). For $k_t$ such that $k_t \varepsilon^2 / \log t \to \infty$ and $k_{N_{t,k}} = o(t)$,

\[
\left| \widehat{f}_t(a, x^*) - f_0(a, x^*) \right| \overset{P}{\to} 0.
\]

Besides, when we use $k_{N_{t,k}} = O(\sqrt{t})$ in our algorithm, which satisfies $k_{N_{t,k}} \varepsilon^2 / \log t \to \infty$ and $k_{N_{t,k}} = o(t)$, the following corollary holds.

**Corollary 4.** For $k_t = \sqrt{t}$, there exists a constant $M > 0$ such that, for $t > \left( \frac{2}{\mathcal{O}^{1/4}_n} \right)^2$,

\[
\mathbb{P} \left( \left| \widehat{f}_t(a, x^*) - f_0(a, x^*) \right| \geq \kappa \right) \\
\leq M \exp \left( - \frac{3k_{N_{t,k}}}{14} \right) + (t^{d+2} + 1) \left( \exp \left( - \frac{3k_{t}\varepsilon}{28} \right) + \exp \left( - \frac{k_{N_{t,k}} \varepsilon^2 \kappa^2}{16(v^2 + w\varepsilon K/4)} \right) \right).
\]

Using these results, we can bound $\mathbb{E} \left[ \left| \widehat{f}_t(a, x^*) - f_0(a, x^*) \right| \right]$ by the following lemma.

**Lemma 3.** For $\kappa > 0$, $\eta_\kappa = \sup\{z : \psi(z; v_d) \leq \kappa\}$, $k_t = \sqrt{t}$, and $t > \left( \frac{2}{\mathcal{O}^{1/4}_n} \right)^2$, there exists a constant $M > 0$ such that

\[
\mathbb{E} \left[ \left| \widehat{f}_t(a, x^*) - f_0(a, x^*) \right| \right] \\
\leq \kappa + C_2 \left( M \exp \left( - \frac{3k_{N_{t,k}}}{14} \right) + (t^{d+2} + 1) \left( \exp \left( - \frac{3k_{t}\varepsilon}{28} \right) + \exp \left( - \frac{k_{N_{t,k}} \varepsilon^2 \kappa^2}{16(v^2 + w\varepsilon K/4)} \right) \right) \right).
\]

**Proof.** For $\kappa > 0$, $\eta_\kappa = \sup\{z : \psi(z; v_d) \leq \kappa\}$, and $t > \left( \frac{2}{\mathcal{O}^{1/4}_n} \right)^2$,

\[
\mathbb{E} \left[ \left| \widehat{f}_t(a, x^*) - f_0(a, x^*) \right| \right]
\]
\[ \leq \kappa + C_2 \mathbb{P} \left( \left| \hat{f}_t(a, x^*) - f_0(a, x^*) \right| \geq \kappa \right) \]
\[ \leq \kappa + C_2 \left( M \exp \left( -\frac{3k_{N_{t,k}}}{14} \right) \right. \]
\[ + \left. \left( T^{d+2} + 1 \right) \left( \exp \left( -\frac{3k_{N_{t,k}} \varepsilon}{28} \right) + \exp \left( -\frac{k_{N_{t,k}} \varepsilon^2 \kappa^2}{16(v^2 + w \varepsilon \kappa/4)} \right) \right) \right). \]

The theoretical results of Yang and Zhu (2002) is based on the assumption that the flexibility of the function is restricted and assignment probabilities are \( > 0 \) for all treatments. Therefore, we can easily check that their results can apply to our case.

## B Preliminaries

### B.1 Mathematical Tools

**Definition 1** (Uniformly Integrable, Hamilton (1994), p. 191). A sequence \( \{A_t\} \) is said to be uniformly integrable if for every \( \varepsilon > 0 \) there exists a number \( c > 0 \) such that
\[ \mathbb{E} \left[ |A_t| \cdot I[|A_t| \geq c] \right] < \varepsilon \]
for all \( t \).

**Proposition 4** (Sufficient Conditions for Uniformly Integrable, Hamilton (1994), Proposition 7.7, p. 191). (a) Suppose there exist \( r > 1 \) and \( M < \infty \) such that \( \mathbb{E}[|A_t|^r] < M \) for all \( t \). Then \( \{A_t\} \) is uniformly integrable. (b) Suppose there exist \( r > 1 \) and \( M < \infty \) such that \( \mathbb{E}[|b_t|^r] < M \) for all \( t \). If \( A_t = \sum_{j=-\infty}^{\infty} h_j \delta_{t-j} \) with \( \sum_{j=-\infty}^{\infty} |h_j| < \infty \), then \( \{A_t\} \) is uniformly integrable.

**Proposition 5** (\( L^r \) Convergence Theorem, Loeve (1977)). Let \( 0 < r < \infty \), suppose that \( \mathbb{E}[|a_n|^r] < \infty \) for all \( n \) and that \( a_n \xrightarrow{p} a \) as \( n \to \infty \). The following are equivalent:

(i) \( a_n \to a \) in \( L^r \) as \( n \to \infty \);

(ii) \( \mathbb{E}[|a_n|^r] \to \mathbb{E}[|a|^r] < \infty \) as \( n \to \infty \);

(iii) \( \{|a_n|^r, n \geq 1\} \) is uniformly integrable.

### B.2 Martingale Limit Theorems

**Proposition 6** (Weak Law of Large Numbers for Martingale, Hall et al. (2014)). Let \( \{S_n = \sum_{i=1}^{n} X_i, \mathcal{H}_t, t \geq 1\} \) be a martingale and \( \{b_n\} \) a sequence of positive constants with \( b_n \to \infty \) as \( n \to \infty \). Then, writing \( X_{ni} = X_i \mathbb{1}[|X_i| \leq b_n], 1 \leq i \leq n \), we have that \( b_n^{-1} S_n \xrightarrow{p} 0 \) as \( n \to \infty \) if

(i) \( \sum_{i=1}^{n} P(|X_i| > b_n) \to 0 \);
(ii) \( b_n^{-1} \sum_{i=1}^n \mathbb{E}[X_{ni} | \mathcal{H}_{t-1}] \overset{p}{\to} 0 \), and;

(iii) \( b_n^{-2} \sum_{i=1}^n \left\{ \mathbb{E}[X_{ni}^2] - \mathbb{E}^2[\mathbb{E}[X_{ni} | \mathcal{H}_{t-1}]] \right\} \to 0 \).

The weak law of large numbers for martingale holds when the random variable is bounded by a constant.

**Proposition 7** (Central Limit Theorem for a Martingale Difference Sequence, Hamilton (1994), Proposition 7.9, p. 194). Let \( \{X_i\}_{i=1}^\infty \) be an \( n \)-dimensional vector martingale difference sequence with \( \overline{X}_T = \frac{1}{T} \sum_{t=1}^T X_t \). Suppose that

(a) \( \mathbb{E}[X_i^2] = \sigma_i^2 \), a positive value with \( \frac{1}{T} \sum_{t=1}^T \sigma_i^2 \to \sigma_0^2 \), a positive value;

(b) \( \mathbb{E}[|X_i|^r] < \infty \) for some \( r > 2 \);

(c) \( \frac{1}{T} \sum_{t=1}^T X_i^2 \overset{p}{\to} \sigma_0^2 \).

Then \( \sqrt{T} \overline{X}_T \overset{d}{\to} \mathcal{N}(0, \sigma^2) \).

On the convergence rate of the central limit theorem for a martingale difference sequence, see Hall and Hayde (1980).

### C Proof of Proposition 2

**Proof.** Let \( \mathcal{P} \) be a function class of \( p : \mathcal{X} \to (0, 1) \), and let us define the following function \( b : \mathcal{P} \to \mathbb{R} \):

\[
b(p) = \mathbb{E} \left[ \frac{e(1, X_t)}{b(X_t)} \right] + \mathbb{E} \left[ \frac{e(0, X_t)}{1 - b(X_t)} \right].
\]

Here, we rewrite \( b(p) \) as follows:

\[
b(p) = \mathbb{E} \left[ \mathbb{E} \left[ \frac{e(1, X_t)}{p(X_t)} + \frac{e(0, X_t)}{1 - p(X_t)} \bigg| X_t \right] \right].
\]

We consider minimizing \( b(p) \) by minimizing \( \tilde{b}(q) = \mathbb{E} \left[ \frac{e(1, X_t)}{q} + \frac{e(0, X_t)}{1 - q} \bigg| X_t \right] \) for \( q \in [\varepsilon, 1 - \varepsilon] \).

The first derivative of \( \tilde{b}(q) \) with respect to \( q \) is given as follows:

\[
\tilde{b}'(q) = -\frac{e(1, X_t)}{q^2} + \frac{e(0, X_t)}{(1 - q)^2}.
\]

The second derivative of \( f \) is given as follows:

\[
\tilde{b}''(q) = 2 \frac{e(1, X_t)}{q^3} + 2 \frac{e(0, X_t)}{(1 - q)^3}.
\]
For $\varepsilon < q < 1 - \varepsilon$, because $\tilde{b}'(q) > 0$, the minimizer $q^*$ of $\tilde{b}$ satisfies the following equation:

$$\frac{-e(1, X_t)}{(q^*)^2} + \frac{e(0, X_t)}{(1 - q^*)^2} = 0.$$ 

This equation is equivalent to

$$-(q^*)^2e(0, X_t) + (1 - q^*)^2e(1, X_t) = 0$$

$$\Leftrightarrow q^*\sqrt{e(0, X_t)} = (1 - q^*)\sqrt{e(1, X_t)}$$

$$\Leftrightarrow q^* = \frac{\sqrt{e(1, X_t)}}{\sqrt{e(1, X_t)} + \sqrt{e(0, X_t)}}.$$ 

Therefore,

$$b^{\text{OPT}}(D = 1 | X_t) = \frac{\sqrt{e(1, X_t)}}{\sqrt{e(1, X_t)} + \sqrt{e(0, X_t)}}.$$ 

\[\square\]

## D Proof of Theorem 1

**Proof.** Note that the estimator is given as follows:

$$\hat{\theta}^{\text{A2IPW}}_T = \frac{1}{T} \sum_{t=1}^{T} \left( \frac{\mathbb{1}[A_t = 1](Y_t - \hat{f}_{t-1}(1, X_t))}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} - \frac{\mathbb{1}[A_t = 0](Y_t - \hat{f}_{t-1}(0, X_t))}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} + \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) \right).$$

Let us note that $z_t$ is defined as

$$\frac{\mathbb{1}[A_t = 1](Y_t - \hat{f}_{t-1}(1, X_t))}{\pi_t(1 \mid x, \mathcal{H}_{t-1})} - \frac{\mathbb{1}[A_t = 0](Y_t - \hat{f}_{t-1}(0, X_t))}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} + \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0.$$ 

The sequence $\{z_t\}_{t=1}^{T}$ is a martingale difference sequence, i.e.,

$$\mathbb{E}[z_t | \mathcal{H}_{t-1}] = \mathbb{E} \left[ \frac{\mathbb{1}[A_t = 1](Y_t - \hat{f}_{t-1}(1, X_t))}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} - \frac{\mathbb{1}[A_t = k](Y_t - \hat{f}_{t-1}(0, X_t))}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} + \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 | \mathcal{H}_{t-1} \right]$$

$$= \mathbb{E} \left[ \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 \right]$$

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We can rewrite that the condition (a) holds.

Step 1: Checking Condition (a) and (c) hold.

Because we assumed the boundedness of following three conditions in the statement.

Therefore, to derive the asymptotic distribution, we consider applying the central limit theorem for a martingale difference sequence introduced in Proposition 7. There are the following three conditions in the statement.

(a) $\mathbb{E}[z_t^2] = \nu_t^2 > 0$ with $(1/T) \sum_{t=1}^{T} \nu_t^2 \rightarrow \nu^2 > 0$;

(b) $\mathbb{E}[|z_t|^r] < \infty$ for some $r > 2$;

(c) $(1/T) \sum_{t=1}^{T} z_t^2 \overset{p}{\rightarrow} \nu^2$.

Because we assumed the boundedness of $z_t$ by assuming the boundedness of $Y_t$, $\hat{f}_{t-1}$, and $1/\pi_t$, the condition (b) holds. Therefore, the remaining task is to show the conditions (a) and (c) hold.

Step 1: Checking Condition (a)

We can rewrite $\mathbb{E}[z_t^2]$ as

$$\mathbb{E}[z_t^2] = \mathbb{E} \left[ \left( \frac{\mathbb{1}[A_t = 1](Y_t - \hat{f}_{t-1}(1, X_t))}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} - \frac{\mathbb{1}[A_t = 0](Y_t - \hat{f}_{t-1}(0, X_t))}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} - \hat{f}_{t-1}(1, X_t) + \hat{f}_{t-1}(0, X_t) \right)^2 \right]$$

$$= \mathbb{E} \left[ \left( \frac{\mathbb{1}[A_t = 1](Y_t - \hat{f}_{t-1}(1, X_t))}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} - \frac{\mathbb{1}[A_t = 0](Y_t - \hat{f}_{t-1}(0, X_t))}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} - \hat{f}_{t-1}(1, X_t) + \hat{f}_{t-1}(0, X_t) - \theta_0 \right)^2 \right]$$

$$= \mathbb{E} \left[ \left( \frac{\mathbb{1}[A_t = 1](Y_t - \hat{f}_{t-1}(1, X_t))}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} - \frac{\mathbb{1}[A_t = 0](Y_t - \hat{f}_{t-1}(0, X_t))}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} - \hat{f}_{t-1}(1, X_t) + \hat{f}_{t-1}(0, X_t) - \theta_0 \right)^2 \right]$$

Therefore, we prove that the RHS of the following equation varnishes asymptotically to show that the condition (a) holds.

$$\mathbb{E}[z_t^2] = \mathbb{E} \left[ \frac{1}{n} \sum_{a=0}^{1} \frac{v(a, X_t)}{\tilde{\pi}(a \mid X_t)} + \left( \theta_0(X_t) - \theta_0 \right)^2 \right] + \mathbb{E} \left[ \frac{1}{n} \sum_{a=0}^{1} \frac{v(a, X_t)}{\tilde{\pi}(a \mid X_t)} + \left( \theta_0(X_t) - \theta_0 \right)^2 \right].$$
Because Π[A_t = 1]Π[A_t = 0] = 0, Π[A_t = k]Π[A_t = k] = Π[A_t = k], and Π[A_t = k]Y_t = Y_t(a)
for k ∈ {1, 0}, we have

\[
E \left[ \left( \frac{\Pi[A_t = k](Y_t - \hat{f}_{t-1}(1, X_t))}{\pi_t(a \mid X_t, \mathcal{H}_{t-1})} \right)^2 \right] = E \left[ \frac{(Y_t(a) - \hat{f}_{t-1}(a, X_t))^2}{\pi_t(a \mid X_t, \mathcal{H}_{t-1})} \right],
\]

\[
E \left[ \left( \frac{\Pi[A_t = 1](Y_t - \hat{f}_{t-1}(1, X_t))}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} \right)^2 \right] = \frac{\Pi[A_t = 0](Y_t - \hat{f}_{t-1}(0, X_t))}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} = 0,
\]

\[
E \left[ \frac{\Pi[A_t = 1](Y_t - \hat{f}_{t-1}(1, X_t))}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} - \frac{\Pi[A_t = 0](Y_t - \hat{f}_{t-1}(0, X_t))}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} \right] = 0.
\]
Using these equations, the RHS of (3) can be calculated as

\[
\mathbb{E} \left[ \frac{\mathbb{I}[A_t = 1]}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} (Y_t - \hat{f}_{t-1}(1, X_t)) \mid X_t, \mathcal{H}_{t-1} \right] - \frac{\mathbb{I}[A_t = 0]}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} (Y_t - \hat{f}_{t-1}(0, X_t)) \\
\times (\hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0) \\
= \mathbb{E} \left[ f_0(1, X_t) - f_0(0, X_t) - \hat{f}_{t-1}(1, X_t) + \hat{f}_{t-1}(0, X_t) \right] (\hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0) \\
\]

Therefore, for the first term of the RHS of (3),

\[
\mathbb{E} \left[ \frac{\mathbb{I}[A_t = 1]}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} (Y_t - \hat{f}_{t-1}(1, X_t)) \mid X_t, \mathcal{H}_{t-1} \right] - \frac{\mathbb{I}[A_t = 0]}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} (Y_t - \hat{f}_{t-1}(0, X_t)) \\
+ \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 \\
= \mathbb{E} \left[ \frac{(Y_t(1) - \hat{f}_{t-1}(1, X_t))^2}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} + \frac{(Y_t(0) - \hat{f}_{t-1}(0, X_t))^2}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} + (\hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0)^2 \\
+ 2 \left( f_0(1, X_t) - f_0(0, X_t) - \hat{f}_{t-1}(1, X_t) + \hat{f}_{t-1}(0, X_t) \right) (\hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0) \right].
\]

For the second term of the RHS of (3),

\[
\mathbb{E} \left[ \sum_{a=0}^{1} \frac{v(a, X_t)}{\pi(a \mid X_t)} + \left( \theta_0(X_t) - \theta_0 \right)^2 \right] \\
= \mathbb{E} \left[ \frac{(Y_t(1) - f_0(1, X_t))^2}{\pi(1 \mid X_t)} + \frac{(Y_t(0) - f_0(0, X_t))^2}{\pi(0 \mid X_t)} + (f_0(1, X_t) - f_0(0, X_t) - \theta_0)^2 \right].
\]

Using these equations, the RHS of (3) can be calculated as

\[
\mathbb{E} \left[ \frac{\mathbb{I}[A_t = 1]}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} (Y_t - \hat{f}_{t-1}(1, X_t)) \mid X_t, \mathcal{H}_{t-1} \right] - \frac{\mathbb{I}[A_t = 0]}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} (Y_t - \hat{f}_{t-1}(0, X_t)) \\
+ \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 \\
- \mathbb{E} \left[ \sum_{a=0}^{1} \frac{v(a, X_t)}{\pi(a \mid X_t)} + \left( \theta_0(X_t) - \theta_0 \right)^2 \right] \\
= \mathbb{E} \left[ \frac{(Y_t(1) - \hat{f}_{t-1}(1, X_t))^2}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} + \frac{(Y_t(0) - \hat{f}_{t-1}(0, X_t))^2}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} + (\hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0)^2 \right].
\]
By taking the absolute value, we can bound the RHS as

\[
\mathbb{E} \left[ \frac{(Y_t(1) - \hat{f}_{t-1}(1, X_t))^2}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} + \frac{(Y_t(0) - \hat{f}_{t-1}(0, X_t))^2}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} + \left( \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 \right)^2 \right].
\]

From the triangle inequality, we have

\[
\mathbb{E} \left[ \left\{ \frac{(Y_t(1) - \hat{f}_{t-1}(1, X_t))^2}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} + \frac{(Y_t(0) - \hat{f}_{t-1}(0, X_t))^2}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} + \left( \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 \right)^2 \right\} \right].
\]
Because all elements are assumed to be bounded and \( b_1^2 - b_2^2 = (b_1 + b_2)(b_1 - b_2) \) for variables \( b_1 \) and \( b_2 \), there exist constants \( \tilde{C}_0 \), \( \tilde{C}_1 \), \( \tilde{C}_2 \), and \( \tilde{C}_f \) such that

\[
\sum_{a \in \{1,0\}} \mathbb{E} \left[ \frac{(Y_t(a) - \hat{f}_{t-1}(a, X_t))^2}{\tilde{\pi}_t(a \mid X_t, \mathcal{H}_{t-1})} - \frac{(Y_t(a) - f_0(a, X_t))^2}{\tilde{\pi}(a \mid X_t)} \right] \\
+ \mathbb{E} \left[ \left( \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 \right)^2 - \left( f_0(1, X_t) - f_0(0, X_t) - \theta_0 \right)^2 \right] \\
+ 2 \mathbb{E} \left[ \left( f_0(1, X_t) - f_0(0, X_t) - \hat{f}_{t-1}(1, X_t) + \hat{f}_{t-1}(0, X_t) \right) \times \left( \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 \right) \right] \\
\leq \tilde{C}_0 \sum_{a \in \{1,0\}} \mathbb{E} \left[ \frac{(Y_t(a) - \hat{f}_{t-1}(a, X_t))^2}{\sqrt{\tilde{\pi}_t(a \mid X_t, \mathcal{H}_{t-1})}} - \frac{(Y_t(a) - f_0(a, X_t))^2}{\sqrt{\tilde{\pi}(a \mid X_t)}} \right] \\
+ \mathbb{E} \left[ \left( \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 \right)^2 - \left( f_0(1, X_t) - f_0(0, X_t) - \theta_0 \right)^2 \right] \\
+ 2 \mathbb{E} \left[ \left( f_0(1, X_t) - f_0(0, X_t) - \hat{f}_{t-1}(1, X_t) + \hat{f}_{t-1}(0, X_t) \right) \times \left( \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 \right) \right] \\
\leq \tilde{C}_1 \sum_{a \in \{1,0\}} \mathbb{E} \left[ \sqrt{\tilde{\pi}(a \mid X_t)} (Y_t - \hat{f}_{t-1}(a, X_t)) - \sqrt{\tilde{\pi}_t(a \mid X_t, \mathcal{H}_{t-1})} (Y_t - f_0(a, X_t)) \right] \\
+ \mathbb{E} \left[ \left( \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 \right)^2 - \left( f_0(1, X_t) - f_0(0, X_t) - \theta_0 \right)^2 \right] \\
+ 2 \mathbb{E} \left[ \left( f_0(1, X_t) - f_0(0, X_t) - \hat{f}_{t-1}(1, X_t) + \hat{f}_{t-1}(0, X_t) \right) \times \left( \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 \right) \right] \\
\leq \tilde{C}_1 \sum_{a \in \{1,0\}} \mathbb{E} \left[ \sqrt{\tilde{\pi}(a \mid X_t)} \hat{f}_{t-1}(a, X_t) - \sqrt{\tilde{\pi}_t(a \mid X_t, \mathcal{H}_{t-1})} f_0(a, X_t) \right] \\
+ \tilde{C}_2 \sum_{a \in \{1,0\}} \mathbb{E} \left[ \sqrt{\tilde{\pi}(a \mid X_t)} - \sqrt{\tilde{\pi}_t(a \mid X_t, \mathcal{H}_{t-1})} \right] \\
+ \tilde{C}_3 \sum_{a \in \{1,0\}} \mathbb{E} \left[ \hat{f}_{t-1}(a, X_t) - f_0(a, X_t) \right].
\]

From \( b_1b_2 - b_3b_4 = (b_1 - b_3)b_4 - (b_4 - b_2)b_1 \) for variables \( b_1, b_2, b_3, \) and \( b_4 \), there exist \( \tilde{C}_2 \) and
\( \tilde{C}_5 \) such that

\[
\begin{align*}
\tilde{C}_1 \sum_{a \in \{1, 0\}} \mathbb{E} \left[ \left| \sqrt{\pi_t(a | X_t)} \hat{f}_{t-1}(a, X_t) - \sqrt{\pi_t(a | X_t, \mathcal{H}_{t-1})} f_0(a, X_t) \right| \right] \\
+ \tilde{C}_2 \sum_{a \in \{1, 0\}} \mathbb{E} \left[ \left| \sqrt{\pi_t(a | X_t)} - \sqrt{\pi_t(a | X_t, \mathcal{H}_{t-1})} \right| \right] \\
+ \tilde{C}_3 \sum_{a \in \{1, 0\}} \mathbb{E} \left[ \left| \hat{f}_{t-1}(a, X_t) - f_0(a, X_t) \right| \right] \\
\leq \tilde{C}_4 \sum_{a \in \{1, 0\}} \mathbb{E} \left[ \left| \sqrt{\pi_t(a | X_t)} - \sqrt{\pi_t(a | X_t, \mathcal{H}_{t-1})} \right| \right] \\
+ \tilde{C}_5 \sum_{a \in \{1, 0\}} \mathbb{E} \left[ \left| \hat{f}_{t-1}(a, X_t) - f_0(a, X_t) \right| \right].
\end{align*}
\]

From \( \pi_t(a | x, \mathcal{H}_{t-1}) - \tilde{\pi}(a | x) \xrightarrow{P} 0 \), we have \( \sqrt{\pi_t(a | x, \mathcal{H}_{t-1})} - \sqrt{\tilde{\pi}(a | x)} \xrightarrow{P} 0 \). From the assumption that the point converges in probability, i.e., for all \( x \in \mathcal{X} \) and \( k \in \{1, 0\} \), \( \sqrt{\pi_t(a | x, \mathcal{H}_{t-1})} - \sqrt{\tilde{\pi}(a | x)} \xrightarrow{P} 0 \) and \( \hat{f}_{t-1}(a, x) - f_0(a, x) \xrightarrow{P} 0 \) as \( t \to \infty \), if \( \sqrt{\pi_t(a | x, \mathcal{H}_{t-1})} \), and \( \hat{f}_{t-1}(a, x) \) are uniformly integrable, for fixed \( x \in \mathcal{X} \), we can prove that

\[
\mathbb{E} \left[ \left| \sqrt{\pi_t(a | X_t, \mathcal{H}_{t-1})} - \sqrt{\tilde{\pi}(a | X_t)} \right| \mid X_t = x, \mathcal{H}_{t-1} \right] = \mathbb{E} \left[ \left| \sqrt{\pi_t(a | x, \mathcal{H}_{t-1})} - \sqrt{\tilde{\pi}(a | x)} \right| \right] \to 0,
\]

\[
\mathbb{E} \left[ \left| \hat{f}_{t-1}(a, X_t) - f_0(a, X_t) \right| \mid X_t = x, \mathcal{H}_{t-1} \right] = \mathbb{E} \left[ \left| \hat{f}_{t-1}(a, x) - f_0(a, x) \right| \right] \to 0,
\]

as \( t \to \infty \) using \( L^r \)-convergence theorem (Proposition 5). Here, we used the fact that \( \hat{f}_{t-1}(a, x) \) and \( \sqrt{\pi_t(a | x, \mathcal{H}_{t-1})} \) are independent from \( X_t \). For fixed \( x \in \mathcal{X} \), we can show that \( \sqrt{\pi_t(a | x, \mathcal{H}_{t-1})} \), and \( \hat{f}_{t-1}(a, x) \) are uniformly integrable from the boundedness of \( \sqrt{\pi_t(a | x, \mathcal{H}_{t-1})} \), and \( \hat{f}_{t-1}(a, x) \) (Proposition 4). From the point convergence of \( \mathbb{E} \left[ \left| \sqrt{\pi_t(a | X_t, \mathcal{H}_{t-1})} - \sqrt{\tilde{\pi}(a | X_t)} \right| \mid X_t = x \right] \) and \( \mathbb{E} \left[ \left| \hat{f}_{t-1}(a, X_t) - f_0(a, X_t) \right| \mid X_t = x \right] \), by using the Lebesgue’s dominated convergence theorem, we can show that

\[
\mathbb{E}_{X_t, \mathcal{H}_{t-1}} \left[ \mathbb{E} \left[ \left| \sqrt{\pi_t(a | X_t, \mathcal{H}_{t-1})} - \sqrt{\tilde{\pi}(a | X_t)} \right| \mid X_t, \mathcal{H}_{t-1} \right] \right] \to 0,
\]

\[
\mathbb{E}_{X_t, \mathcal{H}_{t-1}} \left[ \mathbb{E} \left[ \left| \hat{f}_{t-1}(a, X_t) - f_0(a, X_t) \right| \mid X_t, \mathcal{H}_{t-1} \right] \right] \to 0.
\]

As \( t \to \infty \),

\[
\mathbb{E} \left[ z_t^2 \right] - \mathbb{E} \left[ \sum_{a=0}^{1} \frac{v(a, X_t)}{\sqrt{\pi_t(a | X_t)}} + \left( \theta_0(X_t) - \theta_0 \right)^2 \right] \to 0.
\]

Therefore, for any \( \epsilon > 0 \), there exists \( \hat{t} > 0 \) such that

\[
\frac{1}{T} \sum_{t=1}^{T} \left( \mathbb{E} \left[ z_t^2 \right] - \mathbb{E} \left[ \sum_{a=0}^{1} \frac{v(a, X_t)}{\sqrt{\pi_t(a | X_t)}} + \left( \theta_0(X_t) - \theta_0 \right)^2 \right] \right) \leq \hat{t}/T + \epsilon.
\]
Here, $\mathbb{E} \left[ \sum_{a=0}^{1} \frac{v(a,X_t)}{\pi(a|X_t)} + (\theta_0(X_t) - \theta_0)^2 \right] = \mathbb{E} \left[ \sum_{a=0}^{1} \frac{v(a,X)}{\pi(a|X)} + (\theta_0(X) - \theta_0)^2 \right]$ does not depend on periods. Therefore, $(1/T) \sum_{t=1}^{T} \sigma_t^2 - \sigma^2 \leq \hat{\tau}/T + \epsilon \to 0$ as $T \to \infty$, where

$$
\sigma^2 = \mathbb{E} \left[ \sum_{a=0}^{1} \frac{v(a, X)}{\pi(a | X)} + (\theta_0(X) - \theta_0)^2 \right].
$$

**Step 2: Checking Condition (b)**

From the boundedness of each variable in $z_t$, we can easily show that the condition (b) holds.

**Step 3: Checking Condition (c)**

Let $u_t$ be a martingale difference sequence such that

$$
u_t = z_t^2 - \mathbb{E}[z_t^2 | \mathcal{H}_{t-1}]
= \left( \frac{\mathbb{1}[A_t = 1]}{\pi_t(1 | X_t, \mathcal{H}_{t-1})} - \frac{\mathbb{1}[A_t = 0]}{\pi_t(0 | X_t, \mathcal{H}_{t-1})} \right) X_t
+ \widehat{\theta}_{t-1}(1, X_t) - \widehat{\theta}_{t-1}(0, X_t) - \theta_0
\right)^2

- \mathbb{E} \left[ \left( \frac{\mathbb{1}[A_t = 1]}{\pi_t(1 | X_t, \mathcal{H}_{t-1})} - \frac{\mathbb{1}[A_t = 0]}{\pi_t(0 | X_t, \mathcal{H}_{t-1})} \right) X_t
+ \widehat{\theta}_{t-1}(1, X_t) - \widehat{\theta}_{t-1}(0, X_t) - \theta_0 \right)^2 | \mathcal{H}_{t-1}].
$$

From the boundedness of each variable in $z_t$, we can apply weak law of large numbers for a martingale difference sequence (Proposition 6 in Appendix B), and obtain

$$
\frac{1}{T} \sum_{t=1}^{T} u_t = \frac{1}{T} \sum_{t=1}^{T} \left( z_t^2 - \mathbb{E}[z_t^2 | \mathcal{H}_{t-1}] \right) \overset{p}{\to} 0.
$$

Next, we show that

$$
\frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[z_t^2 | \mathcal{H}_{t-1}] - \sigma_0^2 \overset{p}{\to} 0.
$$

From Markov's inequality, for $\varepsilon > 0$, we have

$$
\mathbb{P} \left( \frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[z_t^2 | \mathcal{H}_{t-1}] - \sigma_0^2 \geq \varepsilon \right) \leq \frac{\mathbb{E} \left[ \frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[z_t^2 | \mathcal{H}_{t-1}] - \sigma_0^2 \right]}{\varepsilon}.
$$

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We then consider showing
\[
\frac{1}{T} \sum_{t=1}^{T} \mathbb{E} \left[ \left| \mathbb{E} \left[ z_t^2 | \mathcal{H}_{t-1} \right] - \sigma_0^2 \right| \right] \to 0.
\]
Here, we have
\[
\begin{align*}
\mathbb{E} \left[ \left| \mathbb{E} \left[ z_t^2 | \mathcal{H}_{t-1} \right] - \sigma_0^2 \right| \right] &= \mathbb{E} \left[ \left| \frac{Y_t(1) - \hat{f}_{t-1}(1, X_t)}{\pi_t(1 | X_t, \mathcal{H}_{t-1})} + \frac{Y_t(0) - \hat{f}_{t-1}(0, X_t)}{\pi_t(0 | X_t, \mathcal{H}_{t-1})} \right| \right]
\end{align*}
\]

By using Jensen’s inequality,
\[
\begin{align*}
\mathbb{E} \left[ \left| \mathbb{E} \left[ z_t^2 | \mathcal{H}_{t-1} \right] - \sigma_0^2 \right| \right] &\leq \mathbb{E} \left[ \left| \frac{Y_t(1) - \hat{f}_{t-1}(1, X_t)}{\pi_t(1 | X_t, \mathcal{H}_{t-1})} + \frac{Y_t(0) - \hat{f}_{t-1}(0, X_t)}{\pi_t(0 | X_t, \mathcal{H}_{t-1})} \right| \right]
\end{align*}
\]
Because \( \hat{f}_{t-1} \) and \( \pi_t \) are constructed from \( \mathcal{H}_{t-1} \), we have

\[
\mathbb{E} \left[ \left[ \mathbb{E} \left[ z_t^2 \mid \mathcal{H}_{t-1} \right] - \sigma_0^2 \right] \right] \\
\leq \mathbb{E} \left[ \left[ \mathbb{E} \left[ \frac{(Y_t(1) - \hat{f}_{t-1}(1, X_t))^2}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} + \frac{(Y_t(0) - \hat{f}_{t-1}(0, X_t))^2}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} \right] + \left( \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 \right)^2 \right] + \frac{(Y_t(1) - f_0(1, X_t))^2}{\pi(1 \mid X_t)} + \frac{(Y_t(0) - f_0(0, X_t))^2}{\pi(0 \mid X_t)} \right] \\
- \left( f_0(1, X_t) - f_0(0, X_t) - \theta_0 \right)^2 \mid X_t, \pi_t \right] \\
\leq \tilde{C}_4 \sum_{a \in \{1, 0\}} \mathbb{E} \left[ \left[ \sqrt{\pi(a \mid X_t)} - \sqrt{\pi_t(a \mid X_t, \mathcal{H}_{t-1})} \right] \right] \\
+ \tilde{C}_5 \sum_{a \in \{1, 0\}} \mathbb{E} \left[ \left( \hat{f}_{t-1}(a, X_t) - f_0(a, X_t) \right) \right] .
\]

From the results of Step 1, there exist \( \tilde{C}_4 \) and \( \tilde{C}_5 \) such that

\[
\mathbb{E} \left[ \left[ \mathbb{E} \left[ z_t^2 \mid \mathcal{H}_{t-1} \right] - \sigma_0^2 \right] \right] \\
\leq \mathbb{E} \left[ \left[ \mathbb{E} \left[ \frac{(Y_t(1) - \hat{f}_{t-1}(1, X_t))^2}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} + \frac{(Y_t(0) - \hat{f}_{t-1}(0, X_t))^2}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} \right] + \left( \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 \right)^2 \right] + \frac{(Y_t(1) - f_0(1, X_t))^2}{\pi(1 \mid X_t)} + \frac{(Y_t(0) - f_0(0, X_t))^2}{\pi(0 \mid X_t)} \right] \\
- \left( f_0(1, X_t) - f_0(0, X_t) - \theta_0 \right)^2 \mid X_t, \pi_t \right] \\
\leq \tilde{C}_4 \sum_{a \in \{1, 0\}} \mathbb{E} \left[ \left[ \sqrt{\pi(a \mid X_t)} - \sqrt{\pi_t(a \mid X_t, \mathcal{H}_{t-1})} \right] \right] \\
+ \tilde{C}_5 \sum_{a \in \{1, 0\}} \mathbb{E} \left[ \left( \hat{f}_{t-1}(a, X_t) - f_0(a, X_t) \right) \right] .
\]
edness of \( z_t \), we have \( \mathbb{E} \left[ \left| \mathbb{E}[z_t^2 | \mathcal{H}_{t-1}] - \sigma_0^2 \right| \right] \to 0 \). Therefore,

\[
P \left( \left| \frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[z_t^2 | \mathcal{H}_{t-1}] - \sigma_0^2 \right| \geq \varepsilon \right) \leq \frac{1}{\varepsilon} \sum_{t=1}^{T} \mathbb{E} \left[ \left| \mathbb{E}[z_t^2 | \mathcal{H}_{t-1}] - \sigma_0^2 \right| \right] \to 0.
\]

As a conclusion,

\[
\frac{1}{T} \sum_{t=1}^{T} z_t^2 - \sigma^2 = \frac{1}{T} \sum_{t=1}^{T} \left( z_t^2 - \mathbb{E} [z_t^2 | \mathcal{H}_{t-1}] + \mathbb{E} [z_t^2 | \mathcal{H}_{t-1}] - \sigma_0^2 \right) \overset{p}{\to} 0.
\]

**Conclusion**

From Steps 1–3, we can use central limit theorem for a martingale difference sequence. Hence, we have

\[
\sqrt{T} \left( \hat{\theta}_T^{\text{A2IPW}} - \theta_0 \right) \overset{d}{\to} \mathcal{N}(0, \sigma_0^2),
\]

where \( \sigma^2 = \mathbb{E} \left[ \sum_{a=0}^{1} \nu(a, X_t) + (\theta_0(X_t) - \theta_0)^2 \right] \). \( \square \)

**E Proof of Theorem 2**

**Proof.** We have

\[
(\theta_0 - \hat{\theta}_T^{\text{A2IPW}})^2 = \left( \frac{1}{T} \theta - \frac{1}{T} \Psi_1 + \cdots + \frac{1}{T} \theta - \frac{1}{T} \Psi_T \right)^2 = \frac{1}{T^2} (\theta - \Psi_1 + \cdots + \theta - \Psi_T)^2.
\]

Let \( z_t \) be \( \theta_0 - \Psi_t \). Then,

\[
\mathbb{E}_\Pi \left[ (\theta - \hat{\theta}_T^{\text{A2IPW}})^2 \right] = \frac{1}{T^2} \mathbb{E}_\Pi \left[ \left( \sum_{t=1}^{T} z_t \right)^2 \right] = \frac{1}{T^2} \mathbb{E}_\Pi \left[ \sum_{t=1}^{T} z_t^2 + 2 \sum_{t=1}^{T} \sum_{s=1}^{t-1} z_t z_s \right].
\]

We use the following result:

\[
\mathbb{E} \left[ \sum_{t=1}^{T} \sum_{s=1}^{t-1} z_t z_s \right]
\]

\[
= \sum_{t=1}^{T} \sum_{s=1}^{t-1} \mathbb{E}_{\mathcal{H}_{t-1}} [ \mathbb{E}_\Pi | \mathcal{H}_{t-1} \mid z_t z_s | \mathcal{H}_{t-1}]
\]

\[
= \sum_{t=1}^{T} \sum_{s=1}^{t-1} \mathbb{E}_{\mathcal{H}_{t-1}} [ \mathbb{E}_\Pi | \mathcal{H}_{t-1} \mid z_t | \mathcal{H}_{t-1}] z_s
\]

\[
= \sum_{t=1}^{T} \sum_{s=1}^{t-1} \mathbb{E}_{\mathcal{H}_{t-1}} [0 \times z_s] = 0.
\]
Therefore,
\[
\mathbb{E}_\Pi \left[ (\theta_0 - \hat{\theta}_T^{AIPW})^2 \right] = \frac{1}{T^2} \mathbb{E}_\Pi \left[ \sum_{t=1}^{T} z_t^2 \right] = \frac{1}{T^2} \sum_{t=1}^{T} \mathbb{E}_\Pi [ z_t^2 ].
\]

As we showed in Step 1 of the proof of Theorem 1, we have
\[
\mathbb{E}_\Pi \left[ (\theta_0 - \hat{\theta}_T^{AIPW})^2 \right]
= \frac{1}{T^2} \sum_{t=1}^{T} \mathbb{E}_\Pi \left[ \frac{(Y_t(1) - \hat{f}_{t-1}(1, X_t))^2}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} + \frac{(Y_t(0) - \hat{f}_{t-1}(0, X_t))^2}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} \right.
\]
\[
+ \left. \left( \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 \right)^2 \right]
\]
\[
+ 2 \left( f_0(1, X_t) - f_0(0, X_t) - \hat{f}_{t-1}(1, X_t) + \hat{f}_{t-1}(0, X_t) \right) \left( \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 \right) \right].
\]

On the other hand, we have
\[
\mathbb{E}_{\Pi^{OPT}} \left[ (\theta_0 - \hat{\theta}_T^{OPT})^2 \right]
= \frac{1}{T^2} \sum_{t=1}^{T} \mathbb{E}_{\Pi^{OPT}} \left[ \left( \frac{1[\hat{A}_t = 1]}{\pi^*(1 \mid X_t)} (Y_t - f_0(1, X_t)) - \frac{1[\hat{A}_t = 0]}{\pi^*(0 \mid X_t)} (Y_t - f_0(0, X_t)) \right.
\]
\[
\left. + f_0(1, X_t) - f_0(0, X_t) - \theta_0 \right)^2 \right],
\]

where \( \hat{A}_t \) denotes the stochastic variable of a treatment under a treatment-assignment probability \( \pi^* \). We have
\[
\frac{1}{T^2} \sum_{t=1}^{T} \mathbb{E}_{\Pi^{OPT}} \left[ \left( \frac{1[\hat{A}_t = 1]}{\pi^*(1 \mid X_t)} (Y_t - f_0(1, X_t)) - \frac{1[\hat{A}_t = 0]}{\pi^*(0 \mid X_t)} (Y_t - f_0(0, X_t)) \right.
\]
\[
\left. + f_0(1, X_t) - f_0(0, X_t) - \theta_0 \right)^2 \right]
\]
\[
= \frac{1}{T^2} \sum_{t=1}^{T} \mathbb{E} \left[ \frac{(Y_t(1) - f_0(1, X_t))^2}{\pi^*(1 \mid X_t)} + \frac{(Y_t(0) - f_0(0, X_t))^2}{\pi^*(0 \mid X_t)} + (f_0(1, X_t) - f_0(0, X_t) - \theta_0)^2 \right].
\]

Therefore, we have
\[
\mathbb{E}_\Pi \left[ (\theta_0 - \hat{\theta}_T^{AIPW})^2 \right] - \mathbb{E}_{\Pi^{OPT}} \left[ (\theta_0 - \hat{\theta}_T^{OPT})^2 \right]
= \frac{1}{T^2} \sum_{t=1}^{T} \mathbb{E} \left[ \frac{(Y_t(1) - \hat{f}_{t-1}(1, X_t))^2}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} + \frac{(Y_t(0) - \hat{f}_{t-1}(0, X_t))^2}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} \right].
\]

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\[ \begin{align*}
&\text{Therefore, we have } \\
&\quad+ \left( \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 \right)^2 \\
&\quad+ 2 \left( f_0(1, X_t) - f_0(0, X_t) - \hat{f}_{t-1}(1, X_t) + \hat{f}_{t-1}(0, X_t) \right) \left( \hat{f}_{t-1}(1, X_t) - \hat{f}_{t-1}(0, X_t) - \theta_0 \right) \\
&\quad- \frac{1}{T^2} \sum_{t=1}^{T} \mathbb{E}_{\mathcal{H}} \left[ \frac{(Y_t(1) - f_0(1, X_t))^2}{\pi^*(1 \mid X_t)} + \frac{(Y_t(0) - f_0(0, X_t))^2}{\pi^*(0 \mid X_t)} \right] \\
&\quad+ \frac{1}{T^2} \sum_{t=1}^{T} \mathbb{E} \left[ \left\{ \frac{(Y_t(1) - \hat{f}_{t-1}(1, X_t))^2}{\pi_t(1 \mid X_t, \mathcal{H}_{t-1})} + \frac{(Y_t(0) - \hat{f}_{t-1}(0, X_t))^2}{\pi_t(0 \mid X_t, \mathcal{H}_{t-1})} \right\} \right] \\
&\quad\leq \frac{1}{T^2} \sum_{t=1}^{T} \mathbb{E} \left[ \left( \frac{(Y_t(1) - f_0(1, X_t))^2}{\pi^*(1 \mid X_t)} + \frac{(Y_t(0) - f_0(0, X_t))^2}{\pi^*(0 \mid X_t)} \right) \left( f_0(1, X_t) - f_0(0, X_t) - \theta_0 \right)^2 \right] \\
&\quad\leq \mathbb{E} \left[ \left( \theta_0 - \hat{\theta}_{T}^{\text{A2IPW}} \right)^2 \right] - \mathbb{E} \left[ \left( \theta_0 - \hat{\theta}_{T}^{\text{OPT}} \right)^2 \right] \\
&\quad\leq \overline{C}_0 \sum_{t=1}^{T} \sum_{a \in \{1, 0\}} \mathbb{E} \left[ \left| \sqrt{\pi^*(a \mid X_t)} - \sqrt{\pi_t(a \mid X_t, \mathcal{H}_{t-1})} \right| \right] \\
&\quad\quad+ \overline{C}_1 \sum_{t=1}^{T} \sum_{a \in \{1, 0\}} \mathbb{E} \left[ \left| \hat{f}_{t-1}(a, X_t) - f_0(a, X_t) \right| \right].
\end{align*} \]

where the expectation of the last equation is taken over random variables including \( \mathcal{H}_{t-1} \).

As we proved in Step 1 of proof of Theorem 1, there exist constants \( \bar{C}_0 \) and \( \bar{C}_1 \) such that

\[ \mathbb{E} \left[ \left( \theta_0 - \hat{\theta}_{T}^{\text{A2IPW}} \right)^2 \right] - \mathbb{E} \left[ \left( \theta_0 - \hat{\theta}_{T}^{\text{OPT}} \right)^2 \right] \]

\[ \leq \frac{\bar{C}_0}{T^2} \sum_{t=1}^{T} \sum_{a \in \{1, 0\}} \mathbb{E} \left[ \left| \sqrt{\pi^*(a \mid X_t)} - \sqrt{\pi_t(a \mid X_t, \mathcal{H}_{t-1})} \right| \right] \]

\[ + \frac{\bar{C}_1}{T^2} \sum_{t=1}^{T} \sum_{a \in \{1, 0\}} \mathbb{E} \left[ \left| \hat{f}_{t-1}(a, X_t) - f_0(a, X_t) \right| \right]. \]

Therefore, we have

\[ \mathbb{E} \left[ \left( \theta_0 - \hat{\theta}_{T}^{\text{A2IPW}} \right)^2 \right] - \mathbb{E} \left[ \left( \theta_0 - \hat{\theta}_{T}^{\text{OPT}} \right)^2 \right] \]

\[ = \frac{1}{T^2} \sum_{t=1}^{T} \sum_{a \in \{1, 0\}} \left\{ 0 \left( \mathbb{E} \left[ \left| \sqrt{\pi^*(a \mid X_t)} - \sqrt{\pi_t(a \mid X_t, \mathcal{H}_{t-1})} \right| \right] \right) \\
+ O \left( \mathbb{E} \left[ \left| f_0(a, X_t) - \hat{f}_{t-1}(a, X_t) \right| \right] \right) \right\}. \]

\[ \square \]
E.1 Proof of Theorem 3

The procedure of this proof mainly follows Balsubramani and Ramdas (2016). For a martingale $M_t$, let $V_t = \sum_{i=1}^t \mathbb{E}[(M_t - M_{t-1})^2 | \mathcal{H}_{t-1}]$. Before proving Theorem 3, we prove the following three lemmas.

**Lemma 4** (Small Sample Bound for a Martingale Difference Sequence). Let $M_t$ be a martingale such that for all $t \geq 1$, $|M_t - M_{t-1}| \leq e^2/2$ with probability 1. Fix any $\delta > 0$, and define $\tau_0 = \min \left\{ s : 2(e - 2) V_s \geq 173 \log \left( \frac{4}{\delta} \right) \right\}$. Then, with probability $1 - \delta$, for all $t \leq \tau_0$,

$$|M_t| \leq 2 \sqrt{\frac{173}{2(e - 2)}} \log \left( \frac{4}{\delta} \right).$$

**Lemma 5** (Uniform Bernstein Bound for Martingales at Any Time). Let $M_t$ be a martingale such that for all $t \geq 1$, $|M_t - M_{t-1}| \leq e^2/2$ with probability 1. Then, with probability $1 - \delta$, for all $t$ simultaneously,

$$|M_t| \leq C_0(\delta) + \sqrt{2C_1 V_t \left( \log \log V_t + \log \left( \frac{4}{\delta} \right) \right)},$$

where $C_0(\delta) = 3(e - 2) + 2 \sqrt{\frac{173}{2(e - 2)}} \log \left( \frac{4}{\delta} \right)$ and $C_1 = 6(e - 2)$.

**Remark 1.** For the Napier’s constant $e$, $e^2/2 \approx 3.694$.

**Lemma 6** (Upper Bound of the Variance). Let $M_t$ be a martingale such that for all $t \geq 1$, $|M_t - M_{t-1}| \leq e^2/2$ with probability 1. Suppose that there exists $C_z$ such that $|(M_t - M_{t-1})^2 - \mathbb{E}[(M_t - M_{t-1})^2 | \mathcal{H}_{t-1}]| \leq C_z$. With probability $1 - \delta$, for all $t$, for sufficiently large $V_t$ and $\sum_{i=1}^t (M_i - M_{i-1})^2$, there is an absolute constant $C_f$ such that

$$V_t \leq C_f \left( \sum_{i=1}^t (M_i - M_{i-1})^2 + \frac{2C_z C_0(\delta)}{e^2} \right),$$

where $C_0(\delta) = 3(e - 2) + 2 \sqrt{\frac{173}{2(e - 2)}} \log \left( \frac{4}{\delta} \right)$.

In this section, we use the following three propositions.

**Proposition 8** (Balsubramani (2014), Lemma 23). Suppose that, for all $\ell \geq 3$ and $t$,

$$\mathbb{E}[(M_t - M_{t-1})^\ell | \mathcal{H}_{t-1}] \leq \frac{1}{2} \ell! \left( e/\sqrt{2} \right)^{2 \ell (e - 2)} \mathbb{E}[(M_t - M_{t-1})^2 | \mathcal{H}_{t-1}]^\ell.$$ Then, for any $\lambda \in \left( -\frac{1}{e^2}, \frac{1}{e^2} \right)$, the process $U^\lambda_t := \exp(\lambda M_t - \lambda^2 V_t)$ is a super martingale.

**Remark 2.** The condition that, for all $\ell \geq 3$ and all $t$, $\mathbb{E}[(M_t - M_{t-1})^\ell | \mathcal{H}_{t-1}] \leq \frac{1}{2} \ell! \left( e/\sqrt{2} \right)^{2 \ell (e - 2)} \mathbb{E}[(M_t - M_{t-1})^2 | \mathcal{H}_{t-1}]$ is satisfied when $|M_t - M_{t-1}| \leq e^2/2$ for all $t$ with probability 1.

**Proposition 9** (Uniform Bernstein Bound for Martingales, Balsubramani (2014), Theorem 5). Let $M_t$ be a martingale such that for all $t \geq 1$, $|M_t - M_{t-1}| \leq e^2$ with probability 1. Fix any
\( \delta < 1 \) and define \( \tau_0 = \min \{ s : 2(e-2)V_s \geq 173 \log \left( \frac{1}{\delta} \right) \} \). Then, with probability \( \geq 1 - \delta \), for all \( t \geq \tau_0 \) simultaneously, \( M_t \leq \frac{2(e-2)(e^2/1 + \sqrt{1/3})V_t + \log \left( \frac{2}{\delta} \right)}{e^2(1+\sqrt{1/3})} \).

**Proposition 10.** Suppose \( b_1, b_2, c \) are positive constants,

\[
 r \geq 8 \max \left( e^4b_1 \log \log (e^4r/4), e^4b_2 \right),
\]

and \( r - \sqrt{b_1 e^4 r \log \log (e^4r/4) + b_2 e^4r - c} \leq 0 \). Then,

\[
 \sqrt{r} \leq \sqrt{b_1 e^4 \log \log (e^4c/2) + b_2 e^4 + \sqrt{c}}.
\]

This proposition is almost the same as Lemma 9 of Balsubramani (2014), but we changed the statement a little. We show the proof as follows.

**Proof of Lemma 10.** Since \( r \geq 8e^4b_2 \),

\[
 0 \leq \frac{r}{8} - e^4b_2 = \frac{r}{4} - e^4b_2 = \frac{r}{4} - b_1 \frac{r}{8b_1} - e^4b_2 \rightarrow 0 \leq \frac{r^2}{4} - b_1 \frac{r}{8b_1} - b_2 e^4r.
\]

Substituting the assumption \( \frac{r}{8b_1} \geq e^4 \log \log (e^4r/4) \) gives

\[
 0 \leq \frac{r^2}{4} - b_1 \frac{r}{8b_1} - b_2 e^4r \leq \frac{r^2}{4} - b_1 re^4 \log \log (e^4r/4) - b_2 e^4r
\]

\[
 \rightarrow \sqrt{b_1 re^4 \log \log (e^4r/4) + b_2 e^4r} \leq \frac{r}{2}.
\]

By substituting this into \( r - \sqrt{b_1 e^4 r \log \log (e^4r/4) + b_2 e^4r - c} \leq 0 \), we have \( r \leq 2c \). Therefore, again using \( r - \sqrt{b_1 e^4 r \log \log (e^4r/4) + b_2 e^4r - c} \leq 0 \),

\[
 0 \geq r - \sqrt{b_1 e^4 \log \log (e^4c/2) + b_2 e^4r - c}
\]

\[
 \geq r - \sqrt{b_1 e^4 \log \log (e^4c/2) + b_2 e^4r - c}.
\]

This is a quadratic in \( \sqrt{r} \). By solving it, we have

\[
 \sqrt{r} \leq \frac{1}{2} \left( \sqrt{b_1 e^4 \log \log (e^4c/2) + b_2 e^4} + \sqrt{b_1 e^4 \log \log (e^4c/2) + b_2 e^4 + 4c} \right)
\]

\[
 \leq \sqrt{b_1 e^4 \log \log (e^4c/2) + b_2 e^4} + \sqrt{c}
\]

We prove Lemmas 4–6 and Theorem 3 as follows.
Proof of Lemma 4

Proof. This proof mostly follows the proof of Theorem 24 of Balsubramani (2014). First, by using Proposition 8, we show that \( 2 \geq \mathbb{E} \left[ \exp \left( \lambda_0 |M_t - \lambda_0^2 V_t \right) \right] \) for any stopping time \( \tau \) and \( \lambda \in \left(-\frac{1}{e^2}, \frac{1}{e^2}\right) \). From Proposition 8, \( U_i^\lambda := \exp(\lambda M_t - \lambda^2 V_t) \) is a super martingale. The condition that, for all \( t \geq 3 \), \( \mathbb{E}((M_t - M_{t-1})^\ell | \mathcal{H}_{t-1}) \leq \frac{1}{2} \ell! \left( \frac{e/\sqrt{2}}{2(\ell-2)} \right)^{2(\ell-2)} \mathbb{E}[(M_t - M_{t-1})^2 | \mathcal{H}_{t-1}] \) holds from the assumption that \( |M_t - M_{t-1}| \leq e^2/2 \) for all \( t \) with probability 1. For \( \lambda_0 \in \left(-\frac{1}{e^2}, \frac{1}{e^2}\right) \), let us consider a situation where \( \lambda \in \{-\lambda_0, \lambda_0\} \) with probability 1/2 each. After marginalizing over \( \lambda \), the resulting process is

\[
\bar{U}_t = \frac{1}{2} \exp(\lambda_0 M_t - \lambda_0^2 V_t) + \frac{1}{2} \exp(-\lambda_0 M_t - \lambda_0^2 V_t)
\]

On the other hand, for any stopping time \( \tau \), from the optimal stopping theorem for a super martingale (Durrett, 2010), we have

\[
\mathbb{E} \left[ \exp(\lambda_0 M_\tau - \lambda_0^2 V_\tau) \right] \leq \mathbb{E} \left[ \exp(\lambda_0 M_0 - \lambda_0^2 V_0) \right] = 1.
\]

Similarly,

\[
\mathbb{E} \left[ \exp(-\lambda_0 M_\tau - \lambda_0^2 V_\tau) \right] \leq \mathbb{E} \left[ \exp(-\lambda_0 M_0 - \lambda_0^2 V_0) \right] = 1.
\]

Combining these results, we have

\[
\mathbb{E} \left[ \bar{U}_t \right] = \mathbb{E} \left[ \frac{1}{2} \exp(\lambda_0 M_t - \lambda_0^2 V_t) + \frac{1}{2} \exp(-\lambda_0 M_t - \lambda_0^2 V_t) \right] \leq 1,
\]

and

\[
1 \geq \mathbb{E} \left[ \frac{1}{2} \exp(\lambda_0 M_t - \lambda_0^2 V_t) \right].
\]

Thus, we proved \( 2 \geq \mathbb{E} \left[ \exp(\lambda_0 |M_\tau| - \lambda_0^2 V_\tau) \right] \).

Next, note that \( \tau_0 = \min \left\{ s : V_s \geq \frac{173}{2(e-2)} \log \left( \frac{4}{\delta} \right) \right\} \). Therefore, by defining the stopping time \( \tau_1 = \min \left\{ s : |M_s| \geq 2 \sqrt{\frac{173}{2(e-2)} \log \left( \frac{4}{\delta} \right)} \right\} \) and using \( \lambda_0 = \sqrt{\frac{2(e-2)}{173}} \approx 0.091 \leq \frac{1}{e^2} \approx 0.135 \),

\[
2 \geq \mathbb{E} \left[ \exp(\lambda_0 |M_{\tau_1}| - \lambda_0^2 V_{\tau_1}) \right] \geq \mathbb{E} \left[ \exp(\lambda_0 |M_{\tau_1}| - \lambda_0^2 V_{\tau_1}) | \tau_1 < \tau_0 \right] \mathbb{P} (\tau_1 < \tau_0) \geq \mathbb{E} \left[ \exp \left( 2\lambda_0 \sqrt{\frac{173}{2(e-2)} \log \left( \frac{4}{\delta} \right)} - \lambda_0^2 \frac{173}{2(e-2)} \log \left( \frac{4}{\delta} \right) \right) | \tau_1 < \tau_0 \right] \mathbb{P} (\tau_1 < \tau_0) \geq \mathbb{E} \left[ \exp \left( \log \left( \frac{4}{\delta} \right) \right) \right] \mathbb{P} (\tau_1 < \tau_0) = \frac{4}{\delta} \mathbb{P} (\tau_1 < \tau_0).
\]

Thus, we obtain \( \mathbb{P} (\tau_1 < \tau_0) \leq \frac{\delta}{2} < \delta \).

\[
\text{Proof of Lemma 5}
\]

Proof. From Proposition 9, with probability \( \geq 1 - \delta/2 \), for all \( t \geq \tau_0 \) simultaneously, \( |M_t| \leq \frac{2(e-2)}{\delta} V_t \) and

\[
|M_t| \leq \sqrt{6(e-2)V_t \left( 2 \log \log \left( \frac{3(e-2)V_t}{|M_t|} \right) + \log \left( \frac{4}{\delta} \right) \right)}.
\]
We therefore have that, with probability \( \geq 1 - \delta/2 \), for all \( t \geq \tau_0 \), simultaneously, \( |M_t| \leq V_t \) and
\[
|M_t| \leq \max \left( 3(e - 2), \sqrt{2C_1 V_t \log \log V_t + C_1 V_t \log \left( \frac{4}{\delta} \right)} \right), \quad (4)
\]
where note that \( C_1 = 6(e - 2) \).

Next, from Lemma 4, with probability \( \geq 1 - \delta/4 \), for all \( t \leq \tau_0 \) simultaneously,
\[
|M_t| \leq 2 \sqrt{\frac{173}{2(e - 2)}} \log \left( \frac{4}{\delta} \right)
\]
By taking a union bound of (4), with probability \( \geq 1 - \delta \), the following inequality holds for all \( t \) simultaneously:
\[
|M_t| \leq \begin{cases} 
2 \sqrt{\frac{173}{2(e - 2)}} \log \left( \frac{4}{\delta} \right) & \text{if } t \leq \tau_0 \\
\frac{2(e - 2)}{e^2(1 + \sqrt{1/3})} V_t \text{ and } \max \left( 3(e - 2), \sqrt{2C_1 V_t \log \log V_t + C_1 V_t \log \left( \frac{4}{\delta} \right)} \right) & \text{if } t \geq \tau_0 
\end{cases}
\]
With probability \( \geq 1 - \delta \), the following relationship holds for all \( t \) simultaneously:
\[
|M_t| \leq C_0(\delta) + \sqrt{C_1 V_t \left( 2 \log \log V_t + \log \left( \frac{4}{\delta} \right) \right)}.
\]

\[\square\]

**Proof of Lemma 6**

Proof. Let \( \tilde{M}_t = \sum_{i=1}^{t} (M_i - M_{i-1})^2 - V_t \), where note that
\[
V_t = \sum_{i=1}^{t} \mathbb{E} \left[ (M_i - M_{i-1})^2 | \mathcal{H}_{i-1} \right].
\]
Suppose that there exists \( C_z \) such that \( |(M_t - M_{t-1})^2 - \mathbb{E} [(M_i - M_{i-1})^2 | \mathcal{H}_{i-1}]| \leq C_z \) with probability 1 in which the existence is guaranteed by the boundedness of \( M_i - M_{i-1} \), i.e., \( |M_i - M_{i-1}| \leq e^2/2 \) for all \( t \) with probability 1. Because \( \tilde{M}_t \) is a martingale, we can apply Proposition 5, i.e., for all \( t \), with probability \( \geq 1 - \delta \)
\[
|\tilde{M}_t| \leq \frac{2C_z}{e^2} \left( C_0(\delta) + \sqrt{C_1 B_t \left( 2 \log \log B_t + \log \left( \frac{4}{\delta} \right) \right)} \right),
\]
where \( B_t = \mathbb{E} \left[ (\sum_{i=1}^{t} (M_i - M_{i-1})^2 - V_t)^2 | \mathcal{H}_{i-1} \right]. \) For \( B_t \), we have
\[
B_t = \sum_{i=1}^{t} \left( \mathbb{E} \left[ (M_i - M_{i-1})^4 | \mathcal{H}_{i-1} \right] - \left( \mathbb{E} \left[ (M_i - M_{i-1})^2 | \mathcal{H}_{i-1} \right] \right)^2 \right)
\]

We consider two cases for

This can be relaxed to

Because \( M_i - M_{i-1} \leq e^2/2 \rightarrow \frac{(M_i - M_{i-1})^2}{e^4/2^4} \leq 1 \), we have \( (M_i - M_{i-1})^2/(e^4/2^4) \geq (M_i - M_{i-1})^4/(e^8/2^4) \), and

Therefore,

This can be relaxed to

\[
- \sum_{i=1}^{t} (M_i - M_{i-1})^2 + V_t - \frac{2C_2}{e^2} \left( C_0(\delta) + \sqrt{C_1 e^4 V_t/4 \left( 2 \log (e^4 V_t/4) + \log \left( \frac{4}{\delta} \right) \right)} \right)
= - \sum_{i=1}^{t} (M_i - M_{i-1})^2 + V_t - \left( \frac{2C_2 C_0(\delta)}{e^2} + \sqrt{\frac{C_2^2 C_1}{e^4} e^4 V_t \left( 2 \log (e^4 V_t/4) + \log \left( \frac{4}{\delta} \right) \right)} \right)
\leq 0.
\]

We consider two cases for \( V_t \). First, we consider a case where

\[
V_t \geq 8 \max \left( e^4 \frac{C_2^2 C_1}{e^4} 2 \log \log (e^4 V_t), e^4 \frac{C_2^2 C_1}{e^4} \log \left( \frac{4}{\delta} \right) \right).
\]

From Proposition 10, we have

\[
\sqrt{V_t} \leq \sqrt{\frac{C_2^2 C_1}{e^4} 2 e^4 \log \log \left( e^{2C_2 C_0(\delta)} + e^4 \sum_{i=1}^{t} (M_i - M_{i-1})^2/2 \right) + e^4 \frac{C_2^2 C_1}{e^4} \log \left( \frac{4}{\delta} \right)}
+ \sqrt{\frac{2C_2 C_0(\delta)}{e^2} + \sum_{i=1}^{t} (M_i - M_{i-1})^2}
= \sqrt{2C_4 C_1 \log \log \left( e^{2C_2 C_0(\delta)} + e^4 \sum_{i=1}^{t} (M_i - M_{i-1})^2/2 \right) + C_4^2 C_1 \log \left( \frac{4}{\delta} \right)}
+ \sqrt{\frac{2C_2 C_0(\delta)}{e^2} + \sum_{i=1}^{t} (M_i - M_{i-1})^2}.
\]
For sufficiently large $\sum_{i=1}^{t}(M_i - M_{i-1})^2$ such that

$$2C_1^2 C_1 \log \log \left( e^{2C_1 C_0(\delta)} + e^{4 \sum_{i=1}^{t}(M_i - M_{i-1})^2/2} \right) \geq C_1^2 C_1 \log \left( \frac{4}{\delta} \right),$$

by using a constant $C_5$, the RHS is bounded as

$$\sqrt{2C_1^2 C_1 \log \log \left( e^{2C_1 C_0(\delta)} + e^{4 \sum_{i=1}^{t}(M_i - M_{i-1})^2/2} \right) + C_1^2 C_1 \log \left( \frac{4}{\delta} \right)}$$

$$+ \sqrt{\frac{2C_1 C_0(\delta)}{e^2} + \sum_{i=1}^{t}(M_i - M_{i-1})^2}$$

$$\leq \sqrt{4C_1^4 C_1 \log \left( e^{2C_1 C_0(\delta)} + e^{4 \sum_{i=1}^{t}(M_i - M_{i-1})^2/2} \right) + \frac{2C_1 C_0(\delta)}{e^2} + \sum_{i=1}^{t}(M_i - M_{i-1})^2}$$

$$\leq \sqrt{4C_1^4 C_1 \left( e^{2C_1 C_0(\delta)} + e^{4 \sum_{i=1}^{t}(M_i - M_{i-1})^2/2} \right) + \frac{2C_1 C_0(\delta)}{e^2} + \sum_{i=1}^{t}(M_i - M_{i-1})^2}.$$

By squaring both sides of

$$\sqrt{\tilde{V}_t} \leq \sqrt{4C_1^4 C_1 \left( e^{2C_1 C_0(\delta)} + e^{4 \sum_{i=1}^{t}(M_i - M_{i-1})^2/2} \right) + \frac{2C_1 C_0(\delta)}{e^2} + \sum_{i=1}^{t}(M_i - M_{i-1})^2}$$

$$= \sqrt{2e^4 C_1^4 C_1 \left( \frac{2C_1 C_0(\delta)}{e^2} + \sum_{i=1}^{t}(M_i - M_{i-1})^2 \right) + \frac{2C_1 C_0(\delta)}{e^2} + \sum_{i=1}^{t}(M_i - M_{i-1})^2},$$

we obtain

$$V_t \leq C_f \left( \sum_{i=1}^{t}(M_i - M_{i-1})^2 + \frac{2C_1 C_0(\delta)}{e^2} \right),$$

where $C_f$ is a constant. When $V_t < 8 \max \left( e^{4C_1^2 C_1/\delta 2} \log \log \left( e^{4V_t} \right), e^{4C_1^2 C_1/\delta 2} \log \left( \frac{4}{\delta} \right) \right)$, the statement clearly holds for sufficiently high $V_t$ such that $V_t < e^{4C_1^2 C_1/\delta 2} \log \log \left( e^{4V_t} \right)$.

**Proof of Theorem 3**

Finally, combining the above results, we show Theorem 3 as follows.

**Proof.** Let us note that we can construct a martingale difference sequence from $z_t = q_t - \theta_0$ as $\{z_t\}_{t=1}^{T}$. Let us suppose that there exists a constant $C$ such that $|z_t| \leq C$. Let $\bar{z}_t$ and $\bar{V}_t$ be $z_t e^2/(2C)$ and $\sum_{i=1}^{t} E[\bar{z}_i^2 | \mathcal{H}_{i-1}]$, respectively. From this boundedness of $z_t$, there
exists a constant $C_z$ such that $|z^2 - \mathbb{E}[z^2|H_{t-1}]| \leq C_z$. For fixed $\delta$, from Proposition 5, with probability $\geq 1 - \delta$, the following true for all $t$ simultaneously:

$$
\left| t \hat{\theta}^{A2IPW}_t - t\theta_0 \right| \leq \frac{2C}{e^2} \left( C_0(\delta) + \sqrt{2C_1 \bar{V}_t^* \left( \log \log \bar{V}_t^* + \log \left( \frac{4}{\delta} \right) \right)} \right).
$$

Here, by using Proposition 6, we have

$$
\bar{V}_t \leq C_f \left( \sum_{i=1}^{t} z_i^2 + \frac{2C_zC_0(\delta)}{e^2} \right).
$$

Then, we have

$$
\left| t \hat{\theta}^{A2IPW}_t - t\theta_0 \right|
\leq \frac{2C}{e^2} \left( C_0(\delta) + \sqrt{2C_1C_f \left( \frac{e^4}{4C^2} \sum_{i=1}^{t} z_i^2 + \frac{2C_zC_0(\delta)}{e^2} \right)} \left( \log \log C_f \left( \frac{e^4}{4C^2} \sum_{i=1}^{t} z_i^2 + \frac{2C_zC_0(\delta)}{e^2} \right) + \log \left( \frac{4}{\delta} \right) \right) \right).
$$

F Proofs of Section 5.3.2

F.1 Proof of Lemma 1

We have

$$
P_{H_1}(\tau > \hat{t}) = 1 - P_{H_1}(\tau \leq \hat{t})
= 1 - P_{H_1} \left( \exists \ell \leq \hat{t} : |t \hat{\theta}^{A2IPW}_t - t\mu| > q_t \right)
\leq 1 - P_{H_1} \left( \left| t \hat{\theta}^{A2IPW}_t - \bar{\mu} \right| > q_t \right)
= P_{H_1} \left( \left| t \hat{\theta}^{A2IPW}_t - \bar{\mu} \right| \leq q_t \right)
= P_{H_1} \left( \left| t \hat{\theta}^{A2IPW}_t - \bar{\mu} \right| = q_t \right)
\leq P_{H_1} \left( t \hat{\theta}^{A2IPW}_t - \bar{\mu} - \hat{\Delta} \leq q_t - \hat{\Delta} \right).
$$

By substituting $q_t = 1.1 \left( \log \left( \frac{1}{\alpha} \right) + \sqrt{2 \sum_{i=1}^{\hat{t}} z_i^2 \left( \log \frac{\log \sum_{i=1}^{\hat{t}} z_i^2}{\alpha} \right)} \right)$,

$$
P_{H_1}(\tau > \hat{t})
$$
\[
\begin{align*}
&\leq \mathbb{P}_{H_t}\left(\tilde{t}\theta_t^{\text{A2IPW}} - \tilde{t}\mu - \tilde{t}\Delta \leq 1.1 \left(\log \left(\frac{1}{\alpha}\right) + \sqrt{\log \sum_{i=1}^\tilde{t} \left(\log \frac{\log \sum_{i=1}^\tilde{t} \frac{z_i^2}{\alpha}}{2}\right)}\right) - \tilde{t}\Delta\right) \\
&= \mathbb{P}_{H_t}\left(\frac{\tilde{t}\theta_t^{\text{A2IPW}} - \tilde{t}\mu - \tilde{t}\Delta}{\sqrt{\sigma^2}} \leq \frac{1.1}{\sqrt{\sigma^2}} \left(\log \left(\frac{1}{\alpha}\right) + \sqrt{\log \sum_{i=1}^\tilde{t} \left(\log \frac{\log \sum_{i=1}^\tilde{t} \frac{z_i^2}{\alpha}}{2}\right)}\right) - \tilde{t}\Delta\right) \\
&\leq \mathbb{P}_{H_t}\left(\frac{\tilde{t}\theta_t^{\text{A2IPW}} - \tilde{t}\mu - \tilde{t}\Delta}{\sqrt{\sigma^2}} \leq \frac{1.1}{\sqrt{\sigma^2}} \left(\log \left(\frac{1}{\alpha}\right) + \sqrt{2C^2\tilde{t} \left(\log \frac{\log \sum_{i=1}^\tilde{t} \frac{z_i^2}{\alpha}}{2}\right)}\right) - \tilde{t}\Delta\right).
\end{align*}
\]

Here, we used $|z_t| \leq C$ for all $t$. Let $\leq$ and $\asymp$ be $\leq$ and $=$ when ignoring constants. By using Azuma-Hoeffding inequality for martingales (Hoeffding, 1963; Azuma, 1967), $|z_t - z_{t-1}| \leq 2C$, and $\tilde{t}\Delta \gg 1.1 \left(\log \left(\frac{1}{\alpha}\right) + \sqrt{2C^2\tilde{t} \left(\log \frac{\log \sum_{i=1}^\tilde{t} \frac{z_i^2}{\alpha}}{2}\right)}\right)$,

\[
\begin{align*}
&\mathbb{P}_{H_t}(\tau > \tilde{t}) \\
&\leq \mathbb{P}_{H_t}\left(\frac{\tilde{t}\theta_t^{\text{A2IPW}} - \tilde{t}\mu - \tilde{t}\Delta}{\sqrt{\sigma^2}} \leq \frac{1.1}{\sqrt{\sigma^2}} \left(\log \left(\frac{1}{\alpha}\right) + \sqrt{2C^2\tilde{t} \left(\log \frac{\log \sum_{i=1}^\tilde{t} \frac{z_i^2}{\alpha}}{2}\right)}\right) - \tilde{t}\Delta\right) \\
&\leq \exp\left(-\frac{\left(\tilde{t}\Delta - 1.1 \left(\log \left(\frac{1}{\alpha}\right) + \sqrt{2C^2\tilde{t} \left(\log \frac{\log \sum_{i=1}^\tilde{t} \frac{z_i^2}{\alpha}}{2}\right)}\right)\right)^2}{8tC^2}\right) \\
&\asymp \exp\left(-\frac{\tilde{t}\Delta^2}{8C^2}\right).
\end{align*}
\]

### F.2 Proof of Theorem 4

For $n_\beta^{\text{OPT}}(\Delta) = \frac{\bar{z}_\beta^2}{2\Delta^2}(z_{1-\alpha/2} - z_\beta)^2$, we have

\[
\mathbb{E}_{H_t}[\tau] = \sum_{n \geq 1} \mathbb{P}_{H_t}(\tau > n)
\leq n_\beta^{\text{OPT}}(\Delta) + \sum_{t \geq n_\beta^{\text{OPT}}(\Delta) + 1} \mathbb{P}_{H_t}(\tau > t)
\leq n_\beta^{\text{OPT}}(\Delta) + \sum_{t \geq n_\beta^{\text{OPT}}(\Delta) - 1} \mathbb{P}_{H_t}(\tau > t)
\leq n_\beta^{\text{OPT}}(\Delta) + \sum_{t \geq n_\beta^{\text{OPT}}(\Delta) - 1} \exp\left(-\frac{t\Delta^2}{8C^2}\right)
= n_\beta^{\text{OPT}}(\Delta) + \exp\left(-\frac{n_\beta^{\text{OPT}}(\Delta) - 1}{8C^2}\right) \Delta^2 + \exp\left(-\frac{n_\beta^{\text{OPT}}(\Delta) - 1}{8C^2}\right) \Delta^2 + \cdots
\]

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\[ n^*_{\beta}(\Delta) + \exp \left( -\frac{n^*_{\beta}(\Delta) - 1}{8C^2} \Delta^2 \right) \sum_{s=1}^{\infty} \exp \left( -\frac{(s-1)\Delta^2}{8C^2} \right). \]

By using the infinite geometric series sum formula,

\[ \sum_{s=1}^{\infty} \exp \left( -\frac{(s-1)\Delta^2}{8C^2} \right) = \frac{1}{1 - \exp \left( -\frac{\Delta^2}{8C^2} \right)}. \]

\[ n^*_{\beta}(\Delta) + \exp \left( -\frac{n^*_{\beta}(\Delta) - 1}{8C^2} \Delta^2 \right) \frac{1}{1 - \exp \left( -\frac{\Delta^2}{8C^2} \right)} \]

By substituting \( \exp \left( -\frac{\Delta^2}{8C^2} \right) \preceq \mathbb{P}_{H_1}(\tau > \tilde{t}) \),

\[ \mathbb{E}_{H_1}[\tau] \leq n^*_{\beta}(\Delta) + \frac{\mathbb{P}_{H_1}(\tau > n^*_{\beta}(\Delta))}{1 - \exp \left( -\frac{\Delta^2}{8C^2} \right)}. \]

Using the inequality, \( 1 - \exp(-r) \leq r \), and \( n^*_{\beta}(\Delta) = \frac{\tilde{\sigma}^2}{\Delta^2} (z_{1-\alpha/2} - z_{\beta})^2 \), we have

\[ \mathbb{E}_{H_1}[\tau] \]
\[ \leq n^*_{\beta}(\Delta) + \frac{8C^2}{\Delta^2} \mathbb{P}_{H_1}(\tau > n^*_{\beta}(\Delta)) \]
\[ = n^*_{\beta}(\Delta) + \frac{8C^2}{\tilde{\sigma}^2} (z_{1-\alpha/2} - z_{\beta})^2 \mathbb{P}_{H_1}(\tau > n^*_{\beta}(\Delta)). \]

## G Additional Experimental Results

### G.1 Setting

In this section, we investigate the empirical performance of the proposed A2IPW and MA2IPW estimators, as well as the ADR estimator introduced in our follow-up study (Kato et al., 2021). The simulation setting follows the framework of Tabord-Meehan (2022) and Athey and Imbens (2016). We generate the covariates \( X_t \) from a beta distribution \( \text{Beta}(2, 5) \) on \( X = [0, 1]^d \). The potential outcomes and covariates follow

\[ Y_t(a) = \kappa_a(X_t) + \nu_a(X_t) \epsilon_{a,t}, \]

where \( \epsilon_{a,t} \sim N(0, 0.1) \).

We adopt this functional form to incorporate both observed covariates \( X_t \) and unobserved noise through \( \epsilon_{a,t} \). In practice, the outcome depends on measurable characteristics \( X_t \), captured through \( \kappa_a(\cdot) \) and \( \nu_a(\cdot) \), as well as latent factors that can differ across treatment arms. The coefficient functions \( \kappa_a \) and \( \nu_a \) thus allow for heteroskedasticity and heterogeneous treatment effects shaped by both observables and unobservables.

We consider three settings with different specifications of \( \kappa_a(\cdot) \) and \( \nu_a(\cdot) \):
Model 1 ATE: $\theta_0 = 0.12$.

- Dimension of $X_t$: $d = 2$.
- $\kappa_0(x) = 0.2$, $\kappa_1(x) = 10x_1^2 \mathbb{1}[x_1 > 0.4] - 5x_2^2 \mathbb{1}[x_2 > 0.4]$.
- $\nu_0(x) = 5$, $\nu_1(x) = 1 + 10x_1^2 \mathbb{1}[x_1 > 0.6] + 5x_2^2 \mathbb{1}[x_2 > 0.6]$.

Model 2 ATE: $\theta_0 = 0.079$.

- Dimension of $X_t$: $d = 10$.
- $\kappa_0(x) = 0.5$, $\kappa_1(x) = \sum_{j=1}^{10} (-1)^{j-1} 10^{-j+2} x_j^2 \mathbb{1}[x_j > 0.4]$.
- $\nu_0(x) = 5$, $\nu_1(x) = 1 + \sum_{j=1}^{10} 10^{-j+2} x_j^2 \mathbb{1}[x_j > 0.6]$.

Model 3 ATE: $\theta_0 = 0.12$.

- Dimension of $X_t$: $d = 10$.
- $\kappa_0(x) = 0.2$, $\kappa_1(x) = \sum_{j=1}^{3} (-1)^{j-1} 10 x_j^2 \mathbb{1}[x_j > 0.4] + \sum_{j=4}^{10} (-1)^{j-1} 5 x_j^2 \mathbb{1}[x_j > 0.4]$.
- $\nu_0(x) = 9$, $\nu_1(x) = 1 + \sum_{j=1}^{3} 10 x_j^2 \mathbb{1}[x_j > 0.6] + \sum_{j=4}^{10} 5 x_j^2 \mathbb{1}[x_j > 0.6]$.

In Section G.2, we evaluate the performance of the proposed estimators in both single-stage and sequential testing settings. In Section G.3, we compare our proposed methods with those of Tabord-Meehan (2022).

G.2 Comparison among A2IPW Estimator, ADR Estimator, Single-stage Testing, and Sequential Testing

We compare the performance of the proposed methods with a randomized controlled trial (RCT) where treatments are assigned with probability 0.5. We also compare with an oracle algorithm that knows the true variances of the potential outcomes and uses the optimal estimator $\hat{\theta}^{OPT}_T$.

For all settings, the null and alternative hypotheses are defined as $H_0 : \theta_0 = 0$ and $H_1 : \theta_0 \neq 0$, respectively. We conduct the following tests:

- **Standard hypothesis testing**: Performed with $T$-statistics when the sample sizes are 1000 and 5000.

- **Sequential testing with Bonferroni correction**: Multiple testing is conducted at sample sizes 1000, 2000, 3000, and 5000.

- **Sequential testing with LIL**: Testing is based on the concentration inequality derived in Theorem 3.

We compare different tests in terms of hypothesis testing power, precision, and efficiency under various scenarios.

We evaluate the methods in terms of power, MSE, and coverage for sample sizes up to 5000. Each simulation is repeated 500 times. Tables 7–9 report the mean squared error
(MSE), standard deviation of the squared error (SMSE), rejection rates (R/R), coverage ratios (CR), and stopping times for LIL and BF-based testing (BC and LIL columns).

For Models 1–3, the A2IPW and ADR estimators generally achieve smaller MSE than the RCT baseline at larger sample sizes. In Table 7 (Model 1), A2IPW with kernel-based nuisance estimators attains lower MSE compared to RCT, reflecting the benefit of adaptive treatment assignment, while still controlling type I error when the null is true (Table 10). Similar trends appear in Tables 8 and 11 (Model 2), although the rejection rates differ owing to the smaller true effect size $\theta_0 = 0.079$. For Model 3 (Tables 9 and 12), the presence of stronger heteroskedasticity causes slightly higher MSE across methods, but A2IPW and ADR still often outperform the RCT in precision. The oracle (not shown in every row but referenced for comparison) serves as a theoretical benchmark, consistently achieving the lowest MSE due to its knowledge of the true variances.

The sequential methods terminate earlier than a fixed-sample analysis if the observed data yield strong evidence. The Bonferroni correction can lead to earlier stops but occasionally increases type I error, whereas the LIL-based approach is often more conservative, as seen by larger average stopping times (BC vs. LIL columns in Tables 7–9). When $\theta_0 = 0$ in Tables 10–12, both sequential approaches correctly fail to reject the null in most cases, albeit sometimes not until nearing the maximum sample size.

G.3 Comparison with the Stratification Tree

In this section, we compare our proposed method with the stratification tree approach introduced in Tabord-Meehan (2022). Specifically, we evaluate the proposed A2IPW estimators against the following alternative methods:

Ad-hoc. In this method, experimental units are stratified using an “ad-hoc” approach, and treatments are assigned to half the sample in each stratum.

Ad-hoc + Neyman. This is a two-stage experiment. In the first stage, the variances of the outcomes are estimated, and treatments are then allocated according to Neyman allocation. The ATE is subsequently estimated by averaging the sample mean of each stratum weighted by the probability that covariates fall into the stratum.

Stratification Tree (Tabord-Meehan, 2022). This method uses a two-stage experiment. In the first stage, a stratification tree is estimated. In the second stage, treatments are assigned using the estimated tree. The tree depth is fixed at three.

Cross-Validated Tree. This method is similar to the Stratification Tree but selects the tree depth via 2-fold cross-validation.

For two-stage experiments, we consider three different sample size ratios between the first and second stages, using 100, 500, and 1500 experimental units for the first stage. For detailed descriptions of each method, refer to Tabord-Meehan (2022).

The total sample size $T$ is set at 5000, and we conducted 1000 independent trials. For each case at round 5000, we report the MSE between $\theta$ and $\hat{\theta}$, the standard deviation of the
squared error, the percentages of hypothesis rejections using $T$-statistics, and the coverage ratios. The results are presented in Tables 7–9.

We consider pilot sample sizes of 100, 500, or 1500 in the first stage for these two-stage methods. Full details appear in Tabord-Meehan (2022). The total sample size is $T = 5000$, and the study is repeated 1000 times for each scenario. Tables 7–9 compare the MSE, SMSE, rejection rates, and coverage (CR) across all methods.

The results generally show that the adaptive methods (A2IPW, ADR) achieve competitive or lower MSE compared to the stratification-based approaches. The performance advantage is especially noticeable when the pilot stage is small (for example, 100 units), since the two-stage stratification designs have less information to guide allocations in the second stage. However, when the pilot grows larger (such as 1500), the performance of the two-stage methods can improve and sometimes approach that of the fully adaptive methods. The cross-validated tree often performs better than the fixed-depth tree, illustrating the importance of tuning the tree depth to capture heterogeneous effects. In scenarios with substantial heteroskedasticity (Model 3), the adaptive weighting in A2IPW and ADR generally yields more stable and accurate estimates relative to the stratification-based methods.

Overall, these findings confirm that adaptive procedures, such as A2IPW and ADR, effectively leverage ongoing data to update treatment allocation probabilities, leading to improved estimation and greater testing power under nonzero effects. Stratification approaches, especially with sufficient pilot data, can also offer good performance but may be more sensitive to the initial estimation of variances or tree-based splits. The choice of method should be guided by practical considerations, including available pilot data, computational resources, and how quickly strong evidence of treatment differences is needed.
Table 7: Simulation results of Model 1.

| Method               | Criteria | MSE   | SMSE  | R/R   | CR   | BC    | LIL    |
|----------------------|----------|-------|-------|-------|------|-------|--------|
|                      |          |       |       |       |      |       |        |
| A2IPW                |          |       |       |       |      |       |        |
| KNN                  | 0.050    | 0.032 | 0.638 | 0.972 | 2228.000 | 2529.696 |
| NW                   | 0.056    | 0.037 | 0.520 | 0.952 | 2392.000 | 2798.364 |
| NN                   | 0.056    | 0.040 | 0.516 | 0.958 | 2394.000 | 2899.466 |
| A2IPW (Oracle)       |          |       |       |       |      |       |        |
| KNN                  | 0.049    | 0.033 | 0.658 | 0.972 | 2234.000 | 2549.920 |
| NW                   | 0.051    | 0.031 | 0.602 | 0.958 | 2212.000 | 2596.902 |
| NN                   | 0.055    | 0.039 | 0.534 | 0.954 | 2416.000 | 2856.816 |
| RCT                  |          |       |       |       |      |       |        |
| Pilot                |          |       |       |       |      |       |        |
| 100                  | 0.053    | 0.037 | 0.610 | 0.964 |       |       |
| 500                  | 0.053    | 0.037 | 0.592 | 0.964 |       |       |
| 1500                 | 0.056    | 0.038 | 0.554 | 0.946 |       |       |
| Ad-hoc Neyman        |          |       |       |       |      |       |        |
| 100                  | 0.054    | 0.038 | 0.564 | 0.962 |       |       |
| 500                  | 0.052    | 0.037 | 0.626 | 0.946 |       |       |
| 1500                 | 0.056    | 0.037 | 0.600 | 0.932 |       |       |
| Strat. Tree          |          |       |       |       |      |       |        |
| 100                  | 0.059    | 0.044 | 0.508 | 0.964 |       |       |
| 500                  | 0.053    | 0.036 | 0.604 | 0.944 |       |       |
| 1500                 | 0.054    | 0.034 | 0.594 | 0.946 |       |       |
| CV Tree              |          |       |       |       |      |       |        |
| 100                  | 0.054    | 0.035 | 0.574 | 0.938 |       |       |
| 500                  | 0.053    | 0.035 | 0.594 | 0.950 |       |       |
| 1500                 | 0.053    | 0.034 | 0.582 | 0.948 |       |       |
Table 8: Simulation results of Model 2.

| Method       | Criteria | Nuisance | MSE  | SMSE | R/R  | CR  | BC          | LIL          |
|--------------|----------|----------|------|------|------|-----|-------------|--------------|
|              |          | KNN      | 0.052| 0.034| 0.302| 0.958| 2748.000 | 3446.008     |
|              |          | NW       | 0.060| 0.043| 0.266| 0.946| 2868.000 | 3540.720     |
|              |          | NN       | 0.056| 0.040| 0.258| 0.952| 2890.000 | 3645.408     |
|              |          | KNN      | 0.052| 0.034| 0.320| 0.954| 2704.000 | 3398.308     |
|              |          | NW       | 0.059| 0.043| 0.472| 0.926| 2550.000 | 3194.026     |
|              |          | NN       | 0.084| 0.074| 0.632| 0.818| 2756.000 | 3473.814     |
|              |          | KNN      | 0.052| 0.034| 0.324| 0.962| 2744.000 | 3431.802     |
|              |          | NW       | 0.053| 0.034| 0.306| 0.946| 2812.000 | 3382.768     |
|              |          | NN       | 0.055| 0.037| 0.288| 0.940| 2878.000 | 3604.940     |
|              |          | KNN      | 0.058| 0.040| 0.264| 0.948| 2862.000 | 3511.908     |

| Pilot        | MSE  | SMSE | R/R  | CR  |
|--------------|------|------|------|-----|
| Ad-hoc       | 0.050| 0.036| 0.286| 0.982|
|              | 0.054| 0.038| 0.294| 0.970|
|              | 0.052| 0.037| 0.294| 0.976|
| Ad-hoc Neyman| 0.054| 0.039| 0.278| 0.966|
|              | 0.052| 0.036| 0.276| 0.970|
|              | 0.051| 0.035| 0.334| 0.982|
| Strat. Tree  | 0.057| 0.046| 0.246| 0.972|
|              | 0.049| 0.034| 0.276| 0.976|
|              | 0.051| 0.034| 0.340| 0.968|
| CV Tree      | 0.051| 0.035| 0.304| 0.976|
|              | 0.050| 0.033| 0.326| 0.966|
|              | 0.049| 0.034| 0.320| 0.978|
Table 9: Simulation results of Model 3.

| Method        | Nuisance | Criteria          |
|---------------|----------|-------------------|
|               |          | MSE    | SMSE   | R/R    | CR     | BC     | LIL    |
| A2IPW         | KNN      | 0.082  | 0.054  | 0.314  | 0.944  | 2774.000 | 3504.320 |
|               | NW       | 0.096  | 0.073  | 0.240  | 0.954  | 2886.000 | 3603.502 |
|               | NN       | 0.093  | 0.068  | 0.238  | 0.948  | 2914.000 | 3523.114 |
|               | ADR      | KNN    | 0.081  | 0.052  | 0.304  | 0.950  | 2720.000 | 3571.318 |
|               | NW       | 0.079  | 0.052  | 0.332  | 0.952  | 2672.000 | 3516.880 |
|               | NN       | 0.088  | 0.058  | 0.276  | 0.946  | 2854.000 | 3508.498 |
| A2IPW (Oracle)| KNN      | 0.082  | 0.055  | 0.302  | 0.934  | 2740.000 | 3537.698 |
|               | NW       | 0.079  | 0.053  | 0.306  | 0.960  | 2692.000 | 3459.326 |
|               | NN       | 0.088  | 0.062  | 0.254  | 0.954  | 2852.000 | 3606.298 |
| RCT           |          | 0.087  | 0.063  | 0.270  | 0.960  | 2816.000 | 3577.846 |

| Method        | Nuisance | Criteria          |
|---------------|----------|-------------------|
|               |          | Pilot             |
|               |          | MSE    | SMSE   | R/R    | CR     |
| Ad-hoc        | 100      | 0.083  | 0.058  | 0.284  | 0.950  |
|               | 500      | 0.084  | 0.062  | 0.284  | 0.954  |
|               | 1500     | 0.080  | 0.055  | 0.314  | 0.976  |
| Ad-hoc Neyman | 100      | 0.083  | 0.061  | 0.274  | 0.956  |
|               | 500      | 0.083  | 0.059  | 0.278  | 0.956  |
|               | 1500     | 0.078  | 0.056  | 0.272  | 0.970  |
| Strat. Tree   | 100      | 0.098  | 0.073  | 0.230  | 0.960  |
|               | 500      | 0.086  | 0.063  | 0.294  | 0.946  |
|               | 1500     | 0.081  | 0.057  | 0.312  | 0.962  |
| CV Tree       | 100      | 0.081  | 0.060  | 0.292  | 0.972  |
|               | 500      | 0.082  | 0.057  | 0.256  | 0.950  |
|               | 1500     | 0.077  | 0.054  | 0.266  | 0.976  |

Table 10: Simulation results of Model 1 when the null hypothesis is true ($\theta_0 = 0$).

| Method        | Nuisance | Criteria          |
|---------------|----------|-------------------|
|               |          | MSE    | SMSE   | R/R    | CR     | BC     | LIL    |
| A2IPW         | KNN      | 0.049  | 0.032  | 0.028  | 0.972  | 3228.000 | 4091.740 |
|               | NW       | 0.056  | 0.038  | 0.044  | 0.956  | 3278.000 | 4099.412 |
|               | NN       | 0.057  | 0.041  | 0.046  | 0.954  | 3280.000 | 4033.838 |
| ADR           | KNN      | 0.050  | 0.032  | 0.030  | 0.970  | 3246.000 | 4131.160 |
|               | NW       | 0.052  | 0.033  | 0.048  | 0.952  | 3296.000 | 4052.690 |
|               | NN       | 0.061  | 0.044  | 0.066  | 0.934  | 3354.000 | 4054.154 |
| RCT           |          | 0.056  | 0.042  | 0.044  | 0.956  | 3368.000 | 4136.404 |
Table 11: Simulation results of Model 2 when the null hypothesis is true ($\theta_0 = 0$).

| Method | Nuisance | MSE   | SMSE  | R/R   | CR   | BC      | LIL       |
|--------|----------|-------|-------|-------|------|---------|-----------|
| A2IPW  | KNN      | 0.052 | 0.034 | 0.042 | 0.958| 3180.000| 4122.806  |
| NW     |          | 0.061 | 0.043 | 0.052 | 0.948| 3300.000| 4264.980  |
| NN     |          | 0.056 | 0.040 | 0.050 | 0.950| 3352.000| 4313.950  |
| ADR    | KNN      | 0.052 | 0.034 | 0.046 | 0.954| 3252.000| 4120.868  |
| NW     |          | 0.059 | 0.043 | 0.070 | 0.930| 3176.000| 4149.514  |
| NN     |          | 0.085 | 0.074 | 0.190 | 0.810| 3314.000| 4249.732  |
| RCT    |          | 0.055 | 0.038 | 0.036 | 0.964| 3276.000| 4109.586  |

Table 12: Simulation results of Model 3 when the null hypothesis is true ($\theta_0 = 0$).

| Method | Nuisance | MSE   | SMSE  | R/R   | CR   | BC      | LIL       |
|--------|----------|-------|-------|-------|------|---------|-----------|
| A2IPW  | KNN      | 0.082 | 0.054 | 0.056 | 0.944| 3172.000| 4209.466  |
| NW     |          | 0.096 | 0.072 | 0.044 | 0.956| 3202.000| 4225.684  |
| NN     |          | 0.095 | 0.069 | 0.064 | 0.936| 3298.000| 4208.704  |
| ADR    | KNN      | 0.081 | 0.052 | 0.050 | 0.950| 3242.000| 4235.044  |
| NW     |          | 0.079 | 0.051 | 0.050 | 0.950| 3344.000| 4201.618  |
| NN     |          | 0.088 | 0.058 | 0.046 | 0.954| 3156.000| 4202.234  |
| RCT    |          | 0.086 | 0.062 | 0.050 | 0.950| 3234.000| 4259.450  |