Experimental Evaluation of Individualized Treatment Rules*

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July 28, 2019

Abstract

In recent years, the increasing availability of individual-level data and the advancement of machine learning algorithms have led to an explosion of methodological development for constructing individualized (or personalized) treatment rules (ITRs). These new tools are being applied in a variety of fields including business, medicine, and politics. However, there exist few methods that empirically evaluate the efficacy of ITRs. We consider common real-world settings, in which policy makers wish to predict the performance of a given ITR prior to its administration in a target population, possibly subject to a budget constraint. In particular, we propose to use a randomized experiment for evaluating the efficacy of ITRs. Unlike existing methods, the proposed methodology takes into account the maximum proportion of units who can receive the treatment. This is an important consideration especially for policy makers who face a budget constraint. Our methodology is based on Neyman’s repeated sampling approach and does not require modeling assumptions. As a result, it is applicable to the empirical evaluation of ITRs even when they are based on complex machine learning models and derived from observational data. We conduct a simulation study to demonstrate the accuracy of the proposed methodology in small samples. We also apply our methods to the Project STAR (Student-Teacher Achievement Ratio) experiment to compare the performance of ITRs that are based on popular machine learning methods used for estimating heterogeneous treatment effects.

Key Words: causal inference, heterogenous treatment effects, machine learning, micro-targeting, precision medicine

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*We thank Naoki Egami, Colin Fogarty, Zhichao Jiang, Susan Murphy, Nicole Pashley, and Stefan Wager for helpful comments. We thank Dr. Hsin-Hsiao Wang who inspired us to write this paper.

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1 Introduction

In recent years, the increasing availability of individual-level data and the rapid development of machine learning methods have led to the application of individualized (or personalized) treatment rules (ITRs) in a variety of fields, which assign different levels of treatments to individuals based on their observed characteristics. Examples include personalized medicine and micro-targeting in business and political campaigns (e.g., Hamburg and Collins, 2010; Imai and Strauss, 2011). In the causal inference literature, a number of researchers have developed methods to estimate ITRs (e.g., Qian and Murphy, 2011; Zhao et al., 2012; Laber and Zhao, 2015; Fu, Zhou and Faries, 2016; Zhou et al., 2017; Athey and Wager, 2018), while others have applied machine learning methods for estimating heterogeneous treatment effects, which can then be used to construct ITRs (e.g., Athey and Imbens, 2016; Imai and Ratkovic, 2013; Künzel et al., 2018; Wager and Athey, 2018).

Despite these methodological advancements and empirical applications, there exist few methods that empirically evaluate the efficacy of ITRs. We consider common real-world settings, in which policy makers wish to predict the performance of a given ITR prior to its administration in a target population, possibly subject to a budget constraint. In particular, we propose to use a randomized experiment for evaluating the efficacy of ITRs. Unlike existing methods, the proposed methodology takes into account the maximum proportion of units who can receive the treatment. This is an important consideration especially for policy makers who face a budget constraint.

Our methodology is based on Neyman (1923)'s repeated sampling approach. Unlike some existing methods, therefore, it does not require any modeling assumptions used to construct ITRs (e.g., Brinkley, Tsiatis and Anstrom, 2010; Cai et al., 2010; Zhang et al., 2012). As a result, it is applicable to the empirical evaluation of ITRs even when they are based on complex machine learning models and derived from observational data. In addition, the proposed approach does not depend on computationally intensive methods such as the bootstrap and posterior sampling (e.g., Athey and Imbens, 2016; Hahn, Murray and Carvalho, 2017; Wager and Athey, 2018). Indeed, the results of the 2017 Atlantic Causal Inference Conference Data Analysis Challenge suggest that these model-based and sampling-based confidence intervals may have poor coverage in practice when estimating heterogeneous treatment effects (see Hahn, Dorie and Murray, 2018 for details). We focus on the evaluation of a given ITR rather than its estimation uncertainty. Under our
framework, the uncertainty comes from the fact that we do not know how an ITR would perform if administered to in the target population and is based solely on the randomization of treatment assignment and the random sampling of experimental units.

We begin by introducing the Population Average Prescriptive Effect (PAPE) as one measure of ITR’s efficacy (Section 2.2). The PAPE is defined as the difference between the average outcomes under an ITR and the random treatment rule, which randomly selects the same number of individuals to be treated as the number of individuals treated under the ITR. Much of the existing methodology literature uses the value or the average outcome under an ITR, as an evaluation metric (e.g., [Qian and Murphy 2011] [Zhao et al. 2012]). The literature usually compares the average outcome under an ITR to a baseline with no treatment. In contrast, we argue that when evaluating the efficacy of an ITR in practice, it is important to hold the number of treated units constant. Otherwise, if a treatment has a non-negative effect on all individuals, for example, we would conclude that a trivial strategy of treating everyone will be most efficacious. While the PAPE has been used by some researchers (e.g., [Imai and Strauss 2011] [Rzepakowski and Jaroszewicz 2012] [Gutierrez and Gérardy 2016] [Fifield 2018]), its statistical properties has not been examined. We propose an unbiased estimator of the PAPE and derive its variance.

We further generalize this idea by considering the PAPE under a budget constraint (Section 2.3). As most policy makers have a limited amount of resources, establishing the priority as to who should receive the treatment is essential. Under this setting, we propose an approximately unbiased estimator of the PAPE and its variance. Because the efficacy of an ITR can vary as a function of budget constraint, we define the Area under the Prescriptive Effect Curve (AUPEC), which averages the PAPE over a specified range of budget constraint (Section 2.4). Again, we propose an approximately unbiased estimator of the AUPEC and derive its variance.

As the third evaluation metric, we propose the Population Average Prescriptive Effect Difference (PAPD), which quantifies the difference in the average outcome under two ITRs with the same budget constraint (Section 2.5). Unlike the usual comparison based on the value of ITRs, the PAPD holds the maximal proportion of treated units constant and hence puts two ITRs on an equal footing. The PAPD also generalizes the PAPE as the latter is a comparison against the random treatment rule. We propose an approximately unbiased estimator of the PAPD. Although the repeated sampling variance of this estimator is unidentifiable, we derive its upper bound,
which yields a conservative estimate of the variance.

Finally, we analytically compare the statistical efficiency of this *ex-post* experimental evaluation over the *ex-ante* experimental evaluation (e.g., Saveski et al. 2017). In the ex-ante evaluation, individuals are randomly assigned to either an ITR or a random treatment rule (Section 2.6). Unfortunately, a definitive conclusion on the statistical efficiency of two approaches is difficult to draw because the comparison depends on many parameters. Nevertheless, we show that under a set of simplifying assumptions, the *ex-post* experimental evaluation presented in this paper is statistically more efficient than the *ex-ante* evaluation. The main reason is that the *ex-post* evaluation utilizes the entire experimental sample to estimate the average outcomes under both the ITR of interest and the random treatment rule, whereas the *ex-ante* evaluation uses a separate part of the sample for each treatment rule.

In Section 3, we conduct a simulation study to evaluate the ITRs based on three commonly used machine learning methods — Bayesian Additive Regression Tree (Hahn, Murray and Carvalho 2017), Causal Forest (Wager and Athey 2018), and LASSO (Tibshirani 1996). The set up of our simulation study follows that of the aforementioned 2017 Atlantical Causal Inference Conference Data Challenge, in which the focus of the competition was the estimation of the conditional average treatment effect (Hahn, Dorie and Murray 2018). We show that even with a sample size as small as 100, the confidence intervals based on the proposed variance estimators have empirical coverage rates close to the nominal rates for the quantities of interest.

In Section 4, we apply our methodology to the Tennessee’s Student/Teacher Achievement Ratio (STAR) Project, which experimentally examines the efficacy of small class sizes on students’ performance. Using this experimental data, we show how to evaluate the ITRs based on the three machine learning methods. We find that these ITRs do not significantly improve upon the random treatment rule when there is no budget constraint in part because small classes have a non-negative effect on many students. However, when we impose a budget constraint, the ITRs based on BART and Causal Forest significantly outperforms the random treatment rule by identifying a subset of students who benefit greatly from small classes. Our analysis shows that in this application, the ITR based on the Causal Forest performs best, followed by that based on BART and then LASSO, when there is a budget constraint.

Finally, Section 5 gives concluding remarks. We briefly discuss how the proposed evaluation
framework can be extended to other settings including dynamic optimal treatment regimes and network experiments.

2 The Proposed Methodology

In this section, we describe the proposed methodology. We introduce four evaluation metrics for ITRs, propose their estimators, and derive their bias and variance under the repeated sampling framework of Neyman (1923). We also compare the statistical efficiency of ex-post experimental evaluation with that of ex-ante experimental evaluation.

2.1 The Setup and Assumptions

Suppose that policy makers wish to predict the performance of a given individualized treatment rule (ITR) \( f \) prior to its administration in a target population, \( \mathcal{P} \). Formally, we define the ITR as a fixed and deterministic map from the covariate space to the binary treatment assignment (Qian and Murphy, 2011; Zhao et al., 2012),

\[
f: \mathcal{X} \rightarrow \{0, 1\}.
\]

where \( \mathcal{X} \) is the support of observed covariates \( \mathbf{X} \). An ITR may be derived separately based on, for example, observational data. We focus on an experimental evaluation of a given ITR rather than its estimation uncertainty. In other words, we consider practically common settings, in which policy makers are interested in knowing how well a particular ITR would perform if administered to a target population.

Assume that we have a simple random sample of \( n \) units from the population of interest, \( \mathcal{P} \). We conduct a completely randomized experiment, in which \( n_1 \) units are randomly assigned to the treatment condition with probability \( n_1/n \) and the rest of the \( n_0(=n-n_1) \) units are assigned to the control condition. Let \( T_i \) denote the treatment assignment indicator variable, which is equal to 1 if unit \( i \) is assigned to the treatment condition. For each unit, we observe the outcome variable \( Y_i \in \mathcal{Y} \) as well as a vector of pre-treatment covariates, \( \mathbf{X}_i \in \mathcal{X} \), where \( \mathcal{Y} \) and \( \mathcal{X} \) are the support of the outcome and covariates, respectively. We assume no interference between units and denote the potential outcome for unit \( i \) under the treatment condition \( T_i = t \) as \( Y_i(t) \) for \( t = 0, 1 \). Then, the observed outcome is given by \( Y_i = Y_i(T_i) \).

We formally state these assumptions as follows.
Assumption 1 (No Interference between Units) The potential outcomes for unit $i$ do not depend on the treatment status of other units. That is, for all $t_1, t_2, \ldots, t_n \in \{0, 1\}$, we have,

$$Y_i(T_1 = t_1, T_2 = t_2, \ldots, T_n = t_n) = Y_i(T_i = t_i)$$

Assumption 2 (Random Sampling of Units) Each of $n$ units, represented by a three-tuple consisting of two potential outcomes and pre-treatment covariates, is assumed to be independently sampled from a super-population $\mathcal{P}$, i.e.,

$$(Y_i(1), Y_i(0), X_i) \overset{i.i.d.}{\sim} \mathcal{P}$$

Assumption 3 (Complete Randomization) For any $i = 1, 2, \ldots, n$, the treatment assignment probability is given by,

$$\Pr(T_i = 1 | Y_i(1), Y_i(0), X_i) = \frac{n_1}{n}$$

where $\sum_{i=1}^{n} T_i = n_1$.

While it is straightforward to allow for unequal treatment assignment probabilities across units under our framework, for the sake of simplicity, we assume complete randomization.

2.2 Evaluation against the Random Treatment Rule

Our goal is to evaluate the efficacy of an individualized treatment rule (ITR). In the literature, researchers often derive an optimal ITR that maximizes the population average value (PAV) (e.g., Qian and Murphy 2011; Zhao et al. 2012; Zhang et al. 2012; Zhou et al. 2017). The PAV is defined as the (super-population) average potential outcome under the ITR,

$$\lambda_f = \mathbb{E}\{Y_i(f(X_i))\}.$$ 

Although the PAV is a reasonable evaluation criteria, we argue that when evaluating the efficacy of an ITR, it is also important to consider the proportion of units which are assigned to the treatment condition. Since a treatment is often costly in practice, the efficacy of an ITR must be examined while holding the number of treated units constant. We do so by comparing an ITR against the random treatment rule, which randomly selects the same number of treated units (see e.g., Imai and Strauss 2011; Rzepakowski and Jaroszewicz 2012; Gutierrez and Gérardy 2016; Fifield 2018). As shown in Section 2.3, this idea naturally generalizes to the setting where policy makers face a budget constraint.
Formally, let $p_f = \Pr(f(X_i) = 1)$ denote the proportion of units in the population assigned to the treatment condition under the individualized treatment assignment rule $f$, where we assume $0 < p_f < 1$. Then, we can define the population average prescription effect (PAPE) of an ITR over the random treatment rule as,

$$\tau_f = \mathbb{E}\{Y_i(f(X_i)) - p_fY_i(1) - (1 - p_f)Y_i(0)\}$$

(1)

where the PAV of the random treatment rule is given by $\mathbb{E}\{p_fY_i(1) - (1 - p_f)Y_i(0)\}$. We consider statistical inference about the PAPE from Neyman’s repeated sampling approach \textbf{[Neyman [1923].} We propose the following estimator of the PAPE,

$$\hat{\tau}_f = \frac{n}{n-1} \left[ \frac{1}{n_1} \sum_{i=1}^{n} Y_i T_i f(X_i) + \frac{1}{n_0} \sum_{i=1}^{n} Y_i (1 - T_i) (1 - f(X_i)) - \frac{\hat{p}_f}{n_1} \sum_{i=1}^{n} Y_i T_i - \frac{1 - \hat{p}_f}{n_0} \sum_{i=1}^{n} Y_i (1 - T_i) \right]$$

(2)

where $\hat{p}_f = \sum_{i=1}^{n} f(X_i)/n$ is a sample estimate of $p_f$. The next theorem shows the unbiasedness of this estimator and derives its variance.

**Theorem 1 (Unbiasedness and Variance of the Estimator for the PAPE)** Under Assumptions 2–3, the bias and variance of the estimator of the PAPE given in equation (2) are given by,

$$\mathbb{E}(\hat{\tau}_f - \tau_f) = 0$$

$$\mathbb{V}(\hat{\tau}_f) = \frac{n^2}{(n-1)^2} \left[ \frac{\mathbb{E}(S_{f1}^2)}{n_1} + \frac{\mathbb{E}(S_{f0}^2)}{n_0} + \frac{1}{n^2} \left\{ \tau_f^2 - np_f(1-p_f)\tau^2 + 2(n-1)(2p_f-1)\tau_f \right\} \right]$$

where

$$\tau = \mathbb{E}(Y_i(1) - Y_i(0)) \quad \text{and} \quad S_{f1}^2 = \frac{1}{n-1} \sum_{i=1}^{n} (Y_i^*(t) - \overline{Y^*(t)})^2$$

for $t = \{0, 1\}$, $Y_i^*(t) = (f(X_i) - \hat{p}_f)Y_i(t)$, and $\overline{Y^*(t)} = \sum_{i=1}^{n} Y_i^*(t)/n$.

Proof is given in Appendix [A.1]. Note that $\mathbb{E}(S_{f1}^2)$ does not equal $\mathbb{V}(Y_i^*(t))$ because the proportion of treated units $p_f$ is unknown and must be estimated. The additional term in the variance accounts for the estimation uncertainty of $p_f$. In addition, the variance of the proposed estimator can be consistently estimated by replacing the unknown terms, i.e., $p_f$, $\tau_f$, $\tau$, $\mathbb{E}(S_{f1}^2)$, with their unbiased estimates, i.e., $\hat{p}_f$, $\hat{\tau}_f$, and

$$\hat{\tau} = \frac{1}{n_1} \sum_{i=1}^{n} T_i Y_i - \frac{1}{n_0} \sum_{i=1}^{n} (1 - T_i) Y_i, \quad \mathbb{E}(\hat{S}_{f1}^2) = \frac{1}{n_t - 1} \sum_{i=1}^{n} 1 \{T_i = t\} (Y_i^* - \overline{Y^*_t})^2.$$

where $Y_i^* = (f(X_i) - \hat{p}_f)Y_i$ and $\overline{Y^*_t} = \sum_{i=1}^{n} 1 \{T_i = t\} Y_i^*/n_t$. 

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2.3 Evaluation with a Budget Constraint

In almost all practical situations, the evaluation of ITRs requires the consideration of a budget constraint. In fact, the efficacy of an ITR matters most when only a fraction of the population can be treated. Here, we generalize the evaluation strategy discussed above by operationalizing a budget constraint as the maximal proportion of treated units, denoted by $p$, and consider the setting, in which this proportion is less than the proportion of units to be treated under an ITR, i.e., $p < p_f$. Note that if $p \geq p_f$, then a budget constraint is not binding and hence the results of Section 2.2 directly apply.

With a budget constraint, we cannot simply treat all units who are predicted to benefit from the treatment. Instead, an ITR must be based on a score function that orders units according to their treatment priority. That is, a unit with a greater score has a higher priority to receive the treatment. Let $s : \mathcal{X} \rightarrow \mathcal{S}$ be such a score function where $\mathcal{S} \subset \mathbb{R}$. For the sake of simplicity, we assume that the score function is bijective, i.e., $s(x) \neq s(x')$ for any $x, x' \in \mathcal{X}$ with $x \neq x'$. This assumption is not restrictive as we can always redefine $\mathcal{X}$ such that the assumption holds. A prominent example of score function is the conditional average treatment effect (CATE),

$$s(x) = \mathbb{E}(Y_i(1) - Y_i(0) \mid X_i = x).$$

A number of researchers have studied how the CATE can be best estimated using various machine learning methods such as regularized regression models and tree-based methods (e.g., Imai and Strauss 2011; Qian and Murphy 2011; Imai and Ratkovic 2013; Athey and Imbens 2016; Grimmer, Messing and Westwood 2017; Künzel et al. 2018; Wager and Athey 2018).

We now define an ITR based on a score function by assigning a unit to the treatment group if and only if its score is higher than a threshold, $c_p$

$$f(X_i, c_p) = 1\{s(X_i) > c_p\}.$$

Since we are considering the case with a binding budget constraint, the threshold $c_p$ corresponds to the maximal proportion of treated units under the budget constraint, i.e.,

$$c_p = \inf\{c \in \mathbb{R} : \Pr(f(X_i, c) = 1) \leq p\}.$$

Following the idea discussed above, we evaluate an ITR $f$ against the random treatment rule, which randomly selects proportion $p$ of units to the treatment group. Thus, the PAPE with a
budget constraint $p$ is defined as,

$$
\tau_f(c_p) = \mathbb{E}\{Y_i(f(X_i, c_p)) - pY_i(1) - (1 - p)Y_i(0)\}. 
$$

We consider the following estimator of the PAPE with a budget constraint,

$$
\hat{\tau}_f(\hat{c}_p) = \frac{1}{n_1} \sum_{i=1}^{n} Y_i T_i f(X_i, \hat{c}_p) + \frac{1}{n_0} \sum_{i=1}^{n} Y_i (1 - T_i) (1 - f(X_i, \hat{c}_p)) - \frac{p}{n_1} \sum_{i=1}^{n} Y_i T_i - \frac{1 - p}{n_0} \sum_{i=1}^{n} Y_i (1 - T_i) \tag{4}
$$

where $\hat{c}_p = \inf\{c \in \mathbb{R} : \sum_{i=1}^{n} f(X_i, c) \leq np\}$. As before, we examine the bias and variance under Neyman’s repeated sampling framework. Since we are also estimating $c_p$, the bias of the proposed estimator in equation (4) is not zero. However, we can derive its upper bound.

**Theorem 2 (Bias and Variance of the Estimator for the PAPE with a Budget Constraint)** Under Assumptions 2–3, the bias of the proposed estimator of the PAPE with a budget constraint $p$ defined in equation (4) can be bounded as follows,

$$
\mathbb{P}(|\mathbb{E}\{\hat{\tau}_f(\hat{c}_p) - \tau_f(c_p)\}| \geq \varepsilon) \leq 1 - B(p + \gamma_p(\varepsilon), [np], n - [np] + 1) + B(p - \gamma_p(\varepsilon), [np], n - [np] + 1)
$$

where any given constant $\varepsilon > 0$, $B(\varepsilon, \alpha, \beta)$ is the incomplete beta function, and

$$
\gamma_p(\varepsilon) = \frac{\varepsilon}{\max_{c \in [c_p - \varepsilon, c_p + \varepsilon]} \mathbb{E}(Y_i(1) - Y_i(0) \mid s(X_i) = c)},
$$

The variance of the estimator is given by,

$$
\mathbb{V}(\hat{\tau}_f(\hat{c}_p)) = \frac{\mathbb{E}(S_{f1}^2)}{n_1} + \frac{\mathbb{E}(S_{f0}^2)}{n_0} + \frac{|np|(n - [np])}{n^2(n - 1)} \{(2p - 1)\kappa_1(X_i, \hat{c}_p)^2 - 2p\kappa_1(X_i, \hat{c}_p)\kappa_0(X_i, \hat{c}_p)\}
$$

where, for $t = 0, 1$,

$$
\hat{S}_{ft}^2 = \frac{1}{n - 1} \sum_{i=1}^{n} (\tilde{Y}_i(t) - \overline{Y}(t))^2, \quad \kappa_t(X_i, \hat{c}_p) = \mathbb{E}(Y_i(1) - Y_i(0) \mid f(X_i, \hat{c}_p) = t),
$$

$$
\tilde{Y}_i(t) = (f(X_i, \hat{c}_p) - p) Y_i(t), \text{ and } \overline{Y}(t) = \sum_{i=1}^{n} \tilde{Y}_i(t)/n.
$$

Proof is given in Appendix A.2. Similar to PAPE, $\mathbb{E}[(\hat{S}_{ft})^2]$ does not equal $\mathbb{V}[(\tilde{Y}_i(t))^2]$ because we must estimate $c_p$. The additional term in the variance accounts for the variance due to estimating $c_p$. As before, the variance can be consistently estimated by replacing each unknown parameter with its sample analogue, i.e., for $t = 0, 1$,

$$
\hat{\mathbb{E}}(S_{ft}^2) = \frac{1}{n_t - 1} \sum_{i=1}^{n} 1\{T_i = t\}(\tilde{Y}_i - \overline{Y}_t)^2 \tag{5}
$$
Figure 1: The Area Under the Prescriptive Effect Curve (AUPEC). The black solid line represents the average outcome under an individualized treatment rule while the red solid line represents the average outcome under the random treatment rule. The shaded area between the curve and the line corresponds to the AUPEC.

\[
\kappa_t(X_i, \hat{c}_p) = \sum_{i=1}^{n} \mathbb{1}\{f(X_i, \hat{c}_p) = t\}T_i Y_i - \sum_{i=1}^{n} \mathbb{1}\{f(X_i, \hat{c}_p) = t\}(1 - T_i) Y_i
\]

where \( \hat{Y}_i = (f(X_i, \hat{c}_p) - p)Y_i \) and \( \bar{Y}_i = \sum_{i=1}^{n} \mathbb{1}\{T_i = t\} \hat{Y}_i / n_t \). To estimate the term that appears in the denominator of \( \gamma_p(\epsilon) \) as part of the upper bound of bias, we may assume that the CATE \( \mathbb{E}(Y_i(1) - Y_i(0) | s(X_i) = c) \) is Lipschitz continuous in \( c \). The Lipschitz continuity of the CATE is often assumed when estimating heterogeneous treatment effects (see e.g., Künzel et al., 2018; Wager and Athey, 2018).

### 2.4 Area Under Prescriptive Effect Curve (AUPEC)

The PAPE defined in equation (3) varies as a function of budget constraint. Figure 1 shows this graphically where the horizontal and vertical axes represent the budget and the average outcome, respectively. In the figure, the red solid curve corresponds to the average outcome under an ITR, i.e., \( \mathbb{E}\{Y_i(f(X_i, c_p))\} \), as a function of budget constraint \( p \), whereas the black solid line represents the average outcome under the random treatment rule. We may wish to evaluate the overall
efficacy of an ITR by computing the area under the red curve minus the area under the black curve. This is shown as a shaded area in Figure 1 and we call it the Area Under the Prescriptive Effect Curve (AUPEC). Formally, we define the AUPEC as,

$$\Gamma_f = \int_0^{p_f} \mathbb{E}\{Y_i(f(X_i, c_p))\}dp + (1 - p_f)\mathbb{E}\{Y_i(f(X_i, c_{p_f}))\} - \frac{1}{2}\mathbb{E}(Y_i(0) + Y_i(1)).$$

Thus, the AUPEC represents the average performance relative to the random treatment rule over the entire range of budget constraint. Although a similar idea is proposed in the literature (see e.g., Rzepakowski and Jaroszewicz 2012), unlike the previous work, we do not require an ITR to assign the maximal number of units to the treatment condition under a budget constraint. For example, treating more than a certain proportion of units may reduce the average outcome because these additional units do not benefit from the treatment. This is indicated by the flatness of the red line after $p_f$ in Figure 1. Recall that $p_f$ represents the the maximal proportion of units an ITR $f$ would assign to the treatment under no budget constraint, i.e., $p_f = \text{Pr}(f(X_i) = 1)$. A large value of the AUPEC implies that the ITR under consideration is effective when compared to the random treatment rule across a wide range of budget constraints.

Now, let $n_f$ represent the maximum number of units in the sample that an ITR $f$ would assign under no budget constraint, i.e., $\hat{p}_f = n_f/n = \sum_{i=1}^n f(X_i)/n$. Then, we propose the following estimator of the AUPEC,

$$\hat{\Gamma}_f = \frac{1}{n_1} \sum_{i=1}^n Y_iT_i \left\{ \frac{1}{n} \left( \sum_{k=1}^{n_f} f(X_i, \hat{c}_{k/n}) + (n - n_f) f(X_i, \hat{c}_{n_f/n}) \right) \right\} + \frac{1}{n_0} \sum_{i=1}^n Y_i(1 - T_i) \left\{ 1 - \frac{1}{n} \left( \sum_{k=1}^{n_f} f(X_i, \hat{c}_{k/n}) + (n - n_f) f(X_i, \hat{c}_{n_f/n}) \right) \right\} - \frac{1}{2n_1} \sum_{i=1}^n Y_iT_i - \frac{1}{2n_0} \sum_{i=1}^n Y_i(1 - T_i)$$ (7)

where $\hat{c}_p = \inf\{c \in \mathbb{R} : \sum_{i=1}^n f(X_i, c)/n \leq p\}$. The next theorem bounds the bias and derives the variance of this estimator under Neyman’s repeated sampling approach.

**Theorem 3 (Bias and Variance of the Estimator for the AUPEC)** Under Assumptions 2-3, the bias of the estimator given in equation (7) can be bounded as follows,

$$\mathbb{P}(\mathbb{E}(\hat{\Gamma}_f - \Gamma_f) \geq \epsilon) \leq 1 - B(p_f + \gamma_{p_f}(\epsilon), \lfloor np_f \rfloor, n - \lfloor np_f \rfloor + 1) + B(p_f - \gamma_{p_f}(\epsilon), \lfloor np_f \rfloor, n - \lfloor np_f \rfloor + 1)$$
where any given constant $\epsilon > 0$, $B(\epsilon, \alpha, \beta)$ is the incomplete beta function, and

$$\gamma_{p_f}(\epsilon) = \frac{\epsilon}{2\max_{c \in [c_{p_f} - \epsilon, c_{p_f} + \epsilon]} \mathbb{E}(Y_i(1) - Y_i(0) \mid s(X_i) = c)}.$$  

The variance is given by,

$$\mathbb{V}(\hat{\Gamma}_f) = \mathbb{E} \left[ -\frac{1}{n} \left\{ \sum_{k=1}^{Z} \frac{k(n-k)}{n^2(n-1)} \kappa_1(X_i, \hat{c}_{k/n}) \kappa_0(X_i, \hat{c}_{k/n}) + \frac{Z(n-Z)^2}{n^2(n-1)} \kappa_1(X_i, \hat{c}_{Z/n}) \kappa_0(X_i, \hat{c}_{Z/n}) \right\} ight. 
- \frac{2}{n^4(n-1)} \sum_{k=1}^{Z-1} \sum_{k'=k+1}^{Z} k(n-k') \kappa_1(X_i, \hat{c}_{k/n}) \kappa_1(X_i, \hat{c}_{k'/n}) 
- \frac{Z^2(n-Z)^2}{n^4(n-1)} \kappa_1(X_i, \hat{c}_{Z/n})^2 - \frac{2(n-Z)^2}{n^4(n-1)} \sum_{k=1}^{Z} k \kappa_1(X_i, \hat{c}_{Z/n}) \kappa_1(X_i, \hat{c}_{k/n}) 
+ \frac{1}{n^2} \sum_{k=1}^{Z} k(n-k) \kappa_1(X_i, \hat{c}_{k/n})^2 \right] 
+ \mathbb{V} \left( \sum_{i=1}^{Z} \frac{i}{n} \kappa_1(X_i, \hat{c}_{i/n}) + \frac{(n-Z)Z}{n} \kappa_1(X_i, \hat{c}_{Z/n}) \right) + \frac{\mathbb{E}(S_{f1}^{12})}{n_1} + \frac{\mathbb{E}(S_{f0}^{12})}{n_0}$$

where $Z$ is a Binomial random variable with size $n$ and success probability $p_f$, and for $t = 0, 1$,

$$S_{ft}^{12} = \frac{1}{n-1} \sum_{i=1}^{n} (Y_i^+(t) - \overline{Y}(t))^2, \quad \kappa_t(X_i, \hat{c}_{k/n}) = \mathbb{E}(Y_i(1) - Y_i(0) \mid f(X_i, \hat{c}_{k/n}) = t),$$

with $Y_i^+(t) = \left[ \frac{1}{n} \left\{ \sum_{k=1}^{n_f} f(X_i, \hat{c}_{k/n}) + (n-n_f) f(X_i, \hat{c}_{n_f/n}) \right\} - \frac{1}{2} \right] Y_i(t)$ and $\overline{Y}(t) = \sum_{i=1}^{n} Y_i^+(t)/n$.

Proof is given in Appendix A.3. Here, $\mathbb{E}[S_{f1}^{1}]$ does not equal $\mathbb{V}[Y_i^+(t)]$ due to the need to estimate the terms $c_{k/n}$ for all $k$. The additional terms account for the variance of estimation. As discussed at the end of Section 2.3, we can consistently estimate the upper bound of bias by assuming that the CATE is Lipschitz continuous. As before, the variance can be consistently estimated by replacing each unknown parameter with its sample analogue, i.e., for $t = 0, 1$,

$$\mathbb{E}(S_{f1}^{12}) = \frac{1}{n_t-1} \sum_{i=1}^{n_t} 1\{T_i = t\} (Y_i^+ - \overline{Y})^2$$

$$\kappa_t(X_i, \hat{c}_{k/n}) = \frac{\sum_{i=1}^{n} 1\{f(X_i, \hat{c}_{k/n}) = t\} T_i Y_i}{\sum_{i=1}^{n} 1\{f(X_i, \hat{c}_{k/n}) = t\} T_i} - \frac{\sum_{i=1}^{n} 1\{f(X_i, \hat{c}_{k/n}) = t\} (1-T_i) Y_i}{\sum_{i=1}^{n} 1\{f(X_i, \hat{c}_{k/n}) = t\} (1-T_i)}$$

where $Y_i^+ = \left[ \frac{1}{n} \left\{ \sum_{k=1}^{n_f} f(X_i, \hat{c}_{k/n}) + (n-n_f) f(X_i, \hat{c}_{n_f/n}) \right\} - \frac{1}{2} \right] Y_i$ and $\overline{Y} = \sum_{i=1}^{n} Y_i^+ / n$. In the extreme cases with $k \to 1$ for $t = 1$ and $k \to n$ for $t = 0$, the denominators in equation (9) are likely to be close to zero. In such cases, we instead use the estimator $\kappa_1(X_i, \hat{c}_{k_{\min}/n})$ for all $k < k_{\min}$.
where $k_{\text{min}}$ is the smallest $k$ such that equation (9) for $\kappa_1(X_i, \hat{c}_{k/n})$ does not suffer from zero in the denominators. Similarly, for $t = 0$, we use $\kappa_0(X_i, \hat{c}_{k_{\text{max}}/n})$ for all $k > k_{\text{max}}$ where $k_{\text{max}}$ is the largest $k$ such that equation (9) does not suffer from zero in the denominators.

For the terms involving the binomial random variable $Z$, we first note that these terms when fully expanded out are the polynomials of $p_f = \mathbb{E}(f(X_i))$. To estimate the polynomials of $p_f$, we can utilize their unbiased estimators as discussed in Stuard and Ord (1994), i.e., $\hat{p}^k_f = s(s-1) \cdots (s-k+1)/(n(n-1) \cdots (n-k+1))$ where $s = \sum_{i=1}^n f(X_i)$ is unbiased for $p_f^k$ for all $k \leq n$. When the sample size is large, this estimation method is not computationally efficient and stable due to the presence of high powers. Hence, we may use the Monte Carlo sampling of $Z$ from a Binomial distribution with size $n$ and success probability $\hat{p}_f$. In our simulation study, we show that this Monte Carlo approach is effective (see Section 3).

To enable a general comparison of efficacy across different datasets, the AUPEC measure can be further normalized to be scale-invariant. We define the normalized AUPEC by shifting $\Gamma_f$ by $\mathbb{E}(Y_i(0))$ and dividing by $\mathbb{E}(Y_i(1) - Y_i(0))$,

$$\Gamma^*_f = \frac{1}{\mathbb{E}(Y_i(1) - Y_i(0))} \left( \int_0^{p_f} \mathbb{E}\{Y_i(f(X_i, c_p))\}dp + (1 - p_f)\mathbb{E}\{Y_i(f(X_i, c_{p_f}))\} - \mathbb{E}(Y_i(0)) \right) - \frac{1}{2}$$

which is invariant to the affine transformation of the outcome variables, $Y_i(1), Y_i(0)$, while the AUPEC $\Gamma_f$ is only invariant to a constant shift. This normalized AUPEC takes a value in $[0, 1]$, and has an intuitive interpretation as the average percentage gain in outcome using the treatment rule $f$ compared to the random treatment rule, under the uniform prior distribution over the percentage treated $p_f$.

The estimator in equation (7) can be extended to a consistent estimator for the normalized AUPEC,

$$\hat{\Gamma}^*_f = \frac{1}{\sum_{i=1}^n Y_i T_i/n_1 - Y_i(1 - T_i)/n_0} \left\{ \frac{1}{nn_1} \sum_{i=1}^n Y_i T_i \left( \sum_{k=1}^{n_f} f(X_i, \hat{c}_{k/n}) + (n - n_f) f(X_i, \hat{c}_{n_f/n}) \right) ight. \\
- \frac{1}{nn_0} \sum_{i=1}^n Y_i (1 - T_i) \left( \sum_{k=1}^{n_f} f(X_i, \hat{c}_{k/n}) + (n - n_f) f(X_i, \hat{c}_{n_f/n}) \right) \right\} - \frac{1}{2}$$

The variance of this estimator, which is based on a ratio of binomial variables, can be estimated using the Taylor expansion of an appropriate order as detailed in Stuard and Ord (1994).
2.5 Relative Efficacy of Two Individualized Treatment Rules

While we have been comparing an ITR against the random treatment rule, policy makers are often interested in evaluating the relative efficacy of two ITRs, \( f \) and \( g \). For example, they may wish to evaluate a new ITR against the ITR that is currently in use. Such a comparison can be done by estimating the difference in the population average value (PAV) between the two ITRs,

\[
\Delta(f, g) = \lambda_f - \lambda_g = \mathbb{E}\{Y_i(f(X_i)) - Y_i(g(X_i))\}. \tag{11}
\]

While this quantity is useful in some settings, the problem is the same as the PAV itself; it fails to take into account the number of units assigned to the treatment condition under each ITR. For example, if a treatment never hurts units, i.e., \( Y_i(1) \geq Y_i(0) \) for all \( i \), then it is not fair to compare an ITR that treats most of the individuals to another ITR that treats only a few. Such a comparison would not account for how good each ITR is in identifying those who benefit most from the treatment and is not informative when policy makers face a budget constraint.

To address this issue, we compare the efficacy of two ITRs under a budget constraint. That is, we aim to estimate the difference in the PAPEs under the same budget constraint \( p \). Formally, we define the Population Average Prescriptive Effect Difference (PAPD) under budget \( p \) as,

\[
\Delta_p(f, g) = \tau_f(c_p) - \tau_g(c_p) = \mathbb{E}\{Y_i(f(X_i, c_p)) - Y_i(g(X_i, c_p))\}
\]

We propose the following estimator of the PAPD,

\[
\hat{\Delta}_p(f, g) = \frac{1}{n_1} \sum_{i=1}^{n} Y_i T_i (f(X_i, \hat{c}_f^p) - g(X_i, \hat{c}_g^p)) + \frac{1}{n_0} \sum_{i=1}^{n} Y_i (1 - T_i) (g(X_i, \hat{c}_g^p) - f(X_i, \hat{c}_f^p)) \tag{12}
\]

where \( \hat{c}_f^p = \inf\{c \in \mathbb{R} : \sum_{i=1}^{n} f(X_i, c) \leq np\} \) and \( \hat{c}_g^p = \inf\{c \in \mathbb{R} : \sum_{i=1}^{n} g(X_i, c) \leq np\} \).

As before, we derive the bias and variance of this estimator under the Neyman’s repeated sampling framework. Although the bias of the proposed estimator in equation \( 12 \) is not zero, we derive its upper bound as done in Theorems 2 and 3. Unlike the previous cases considered in this paper, however, the variance is not identifiable either in this case. Hence, we derive its upper bound, yielding a conservative variance estimator.

**Theorem 4 (Bias and Variance of the Estimator for the PAPD with a Budget Constraint)** Under Assumptions 2–3, the bias of the proposed estimator of the PAPD with a budget constraint \( p \) defined in equation \( 12 \) can be bounded as follows,

\[
\mathbb{P}(|\mathbb{E}\{\hat{\Delta}_p(f, g) - \Delta_p(f, g)\}| \geq \epsilon) \leq 1 - 2B(p + \gamma_p(\epsilon), [np], n - [np] + 1) + 2B(p - \gamma_p(\epsilon), [np], n - [np] + 1)
\]
where any given constant \( \epsilon > 0 \), \( B(\alpha, \beta) \) is the incomplete beta function, and

\[
\gamma_p(\epsilon) = \max_{c \in [c_p, c_p+\epsilon]} \frac{\epsilon}{\max_{d \in [c_p, c_p+\epsilon]} \{E(Y_i(1) - Y_i(0) \mid s_f(X_i) = c), E(Y_i(1) - Y_i(0) \mid s_g(X_i) = d)\}}.
\]

The variance of the estimator is bounded by,

\[
\mathbb{V}(\hat{\Delta}(f, g)) \leq \frac{E(S_{fgt}^2)}{n_1} + \frac{E(S_{fg0}^2)}{n_0} + \frac{|np|}{n^2(n-1)} \left( \kappa_f(X_i, \hat{c}_f)^2 + \kappa_g(X_i, \hat{c}_g)^2 \right) + 2\frac{|np| \max\{|np|, n - |np|\}}{n^2(n-1)} |\kappa_f(X_i, \hat{c}_f)\kappa_g(X_i, \hat{c}_g)|
\]

where for \( t = 0, 1 \), \( \kappa_f(X_i, \hat{c}_f) = E(Y_i(1) - Y_i(0) \mid f(X_i, \hat{c}_f) = t) \), \( \kappa_g(X_i, \hat{c}_g) = E(Y_i(1) - Y_i(0) \mid g(X_i, \hat{c}_g) = t) \),

\[
S_{fgt}^2 = \frac{1}{n-1} \sum_{i=1}^{n} (\tilde{Y}_i^*(t) - \bar{Y}^*(t))^2,
\]

\( \tilde{Y}_i^*(t) = (f(X_i, \hat{c}_f) - g(X_i, \hat{c}_g)) Y_i(t) \) and \( \bar{Y}^*(t) = \sum_{i=1}^{n} \tilde{Y}_i^*(t)/n \).

Proof is given in Appendix A.4. The upper bound of the variance can be estimated by replacing the unknown parameters with their sample analogues in a manner similar to those given in equations (5) and (6). Unlike the case of the PAPE under a budget constraint (see Theorem 2), the variance of the PAPD estimator under a budget constraint is unidentifiable. In the previous case, we have only score \( s_f(X) \), and the statistic \( \hat{c}_p \) helps us anchor its distribution because of the identity, \( \Pr(s_f(X) > \hat{c}_p) = |np|/n \). In addition, the comparison with the random treatment rule does not suffer from this unidentifiability problem because its uniform scoring rule allows us to identify their joint distribution. In the current case, however, we have two general scores, \( \hat{c}_f \) and \( \hat{c}_g \), and we can only identify their marginal distributions from the observed data, so their joint distribution is unidentifiable.

### 2.6 Comparison with the Ex-ante Experimental Evaluation

So far, we have considered an ex-post evaluation, in which we first conduct a randomized experiment and then evaluate ITRs using the data from the experiment. Alternatively, researchers may consider an ex-ante experimental evaluation, in which we conduct a randomized experiment to directly evaluate ITRs by considering the application of each ITR as a treatment. We compare these ex-ante and ex-post evaluations in terms of their statistical efficiency. As we show below, in general, the ex-post evaluation tends to be more efficient than the ex-ante evaluation. The main
reason is that the ex-post evaluation uses the entire sample to estimate the PAV for both the ITR of interest and a random assignment rule. In contrast, the ex-ante evaluation uses separate parts of the sample for the estimation of the PAV for the two treatment rules.

Suppose we have a simple random sample of \( n \) units from the same target population, \( \mathcal{P} \). Consider a completely randomized experiment, in which a total of \( n_f \) units are randomly assigned to an ITR \( f \) while the remaining units \( n_r = n - n_f \) are assigned to the random treatment rule with the probability of treatment assignment equal to \( n_{r1}/n_r \). Let \( F_i \) be an indicator variable, which is equal to 1 if unit \( i \) is assigned to the ITR \( f \) and is equal to 0 otherwise. Under the random treatment rule, the number of units that are randomly assigned to the treatment condition is \( n_{r1} \) while \( n_{r0} = n_r - n_{r1} \) units are assigned to the control condition. As before, we use \( T_i \) to represent the treatment indicator.

**Assumption 4 (Complete Randomization in the Ex-ante Evaluation)** For any \( i = 1, 2, \ldots, n \), the probability of being assigned to the individualized treatment rule rather than the random treatment rule is given by,

\[
Pr(F_i = 1 \mid Y_i(1), Y_i(0), X_i) = \frac{n_f}{n}
\]

where \( \sum_{i=1}^{n} F_i = n_f \). Among those who are assigned to the random treatment rule, i.e., \( F_i = 0 \), the probability of treatment assignment is given by,

\[
Pr(T_i = 1 \mid Y_i(1), Y_i(0), X_i, F_i = 0) = \frac{n_{r1}}{n_r}
\]

where \( \sum_{i=1}^{n} (1 - F_i)T_i = n_{r1} \).

Using this experimental data, we wish to estimate the PAPE defined in equation (1). One potential complication is that we have to adjust for the number of treated units as done throughout this paper since the number of treated units under the random treatment rule may differ from that under the ITR, i.e., \( \hat{\rho}_f \neq n_{r1}/n_r \) where \( \hat{\rho}_f = \sum_{i=1}^{n} f(X_i)/n \). On the other hand, it is possible to choose the number of treated units under the random treatment rule such that the equality is enforced if the covariate data for the group assigned to the ITR are available prior to the randomization of treatment assignment. We propose the following estimator of the PAPE for the ex-ante experimental evaluation that accounts for a potential difference in the proportion of treated units between the ITR and the random treatment rule by appropriately weighting the
latter,
\[
\hat{\tau}_f^* = \frac{n}{n-1} \left( \frac{1}{n_f} \sum_{i=1}^{n} F_i f(X_i) Y_i - \hat{p}_f \sum_{i=1}^{n} (1 - F_i) T_i Y_i - \frac{1 - \hat{p}_f}{n_{r0}} \sum_{i=1}^{n} (1 - F_i)(1 - T_i) Y_i \right) 
\]  

(13)

The \textit{ex-ante} evaluation differs from the \textit{ex-post} evaluation in two ways. First, the \textit{ex-ante} estimator requires two separate random assignments (\(T_i\) and \(F_i\)) while the \textit{ex-post} estimator only involves one. Intuitively, an additional layer of randomization increases variance. Second, the \textit{ex-ante} evaluation requires a separate group that follows an ITR, whereas all individuals in the \textit{ex-post} evaluation are simply randomly assigned either to the treatment or control group. As a result, in the \textit{ex-post} evaluation, the PAV of the random treatment rule is estimated using the entire sample. Together, we expect the \textit{ex-ante} evaluation to be less efficient than the \textit{ex-post} evaluation. We confirm this intuition under a set of simplifying assumptions below.

Before comparing two modes of evaluation, we derive the bias and variance of the \textit{ex-ante} evaluation estimator under Neyman’s repeated sampling framework. In the current case, the uncertainty comes from three types of randomness: (1) the random assignment to the individualized or random treatment rule, (2) the randomized treatment assignment under the random assignment rule, and (3) the simple random sampling of units from the target population. The next theorem shows that this estimator is unbiased and the variance is identifiable.

\textbf{Theorem 5 (Bias and Variance of the Ex-Ante Evaluation Estimator for PAPE) Under Assumptions 2, 1, and 4, the bias and variance of the estimator of the PAPE given in equation (13) are given by,}

\[
\mathbb{E}(\hat{\tau}_f^* - \tau_f) = 0 \\
\mathbb{V}(\hat{\tau}_f^*) = \frac{n^2}{(n-1)^2} \left[ \mathbb{E} \left\{ \frac{S_f^2}{n_f} + \frac{\hat{p}_f^2}{n_{r1}} + \frac{(1 - \hat{p}_f)^2}{n_{r0}} \right\} + \frac{1}{n^2} \left\{ \tau_f^2 - np_f(1 - p_f)\tau_f^2 + 2(n-1)(2p_f - 1)\tau_f \right\} \right]
\]

\text{where}

\[
S_f^2 = \frac{1}{n-1} \sum_{i=1}^{n} (Y_i(f(X_i)) - \bar{Y}(f(X)))^2, \quad S_t^2 = \frac{1}{n-1} \sum_{i=1}^{n} (Y_i(t) - \bar{Y}(t))^2
\]

for \(t = 0, 1\).

Proof is given in Appendix A.5. To estimate the variance, we replace the terms with their unbiased estimates.
We now examine the relative statistical efficiency of the *ex-post* and *ex-ante* experimental evaluations. This can be done by directly comparing the variances derived in Theorems 1 and 5. To facilitate the comparison, we assume \( n_1 = n_0 = n_r = n_f = n/2 \). In words, the *ex-ante* evaluation sets the treatment assignment probability to 1/2, and the *ex-post* evaluation also sets the probability of being assigned to the ITR to 1/2. Finally, we also assume \( n_r1 = n_r0 = n/4 \), implying that in the *ex-post* evaluation the treatment assignment probability under the random treatment rule also equals 1/2. Under this setting, the difference in the variance of the PAPE estimator between the *ex-ante* and *ex-post* evaluations is given by,

\[
\begin{align*}
\text{V}(\hat{\tau}_f) - \text{V}(\hat{\tau}_f) \\
= \frac{2n}{(n-1)^2} \left[ \mathbb{E} \left\{ p_f^2 S_1^2 + (1 - p_f)^2 S_0^2 \right\} + 2 \text{Cov}(f(X_i)Y_i(1), (1 - f(X_i))Y_i(0)) \\
+ 2p_f \text{Cov}(f(X_i)Y_i(1), Y_i(1)) + 2(1 - p_f) \text{Cov}((1 - f(X_i))Y_i(0), Y_i(0)) \right] \\
= \frac{2n}{(n-1)^2} \left[ p_f^2 \mathbb{V}(Y_i(1)) + (1 - p_f)^2 \mathbb{V}(Y_i(0)) - 2p_f(1 - p_f)\mathbb{E}(Y_i(0) | f(X_i) = 0)\mathbb{E}(Y_i(1) | f(X_i) = 1) \\
+ 2p_f \left\{ \mathbb{E}(Y_i^2(1) | f(X_i) = 1) - \mathbb{E}(Y_i(1))\mathbb{E}(Y_i(1) | f(X_i) = 1) \right\} \\
+ 2(1 - p_f)^2 \left\{ \mathbb{E}(Y_i^2(0) | f(X_i) = 0) - \mathbb{E}(Y_i(0))\mathbb{E}(Y_i(0) | f(X_i) = 0) \right\} \right]
\end{align*}
\] 

(14)

The details of the derivation are given in Appendix A.6.1.

Suppose now that the ITR correctly assigns individuals on average, i.e., \( \mathbb{E}(Y_i(t) | f(X_i) = t) \geq \mathbb{E}(Y_i(t) | f(X_i) = 1 - t) \) for \( t = 0, 1 \). Under this assumption, the last two terms in the square bracket are positive, i.e.,

\[
\mathbb{E}(Y_i^2(t) | f(X_i) = t) - \mathbb{E}(Y_i(t))\mathbb{E}(Y_i(t) | f(X_i) = t) \geq \mathbb{V}(Y_i(t) | f(X_i) = t)
\]

for \( t = 0, 1 \). Hence, the only term that is possibly negative in equation (14) is the third term in the square bracket. This suggests that the *ex-post* evaluation is more efficient than *ex-ante* evaluation if this term is sufficiently small.

Unfortunately, it is difficult to determine the sign of this variance difference in generality. One reason for this difficulty is that the proposed *ex-post* evaluation estimator \( \hat{\tau}_f \) in equation (2) is not invariant to a constant shift of the outcome variable due to the fact that \( p_f \) is estimated. That is, adding a constant \( \delta \) to \( Y \) will change the value of \( \hat{\tau}_f \). Although this does not change the unbiasedness of \( \hat{\tau}_f \), it does alter the variance shown in Theorem 1. Specifically, the variance will
have an additional term:

$$2p_f(1 - p_f) \left[ \delta^2 + \{(1 - p_f)\mathbb{E}(Y_i(1) + Y_i(0) \mid f(X_i) = 1) + p_f\mathbb{E}(Y_i(1) + Y_i(0) \mid f(X_i) = 0)\} \delta \right]$$

It is natural to choose the value of $\delta$ to minimize this extra term of the variance, which yields the following optimal value,

$$\delta^* = -\frac{1}{2} \{(1 - p_f)\mathbb{E}(Y_i(1) + Y_i(0) \mid f(X_i) = 1) + p_f\mathbb{E}(Y_i(1) + Y_i(0) \mid f(X_i) = 0)\}$$

(15)

Roughly speaking, the optimal value of $\delta$ balances the two potential outcomes around zero after a constant shift, i.e., $\frac{1}{n} \sum_{i=1}^{n} \{(Y_i(1) + \delta^*) + (Y_i(0) + \delta^*)\}/2 \approx 0$.

Now, for simplicity, assume that $\mathbb{E}(Y_i(1) + Y_i(0) \mid f(X_i) = 1) = \mathbb{E}(Y_i(1) + Y_i(0) \mid f(X_i) = 0) = 0$. This guarantees that the optimal choice of $\delta$ is zero and hence no adjustment in variance is necessary. Under this assumption, we can bound equation (14) from below as follows (see Appendix A.6.2 for details),

$$\mathbb{V}(\hat{\tau}_f) - \mathbb{V}(\hat{\tau}_f) = \frac{2n}{(n-1)^2} \left[ p_f^2\mathbb{V}(Y_i(1)) + (1 - p_f)^2\mathbb{V}(Y_i(0)) + 2p_f^2\mathbb{V}(Y_i(1) \mid f(X_i) = 1) + 2(1 - p_f)^2\mathbb{V}(Y_i(0) \mid f(X_i) = 0) \\
+2p_f(1 - p_f) \left[ (1 - p_f)\mathbb{E}(Y_i(0) \mid f(X_i) = 0) \right]^2 + p_f\left[ \mathbb{E}(Y_i(1) \mid f(X_i) = 1) \right]^2 \right] \geq 0$$

This implies that under this simplifying assumption the ex-post evaluation is more efficient than the ex-ante evaluation. Thus, our analysis suggests that the ex-post evaluation may result in a smaller variance than the ex-ante evaluation.

3 A Simulation Study

We conduct a simulation study to examine the finite sample performance of the proposed methodology. We show that the empirical coverage probability of the confidence interval based on the proposed variance converges quickly to its nominal rate. We also find that as expected the bias is minimal even when the proposed estimator is not unbiased and the variance bounds are tight.

3.1 Data Generation Process

We base our data generating process (DGP) on the one used in the 2017 Atlantic Causal inference Conference (ACIC) Data Analysis Challenge (see Hahn, Dorie and Murray 2018 for details). The
focus of this competition was the estimation and inference for the conditional average treatment effect in observational studies. A total of 8 covariates $X$ are taken from the Infant Health and Development Program [Brooks-Gunn, Liaw and Klebanov [1992], which originally had 58 covariates and $n = 4,302$ observations. In our simulation, we assume that the population distribution of covariates equals the empirical distribution based on this data set. Therefore, we obtain each simulation sample via bootstrap. We vary the sample size by setting it to either 100, 500, or 2,000.

We use the same outcome model as the one used in the competition,

$$
\mathbb{E}(Y_i(t) \mid X_i) = \mu(X_i) + \tau(X_i)t
$$

(16)

where

$$
\pi(x) = \frac{1}{1 + e^{3(x_1+x_{43}+0.3(x_{10}-1))-1}}
$$

$$
\mu(x) = -\sin(\Phi(\pi(x))) + x_{43}
$$

$$
\tau(x) = \xi(x_3x_{24} + (x_{14} - 1) - (x_{15} - 1))
$$

with $\Phi(\cdot)$ representing the standard Normal CDF and $x_j$ indicating a specific covariate in the data set (see Hahn, Dorie and Murray [2018]). One important difference from the competition is that we assume a complete randomized experiment whereas the original DGP used the treatment assignment mechanism as a function of covariates to emulate an observational study. As in the original competition, we focus on two scenarios regarding the treatment effect size by setting $\xi$ equal to 2 ("high") and 1/3 ("low"). Although the original DGP included four different types of errors, we focus on the independently, and identically distributed $\sigma(X_i)\epsilon_i$ where $\sigma(x) = 0.25\sqrt{\mathbb{V}(\mu(x) + \pi(x)\tau(x))}$ and $\epsilon_i \sim \mathcal{N}(0, 1)$.

To compute the true value of our causal quantities of interest, we use the outcome model specified in equation (16) and evaluate each quantity in the entire original data set. For example, we compute the PAPE as,

$$
\tau_f = \frac{1}{n} \sum_{i=1}^{n} \{ \mathbb{E}(Y_i(f(X_i)) \mid X_i) - p_f \mathbb{E}(Y_i(1) \mid X_i) - (1 - p_f) \mathbb{E}(Y_i(0) \mid X_i) \}
$$

where $p_f = \frac{1}{n} \sum_{i=1}^{n} f(X_i)/n$. This computation gives the true value in our simulation setting because we assume the population distribution of covariates is equal to the empirical distribution of the original data set.
For illustration, we evaluate the Bayesian Additive Regression Trees (BART) (see Chipman et al., 2010; Hill, 2011; Hahn, Murray and Carvalho, 2017), which had the best overall performance in the original competition. We also compare this model with two other popular methods: Causal Forest, which is a variant of random forest designed specifically for the estimation of heterogeneous causal effects (Wager and Athey, 2018) as well as the LASSO, which includes all main effect terms and two-way interaction effect terms between the treatment and all covariates (Tibshirani, 1996). All three models are trained on the original data from the 2017 ACIC Data Challenge. The number of trees were tuned through the 5-fold cross validation for BART and Causal Forest. The regularization parameter was tuned similarly for LASSO. All models were cross-validated on the PAPE metric. For implementation, we use R 3.4.2 with the following packages: bartMachine (version 1.4.2) for BART, grf (version 0.10.2) for Causal Forest, and glmnet (version 2.0.13) for LASSO. Once the models are trained, then an ITR is derived based on the magnitude of the estimated conditional average treatment effect \( \tau(x) \) under each model, i.e., \( f(X_i) = 1\{\tau(X_i) > 0\} \).

### 3.2 Results

Table 1 presents the bias and standard deviation of each estimator as well as the coverage probability of its 95% confidence intervals based on the normal approximation. They are based on 1,000 Monte Carlo trials following the procedure described above. The results are shown separately for two scenarios: high and low treatment effects. Under each scenario, we use three different sample sizes. We first estimate the PAPE for BART \( \tau_f \) without a budget constraint. We also estimate the PAPE with a budget constraint of 20% as the maximal proportion of treated units, \( \tau_f(c_{0.2}) \). Finally, we estimate the AUPEC for BART \( \Gamma_f \). In addition, we compare the performance of BART with the other methods by computing the difference in the PAPE or PAPD between BART and Causal Forest (\( \Delta(f, g) \)), and between BART and LASSO (\( \Delta(f, h) \)). We find that under both scenarios and across sample sizes, the bias of our estimator is small. Moreover, the coverage rate of 95% confidence intervals is close to their nominal rate even when the sample size is quite small. Although we can only bound the variance when estimating the PAPD between two ITRs (i.e., \( \Delta_{0.2}(f, g) \) and \( \Delta_{0.2}(f, h) \)), the coverage stay close to 95% as we empirically observe the bounded covariance term to have a small effect on the entire variance.

We next compare the relative efficiency between the \textit{ex-ante} and \textit{ex-post} experimental evalua-
Table 1: The Results of the Simulation Study. The table presents the bias and standard deviation of each estimator as well as the coverage of its 95% confidence intervals under the “Low treatment effect” and “High treatment effect” scenarios. The first three estimators shown here are for BART \( \hat{\tau}_f \): Population Average Prescription effect (PAPE; \( \hat{\tau}_f \)), PAPE with a budget constraint of 20% treatment proportion (\( \hat{\tau}_f(c_{0.2}) \)), Area Under the Prescriptive Effect Curve (AUPEC; \( \hat{\Gamma}_f \)). We also present the results for the difference in the PAPE between BART and Causal Forest \( g \) (\( \hat{\Delta}_{0.2}(f, g) \)) and between BART and LASSO \( h \) (\( \hat{\Delta}_{0.2}(f, h) \)) under the budget constraint.

The simulation data we use for the ex-ante evaluation are identical to those used for the ex-post evaluation so that we can make a fair comparison. We assign half of the sample to the ITR and the other half to the random treatment rule, i.e., \( n_f = n_r = n/2 \). Within the random treatment rule arm, the probability of receiving the treatment is 50%, which is identical to the treatment assignment probability for the ex-post evaluation, i.e., \( n_{r1}/n_r = n_{r0}/n_r = n_1/n = n_0/n = 1/2 \).

Figure 2 presents the result of this comparison for BART by plotting the standard deviation of the PAPE estimator for the ex-ante evaluation (horizontal axis) against that for the ex-post evaluation (vertical axis). We do not present the results for Causal Forest and LASSO as they are sufficiently similar. For both low (red line with solid circles) and high (blue line with solid squares) treatment effect scenarios, the ex-post evaluation estimator is substantially more efficient.
Figure 2: Comparison of Ex-Post and Ex-ante PAPE Estimation for the Individualized Treatment Rule based on BART. The standard deviation of the PAPE estimator for the ex-ante evaluation (horizontal axis) is plotted against that for the ex-post evaluation (vertical axis). Two lines represent different scenarios (low and high treatment effect), and each node represents a different sample size.

than the ex-ante evaluation estimator. This finding is consistent with the analytical result derived under a set of simplifying assumptions in Section 2.6.

4 An Empirical Application

We apply the proposed methodology to the data from the Tennessee’s Student/Teacher Achievement Ratio (STAR) project, which was a four-year longitudinal study experimentally evaluating the impacts of class size in early education on various outcomes [Mosteller, 1995]. As shown below, we find that in this specific application Causal Forest outperforms BART and LASSO when there is a budget constraint.

4.1 Data and Setup

The STAR project randomly assigned over 7,000 students across 79 schools to three different groups: small class (13 to 17 students), regular class (22 to 25 students), and regular class with a full-time teacher’s aid. The experiment began when students entered kindergarten and continued through third grade. To create a binary treatment, we focus on the first two groups: small class and regular class without an aid. The treatment effect heterogeneity is important here because
reducing class size is costly, requiring additional teachers and classrooms. Policy makers who face a budget constraint may be interested in finding out which groups of students benefit most from a small class size so that the priority can be given to those students.

We use a total of 10 pre-treatment covariates $\mathbf{X}_i$ that include four demographic characteristics of students (gender, race, birth month, birth year) and six school characteristics (urban/rural, enrollment size, grade range, number of students on free lunch, number of students on school buses, and percentage of white students). Our treatment variable is the class size to which they were assigned at kindergarten: small class $T_i = 1$ and regular class without an aid $T_i = 0$. For the outcome variables $Y_i$, we use three standardized test scores measured at third grade: SAT math, reading, and writing scores.

The resulting data set has a total of 1,911 observations. We randomly select approximately 70% of the sample (i.e., 1,338 observations) as the training data and the reminder of the sample (i.e., 573 observations) as the evaluation data. We train the same three machine learning models as the ones used in our simulation study. For Causal Forest, we set `tune.parameters = TRUE`. For BART, tuning was done on the number of trees. For LASSO, we tuned the regularization parameter. All tuning was done through the 5-fold cross validation procedure on the training set using the PAPE as the evaluation metric. We then create an ITR as $1\{\hat{\tau}(x) > 0\}$ where $\hat{\tau}(x)$ is the estimated conditional average treatment effect obtained from each fitted model. We will evaluate these ITRs using the evaluation sample.

4.2 Results

The upper panel of Table 2 presents the estimated PAPE for the ITRs based on BART, Causal Forest, and LASSO without a budget constraint. We find that without a budget constraint, none of the ITRs based on the machine learning methods significantly improves upon the random treatment rule with two exceptions. The ITR based on Causal Forest performs worse than the random treatment rule for the SAT reading score by more than 19 points (with a standard error of 4.4 points). In addition, the ITR based on LASSO performs worse for the SAT math score by about 16 points (with a standard error of 4.7 points) relative to the random treatment rule.

The results change substantially when we impose a budget constraint. The lower panel of Table 2 presents the results with a budget constraint where the maximum proportion of treated
Table 2: The Estimated Population Average Prescription Effect (PAPE) for BART, Causal Forest, and LASSO with and without a Budget Constraint. For each of the three outcomes, the point estimate, the standard error, and the proportion treated are shown. The budget constraint considered here implies that the maximum proportion treated is 20%.

Table 3 directly compares these three ITRs based on Causal Forest, BART, and LASSO by estimating the Population Average Prescriptive Effect Difference (PAPD) under the same budget constraint as above. Causal Forest statistically significantly outperforms BART and LASSO in
essentially all cases (the exception is SAT writing for BART but its 95% confidence interval only slightly overlaps with zero). Lastly, the difference between BART and LASSO is statistically significant for SAT math and writing scores.

Finally, Figure 3 presents the estimated PAPE (solid red line) across a range of budget constraints with pointwise 95% confidence intervals. The area between this line and the black horizontal line at zero corresponds to the Area Under the Prescriptive Effect Curve (AUPEC) (see Figure A1 in Appendix A.7 for the plots showing the corresponding estimated Prescriptive Effect Curves). The results are shown for the ITRs based on BART (left column), Causal Forest (middle column), and LASSO (right column) and for each test score (rows). In each plot, the horizontal axis represents the budget constraint as the maximum proportion treated, and the point estimate and standard error of the AUPEC are shown.

Across three test scores, both BART and Causal Forest identify students who benefit positively from small class sizes when the maximum proportion treated is relatively small. In contrast, LASSO has a difficulty in finding these individuals. As the budget constraint is relaxed, the ITRs based on BART and Causal Forest yields the PAPE similar to the one under the random assignment rule. This suggests that they are “over-treating” students, meaning that those who do not necessarily benefit from small class are also treated when little or no budget constraint is imposed.

5 Concluding Remarks

As the application of individualized treatment rules (ITRs) becomes more widespread in a variety of fields, a rigorous performance evaluation of ITRs becomes essential before policy makers deploy them in a target population. We believe that the inferential approach proposed in this paper provides a robust and widely applicable tool to experimentally evaluate the efficacy of ITRs. Furthermore, we provide evidence that ex-post evaluation of ITRs is more efficient than ex-ante evaluation. This opens up opportunities to utilize the existing randomized controlled trial data for the efficient evaluation of ITRs before they are administered in the real world. In addition, although we do not focus on the estimation of ITRs in this paper, the proposed evaluation metrics can be used to tune hyper-parameters when cross validating machine learning algorithms as done in our empirical application. In future research, we plan to consider the extensions of the
Figure 3: Estimated Area Under the Prescriptive Effect Curve (AUPEC). A solid red line in each plot represents the Population Average Prescriptive Effect (PAPE) across a range of budget constraint (horizontal axis) with pointwise 95% confidence interval. The area between this line and the black horizontal line at zero corresponds to the AUPEC. The results are presented for the individualized treatment rules based on BART (left column), Causal Forest (middle column), and LASSO (right column), whereas each row presents the results for a different outcome.
proposed methodology to other settings, including non-binary treatments, dynamic treatments, and treatment allocations in the presence of interference between units.

References


Hahn, P Richard, Jared Murray and Carlos M Carvalho. 2017. “Bayesian regression tree models for causal inference: regularization, confounding, and heterogeneous effects.”.


A Supplementary Appendix

A.1 Proof of Theorem 1

To prove Theorem 1, we first consider the sample average prescription effect (SAPE),

\[ \tau_f^s = \frac{1}{n} \sum_{i=1}^{n} \{ Y_i(f(X_i)) - \hat{p}_f Y_i(1) - (1 - \hat{p}_f) Y_i(0) \}. \]  

(A1)

and its unbiased estimator,

\[ \hat{\tau}_f^s = \frac{1}{n_1} \sum_{i=1}^{n} Y_i T_i f(X_i) + \frac{1}{n_0} \sum_{i=1}^{n} Y_i (1 - T_i) (1 - f(X_i)) - \hat{p}_f \frac{n}{n_1} \sum_{i=1}^{n} Y_i T_i - \frac{1 - \hat{p}_f}{n_0} \sum_{i=1}^{n} Y_i (1 - T_i) \]  

(A2)

This estimator differs from the estimator of the PAPE by a small factor, i.e., \( \hat{\tau}_f^s = (n - 1)/n \tau_f \).

The following lemma derives the bias and variance in the finite sample framework.

**Lemma 1 (Bias and Variance of the Estimator for the SAPE)** Under Assumptions 2, 1, and 3, the bias and variance of the estimator of the PAPE given in equation (A2) for estimating the SAPE defined in equation (A1) are given by,

\[ \mathbb{E}(\hat{\tau}_f^s | \{Y_i(1), Y_i(0), X_i\}_{i=1}^{n}) = \tau_f^s \]

\[ \mathbb{V}(\hat{\tau}_f^s | \{Y_i(1), Y_i(0), X_i\}_{i=1}^{n}) = \frac{1}{n} \left( \frac{n_0}{n_1} S_{f1}^2 + \frac{n_1}{n_0} S_{f0}^2 + 2 S_{f01} \right) \]

where

\[ S_{f01} = \frac{1}{n-1} \sum_{i=1}^{n} (Y^*_i(0) - \overline{Y}^*_0)(Y^*_i(1) - \overline{Y}^*_1) \].

**Proof** For the sake of notational simplicity, let \( \mathcal{O}_n = \{Y_i(1), Y_i(0), X_i\}_{i=1}^{n} \). Then, we take the expectation with respect to the experimental treatment assignment, i.e., \( T_i \),

\[ \mathbb{E}(\hat{\tau}_f^s | \mathcal{O}_n) = \mathbb{E} \left( \frac{1}{n_1} \sum_{i=1}^{n} f(X_i) T_i Y_i(1) + \frac{1}{n_0} \sum_{i=1}^{n} (1 - f(X_i))(1 - T_i) Y_i(0) \right) \]

\[ - \frac{\hat{p}_f}{n_1} \sum_{i=1}^{n} T_i Y_i(1) - \frac{1 - \hat{p}_f}{n_0} \sum_{i=1}^{n} (1 - T_i) Y_i(0) \right) \]

\[ = \frac{1}{n} \sum_{i=1}^{n} Y_i(1) f(X_i) + \frac{1}{n} \sum_{i=1}^{n} Y_i(0)(1 - f(X_i)) - \frac{\hat{p}_f}{n} \sum_{i=1}^{n} Y_i(1) - \frac{1 - \hat{p}_f}{n} \sum_{i=1}^{n} Y_i(0) \]

\[ = \tau_f^s \]

To derive the variance, we first rewrite the proposed estimator as,

\[ \hat{\tau}_f^s = \tau_f^s + \sum_{i=1}^{n} D_i (f(X_i) - \hat{p}_f) \left( \frac{Y_i(1)}{n_1} + \frac{Y_i(0)}{n_0} \right) \]
where \( D_i = T_i - n_1/n \). Thus, noting \( E(D_i) = 0, E(D_i^2) = n_0 n_1 / n^2 \), and \( E(D_i D_j) = -n_0 n_1 / \{n^2(n-1)\} \) for \( i \neq j \), after some algebra, we have,

\[
\nabla(\hat{\tau}_f \mid O_n) = \nabla(\hat{\tau}_f - \tau_f \mid O_n)
\]

\[
= \mathbb{E} \left[ \sum_{i=1}^{n} D_i \left( \frac{Y_i^*(1)}{n_1} + \frac{Y_i^*(0)}{n_0} \right) \right] \bigg| O_n = \frac{1}{n} \left( n_0 S_{f1}^2 + \frac{n_1}{n_0} S_{f0}^2 + 2S_{f01} \right)
\]

Now, we prove Theorem 1. Using Lemma 1 and the law of iterated expectation, we have,

\[
\mathbb{E}(\hat{\tau}_f) = \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \{ Y_i(f(X_i)) - \hat{p}_f Y_i(1) - (1 - \hat{p}_f) Y_i(0) \} \right]
\]

We compute the following expectation for \( t = 0, 1 \),

\[
\mathbb{E} \left[ \sum_{i=1}^{n} \hat{p}_f Y_i(t) \right] = \mathbb{E} \left[ \sum_{i=1}^{n} \frac{\sum_{j=1}^{n} f(X_j)}{n} Y_i(t) \right]
\]

\[
= \frac{1}{n} \mathbb{E} \left[ \sum_{i=1}^{n} f(X_i) Y_i(t) + \sum_{j=1}^{n} \sum_{i \neq j} f(X_j) Y_i(t) \right]
\]

\[
= \mathbb{E} \{ f(X_i) Y_i(t) \} + (n-1)p_f \mathbb{E}(Y_i(t)).
\]

Putting them together yields the following bias expression,

\[
\mathbb{E}(\hat{\tau}_f) = \mathbb{E} \left[ \{ Y_i(f(X_i)) - \frac{1}{n} f(X_i) \{ Y_i(1) - Y_i(0) \} \} - \frac{n-1}{n} p_f \{ Y_i(1) - Y_i(0) \} - Y_i(0) \right]
\]

\[
= \tau_f - \frac{1}{n} \mathbb{E} \left[ \{ f(X_i) Y_i(1) - (1 - f(X_i)) Y_i(0) \} - \{ p_f Y_i(1) - (1 - p_f) Y_i(0) \} \right]
\]

\[
= \tau_f - \frac{1}{n} \text{Cov}(f(X_i), Y_i(1) - Y_i(0))
\]

We can further rewrite the bias as,

\[
- \frac{1}{n} \text{Cov}(f(X_i), Y_i(1) - Y_i(0))
\]

\[
= \frac{1}{n} p_f \{ \mathbb{E}(Y_i(1) - Y_i(0) \mid f(X_i) = 1) - \mathbb{E}(Y_i(1) - Y_i(0)) \}
\]

\[
= \frac{1}{n} p_f (1 - p_f) \{ \mathbb{E}(Y_i(1) - Y_i(0) \mid f(X_i) = 1) - \mathbb{E}(Y_i(1) - Y_i(0) \mid f(X_i) = 0) \}
\]

\[
= \frac{1}{n} \tau_f.
\]

(A3)

This implies that the estimator for the PAPE is unbiased, i.e., \( \mathbb{E}(\hat{\tau}_f) = \tau_f \).

To derive the variance, Lemma 1 implies,

\[
\nabla(\hat{\tau}_f) = \frac{n^2}{(n-1)^2} \left[ \nabla \left( \frac{1}{n} \sum_{i=1}^{n} \{ Y_i^*(1) - Y_i^*(0) \} \right) \right] + \mathbb{E} \left\{ \frac{1}{n} \left( \frac{n_0}{n_1} S_{f1}^2 + \frac{n_1}{n_0} S_{f0}^2 + 2S_{f01} \right) \right\}
\]

(A4)
Applying Lemma 1 of Nadeau and Bengio (2000) to the first term within the square brackets yields,

\[ \mathbb{V} \left( \frac{1}{n} \sum_{i=1}^{n} \{ Y_i^* - Y_i^* (0) \} \right) = \text{Cov} (Y_i^* (1) - Y_i^* (0), Y_j^* (1) - Y_j^* (0)) + \frac{1}{n} \mathbb{E}(S_f^2 + S_p^2 - 2S_{fp}) \quad (A5) \]

where \( i \neq j \). Focusing on the covariance term, we have,

\[
\text{Cov} (Y_i^* (1) - Y_i^* (0), Y_j^* (1) - Y_j^* (0))
\]

\[
= \text{Cov} \left( \left\{ f(X_i) - \frac{1}{n} \sum_{i'=1}^{n} f(X_{i'}) \right\} (Y_i (1) - Y_i (0)), \left\{ f(X_j) - \frac{1}{n} \sum_{j'=1}^{n} f(X_{j'}) \right\} (Y_j (1) - Y_j (0)) \right)
\]

\[
= -2 \text{Cov} \left( \frac{n-1}{n} f(X_i) (Y_i (1) - Y_i (0)), \frac{1}{n} f(X_i) (Y_j (1) - Y_j (0)) \right)
\]

\[
+ \sum_{i' \neq i, j} \text{Cov} \left( \frac{1}{n} f(X_{i'}) (Y_i (1) - Y_i (0)), \frac{1}{n} f(X_{j'}) (Y_j (1) - Y_j (0)) \right)
\]

\[
+ 2 \sum_{i' \neq i, j} \text{Cov} \left( \frac{1}{n} f(X_j) (Y_i (1) - Y_i (0)), \frac{1}{n} f(X_{i'}) (Y_j (1) - Y_j (0)) \right)
\]

\[
+ \text{Cov} \left( \frac{1}{n} f(X_j) (Y_i (1) - Y_i (0)), \frac{1}{n} f(X_i) (Y_j (1) - Y_j (0)) \right)
\]

\[
= - \frac{2(n-1)\tau}{n^2} \text{Cov} (f(X_i), f(X_j) (Y_i (1) - Y_i (0))) + \frac{(n-2)\tau^2}{n^2} \mathbb{V} (f(X_i))
\]

\[
+ \frac{2(n-2)\tau}{n^2} pf \text{Cov} (f(X_i), Y_i (1) - Y_i (0))
\]

\[
+ \frac{1}{n^2} \{ \text{Cov}^2 (f(X_i), Y_i (1) - Y_i (0)) + 2 pf \tau \text{Cov} (f(X_i), Y_i (1) - Y_i (0)) \}
\]

\[
= \frac{1}{n^2} \text{Cov}^2 (f(X_i), Y_i (1) - Y_i (0)) + \frac{(n-2)\tau^2}{n^2} pf (1 - pf)
\]

\[
+ \frac{2(n-1)\tau}{n^2} \text{Cov} (f(X_i), (pf - f(X_i))(Y_i (1) - Y_i (0)))
\]

\[
= \frac{1}{n^2} \{ \tau_f^2 + (n-2) pf (1 - pf) \tau^2 + 2(n-1) \tau \{ + pf \tau_f - (1 - pf) \mathbb{E}(Y_i (f(X_i)) - Y_i (0)) \}
\]

\[
= \frac{1}{n^2} \{ \tau_f^2 + (n-2) pf (1 - pf) \tau^2 + 2(n-1) \tau \{ + pf (2pf - 1) - (1 - pf) pf \tau \}
\]

\[
= \frac{1}{n^2} \{ \tau_f^2 - npf (1 - pf) \tau^2 + 2(n-1)(2pf - 1) \tau_f \}
\]

where the third equality follows from the formula for the covariance of products of two random variables (Bohnstedt and Goldberger 1969). Finally, combining this result with equations (A4) and (A5) yields,

\[
\mathbb{V} (\hat{\tau_f}) = \frac{n^2}{(n-1)^2} \left[ \frac{E(S_{f1}^2)}{n_1} + \frac{E(S_{p0}^2)}{n_0} + \frac{1}{n^2} \{ \tau_f^2 - npf (1 - pf) \tau^2 + 2(n-1)(2pf - 1) \tau_f \} \right]
\]

\[ \square \]
A.2 Proof of Theorem 2

We begin by deriving the variance expression. The derivation proceeds in the same fashion as the one for Theorem 1. The only non-trivial change is the derivation of the covariance term, which we detail below. First, we note that

\[
\Pr(f(X_i, \hat{c}_p) = 1) = \int_{-\infty}^{\infty} \Pr(f(X_i, c) = 1 \mid \hat{c}_p = c) P(\hat{c}_p = c) dc
\]

\[
= \int_{-\infty}^{\infty} \frac{|np|}{n} P(\hat{c}_p = c) dc
\]

where the second equality follows from the fact that once conditioned on \( \hat{c}_p = c \), exactly \(|np|\) out of \( n \) units will be assigned to the treatment condition. Given this result, we can compute the covariance as follows,

\[
\text{Cov}(\tilde{Y}_i(1) - \bar{Y}_i(0), \tilde{Y}_j(1) - \bar{Y}_j(0)) = \text{Cov}((f(X_i, \hat{c}_p) - p)(Y_i(1) - Y_i(0)), (f(X_j, \hat{c}_p) - p)(Y_j(1) - Y_j(0)))
\]

\[
= \text{Cov}(f(X_i, \hat{c}_p)(Y_i(1) - Y_i(0)), f(X_j, \hat{c}_p)(Y_j(1) - Y_j(0)))
\]

\[
- 2p \text{Cov}((Y_i(1) - Y_i(0)), f(X_j, \hat{c}_p)(Y_j(1) - Y_j(0)))
\]

\[
= \frac{|np|(|np| - n)}{n^2(n - 1)} \kappa_1(X_i, \hat{c}_p)^2 + \frac{2p|np|(n - |np|)}{n^2(n - 1)} (\kappa_1(X_i, \hat{c}_p)^2 - \kappa_1(X_i, \hat{c}_p)\kappa_0(X_i, \hat{c}_p))
\]

\[
= (2p - 1) \frac{|np|(n - |np|)}{n^2(n - 1)} \kappa_1(X_i, \hat{c}_p)^2 - 2p \frac{|np|(n - |np|)}{n^2(n - 1)} \kappa_1(X_i, \hat{c}_p)\kappa_0(X_i, \hat{c}_p)
\]

\[
= |np|(n - |np|) \{(2p - 1)\kappa_1(X_i, \hat{c}_p)^2 - 2p\kappa_1(X_i, \hat{c}_p)\kappa_0(X_i, \hat{c}_p)\}
\]

Combining this covariance result with the expression for the marginal variances yields the desired variance expression for \( \hat{\tau}_f(\hat{c}_p) \).

Next, we derive the upper bound of bias. Using the same technique as the proof of Theorem 1, we can rewrite the expectation of the proposed estimator as,

\[
\mathbb{E}(\hat{\tau}_f(c_p)) = \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \{ Y_i (f(X_i, \hat{c}_p)) - pY_i(1) - (1 - p)Y_i(0) \} \right]
\]

Now, define \( F(c) = \mathbb{P}(s(X_i) \leq c) \). Without loss of generality, assume \( \hat{c}_p > c_p \) (If this is not the case, we simply switch the upper and lower limits of the integrals below). Then, the bias of the estimator is given by,

\[
|\mathbb{E}(\hat{\tau}_f(\hat{c}_p)) - \tau_f(c_p)| = \left| \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} \{ Y_i (f(X_i, \hat{c}_p)) - Y_i (f(X_i, c_p)) \} \right] \right|
\]

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The derivation of the variance expression in Theorem 3 proceeds in the same fashion as Theorem 1. A.3 Proof of Theorem 3

Let \( \hat{c}_p \) and \( F(\hat{c}_p) \) be the \( np \)th order statistic of \( n \) independent uniform random variables, and thus follows the Beta distribution with the shape and scale parameters equal to \( np \) and \( n - np + 1 \), respectively. Therefore, we have,

\[
\mathbb{P}(|F(\hat{c}_p) - p| > \epsilon) = 1 - B(p + \epsilon, [np], n - [np] + 1) + B(p - \epsilon, [np], n - [np] + 1)
\]

(A6)

where \( B(\epsilon, \alpha, \beta) \) is the incomplete beta function, i.e.,

\[
B(\epsilon, \alpha, \beta) = \int_0^\epsilon t^{\alpha-1}(1-t)^{\beta-1}dt
\]

Combining with the result above, the desired result follows.

A.3 Proof of Theorem 3

The derivation of the variance expression in Theorem 3 proceeds in the same fashion as Theorem 1 (see Appendix A.2) with the only non-trivial change being the calculation of the covariance term. Note \( \text{Pr}(f(X_i, \hat{c}_{k/n}) = 1) = k/n \) for \( t = 0, 1 \) and \( n_f = Z \sim \text{Binom}(n, p_f) \). Then, we have:

\[
\text{Cov}(Y_i^+(1) - Y_i^+(0), Y_j^+(1) - Y_j^+(0))
\]

\[=
\begin{align*}
\mathbb{E} \left[ \left( \sum_{k=1}^{n_f} f(X_i, \hat{c}_{k/n}) + \sum_{k=n_f+1}^n f(X_i, \hat{c}_{n_f/n}) \right) \left( \sum_{k=1}^{n_f} f(X_j, \hat{c}_{k/n}) + \sum_{k=n_f+1}^n f(X_j, \hat{c}_{n_f/n}) \right) - \frac{1}{2} \right] (Y_i(1) - Y_i(0)),
\end{align*}
\]

\[=
\begin{align*}
\mathbb{E} \left[ \left( \sum_{k=1}^{Z} f(X_i, \hat{c}_{k/n}) + \sum_{k=Z+1}^n f(X_i, \hat{c}_{Z/n}) \right) \left( \sum_{k=1}^{Z} f(X_j, \hat{c}_{k/n}) + \sum_{k=Z+1}^n f(X_j, \hat{c}_{Z/n}) \right) - \frac{1}{2} \right] (Y_i(1) - Y_i(0)) | Z)
\end{align*}
\]

\[+
\begin{align*}
\mathbb{E} \left[ \left( \sum_{k=1}^{Z} f(X_i, \hat{c}_{k/n}) + \sum_{k=Z+1}^n f(X_i, \hat{c}_{Z/n}) \right) \left( \sum_{k=1}^{Z} f(X_j, \hat{c}_{k/n}) + \sum_{k=Z+1}^n f(X_j, \hat{c}_{Z/n}) \right) - \frac{1}{2} \right] (Y_i(1) - Y_i(0)) | Z)
\]

\[=
\begin{align*}
\mathbb{E} \left[- \frac{1}{n} \left\{ \sum_{k=1}^{Z} \frac{k(n-k)}{n^2(n-1)} \kappa_1(X_i, \hat{c}_{k/n}) \kappa_0(X_i, \hat{c}_{k/n}) + \frac{Z(n-Z)^2}{n^2(n-1)} \kappa_1(X_i, \hat{c}_{Z/n}) \kappa_0(X_i, \hat{c}_{Z/n}) \right\}
\right]
\end{align*}
\]

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\begin{equation*}
- \frac{2}{n^4(n-1)} \sum_{k=1}^{Z-1} \sum_{k'=k+1}^{Z} k(n-k') \kappa_1(\mathbf{X}_i, \hat{c}_{k/n}) \kappa_1(\mathbf{X}_i, \hat{c}_{k'/n}) \\
- \frac{Z^2(n-Z)^2}{n^4(n-1)} \kappa_1(\mathbf{X}_i, \hat{c}_{Z/n})^2 - \frac{2(n-Z)^2}{n^4(n-1)} \sum_{k=1}^{Z} k \kappa_1(\mathbf{X}_i, \hat{c}_{Z/n}) \kappa_1(\mathbf{X}_i, \hat{c}_{k/n}) \\
+ \frac{1}{n^2} \sum_{k=1}^{Z} k(n-k) \kappa_1(\mathbf{X}_i, \hat{c}_{k/n})^2 \Bigg) + \nabla \left( \sum_{i=1}^{n} \frac{i}{n} \kappa_1(\mathbf{X}_i, \hat{c}_{i/n}) + \frac{(n-Z)Z}{n} \kappa_1(\mathbf{X}_i, \hat{c}_{Z/n}) \right)
\end{equation*}

where the last equality is based on the results from Appendix A.2.

For the bias, we can rewrite \( \Gamma_f \) as,
\begin{equation*}
\Gamma_f = \int_0^{p_f} \mathbb{E}\{Y_i(f(\mathbf{X}_i, c_p))\} \, dp + (1 - p_f) \mathbb{E}\{Y_i(f(\mathbf{X}_i, \hat{c}_{p_f}))\}
\end{equation*}

and similarly its estimator \( \hat{\Gamma}_f \) as,
\begin{equation*}
\hat{\Gamma}_f = \int_0^{\hat{p}_f} \mathbb{E}\{Y_i(f(\mathbf{X}_i, c_p))\} \, dp + (1 - \hat{p}_f) \mathbb{E}\{Y_i(f(\mathbf{X}_i, \hat{c}_{p_f}))\}
\end{equation*}

Therefore, the bias of the estimator is:
\begin{align*}
\mathbb{E}(\hat{\Gamma}_f) - \Gamma_f & \leq \mathbb{E} \left[ |p_f - \hat{p}_f| \max_{c \in \{\min\{p_f, p_f\}, \max\{p_f, p_f\}\}} \mathbb{E}\{Y_i(f(\mathbf{X}_i, c)) - Y_i(f(\mathbf{X}_i, c_p))\} \right] \\
& \quad + \mathbb{E}\{Y_i(f(\mathbf{X}_i, c_p))\} - \mathbb{E}\{Y_i(f(\mathbf{X}_i, \hat{c}_{p_f}))\} \right] \\
& \leq (\epsilon + 1) \max_{c \in [\hat{c}_{p_f} - \epsilon, \hat{c}_{p_f} + \epsilon]} |\mathbb{E}\{Y_i(f(\mathbf{X}_i, c)) - Y_i(f(\mathbf{X}_i, c_p))\}| \\
& \leq (\epsilon + 1) \epsilon \max_{c \in [\hat{c}_{p_f} - \epsilon, \hat{c}_{p_f} + \epsilon]} |\mathbb{E}(Y_i(1) - Y_i(0) \mid s(\mathbf{X}_i) = c)|
\end{align*}

Now, taking the bound \( \epsilon(1 + \epsilon) \leq 2\epsilon \) for \( 0 \leq \epsilon \leq 1 \) in equation (A6) of Appendix A.2, we have the desired result. \( \square \)

### A.4 Proof of Theorem 4

The proof of the bounds for the bias and variance of the proposed estimator largely follows the proof given in Appendix A.2. The only significant difference is the calculation of the covariance term, which is given below:

\begin{align*}
\text{Cov}(Y_i^*(1) - Y_i^*(0), Y_j^*(1) - Y_j^*(0)) & = \text{Cov} \left( f(\mathbf{X}_i, \hat{c}_{i/p}) - g(\mathbf{X}_i, \hat{c}_{i/p}^g)(Y_i(1) - Y_i(0)), f(\mathbf{X}_j, \hat{c}_{j/p}) - g(\mathbf{X}_j, \hat{c}_{j/p}^g)(Y_j(1) - Y_j(0)) \right) \\
& = \text{Cov}(f(\mathbf{X}_i, \hat{c}_{i/p}^f)(Y_i(1) - Y_i(0)), f(\mathbf{X}_j, \hat{c}_{j/p}^f)(Y_j(1) - Y_j(0))) \\
& \quad + \text{Cov}(g(\mathbf{X}_i, \hat{c}_{i/p}^g)(Y_i(1) - Y_i(0)), g(\mathbf{X}_j, \hat{c}_{j/p}^g)(Y_j(1) - Y_j(0))) \\
& \quad - 2 \text{Cov}(f(\mathbf{X}_i, \hat{c}_{i/p}^f)(Y_i(1) - Y_i(0)), g(\mathbf{X}_j, \hat{c}_{j/p}^g)(Y_j(1) - Y_j(0))) \\
& = \frac{|np|(|np| - n)}{n^2(n-1)} \left( \kappa_1^f(\mathbf{X}_i, \hat{c}_{i/p}^f)^2 + \kappa_1^g(\mathbf{X}_i, \hat{c}_{i/p}^g)^2 \right)
\end{align*}
\(-2 \text{Cov}(f(X_i, \hat{c}_g^p)(Y_i(1) - Y_i(0)), g(X_j, \hat{c}_g^p)(Y_j(1) - Y_j(0)))\).

Since the covariance term \(\text{Cov}(f(X_i, \hat{c}_g^p)(Y_i(1) - Y_i(0)), g(X_j, \hat{c}_g^p)(Y_j(1) - Y_j(0)))\) is unidentifiable without the covariance of the distribution of the scoring functions \(s_f(X)\) and \(s_g(X)\), we derive the bounds by noting that the maximum covariance occurs when the scoring functions of \(f\) and \(g\), i.e., \(s_f(X_i)\) and \(s_g(X_i)\), are perfectly correlated. This observation leads to the following result,

\[
\text{Cov}(Y_i^*(1) - Y_i^*(0), Y_j^*(1) - Y_j^*(0)) \\
\leq \frac{|np|(|np| - n)}{n^2(n - 1)} \left( \kappa_1^f(X_i, \hat{c}_g^p)^2 + \kappa_0^g(X_i, \hat{c}_g^p)^2 \right) + \frac{2|np| \max\{|np|, n - |np|\}}{n^2(n - 1)} \kappa_1^f(X_i, \hat{c}_g^p) \kappa_0^g(X_i, \hat{c}_g^p)
\]

which can then be used to obtain the results of Theorem 3.

\(\Box\)

### A.5 Proof of Theorem 5

The proof proceeds in a manner similar to that of Appendix A.1. We first consider the following estimator,

\[
\hat{\tau}_f^{**} = \frac{1}{n_f} \sum_{i=1}^{n} \left\{ Y_i T_i + Y_i(1 - f(X_i)) \right\} F_i - \frac{1}{n_r} \sum_{i=1}^{n} \left\{ Y_i T_i + Y_i(1 - T_i) \right\}(1 - F_i) \tag{A7}
\]

This estimator differs from the \textit{ex-ante} estimator of the PAPE \(\hat{\tau}_f^a\), by a small factor, i.e., \(\hat{\tau}_f^{**} = (n - 1)/n\hat{\tau}_f^a\). The following lemma derives the bias and variance of this estimator. Using this lemma, the results of Theorem 5 can be obtained immediately.

**Lemma 2 (Bias and Variance of the Naive Estimator)** Under Assumptions 2, 1, and 4, the bias and variance of the estimator given in equation (A7) for estimating the PAPE defined in equation (1) are given by,

\[
\mathbb{E}(\hat{\tau}_f^{**}) = \frac{n - 1}{n} \tau_f \\
\mathbb{V}(\hat{\tau}_f^{**}) = \frac{\mathbb{E}(S_f^2)}{n_f} + \mathbb{E} \left\{ \frac{\hat{p}_f^2 S_f^2}{n_r} + \left( \frac{1 - \hat{p}_f)^2 S_0^2}{n_r} \right) \right\} + \frac{1}{n^2} \left\{ \tau_f^2 - np_f(1 - p_f)\tau_f^2 + 2(n - 1)(2p_f - 1)\tau_f \right\}
\]

**Proof** We first derive the bias expression. First, we take the expectation with respect to \(T_i\),

\[
\mathbb{E} \left[ \frac{1}{n_f} \sum_{i=1}^{n} \left\{ Y_i f(X_i) + Y_i(1 - f(X_i)) \right\} F_i - \frac{1}{n_r} \sum_{i=1}^{n} \left\{ Y_i T_i + Y_i(1 - T_i) \right\}(1 - F_i) \middle| X_i, Y_i(1), Y_i(0), F_i \right] \\
= \frac{1}{n_f} \sum_{i=1}^{n} \left\{ Y_i f(X_i) + Y_i(1 - f(X_i)) \right\} F_i - \frac{1}{n_r} \sum_{i=1}^{n} \left\{ Y_i(1) \frac{\sum_{i=1}^{n} f(X_i)}{n_f} + Y_i(0) \left( 1 - \frac{\sum_{i=1}^{n} f(X_i)}{n_f} \right) \right\} (1 - F_i)
\]

Then we take the expectation with respect to \(F_i\):

\[
\mathbb{E} \left[ \frac{1}{n_f} \sum_{i=1}^{n} \left\{ Y_i f(X_i) + Y_i(1 - f(X_i)) \right\} F_i 
\right]
\]
\[-\frac{1}{n_r} \sum_{i=1}^{n} \left\{ Y_i(1) \sum_{i=1}^{n} f(X_i) - Y_i(0) \left( 1 - \frac{\sum_{i=1}^{n} f(X_i)}{n_f} \right) \right\} (1 - F_i) \mid X_i, Y_i(1), Y_i(0) \]

\[= \frac{1}{n} \sum_{i=1}^{n} Y_i(f(X_i)) - \frac{1}{n_f} \sum_{i=1}^{n} \sum_{j=1}^{n} \mathbb{E} \left[ Y_i(1) f(X_j)(1 - F_i) + Y_i(0) \left( \frac{n_f}{n} - f(X_j) \right) (1 - F_i) \mid X_i, Y_i(1), Y_i(0) \right] \]

\[= \frac{1}{n} \sum_{i=1}^{n} Y_i(f(X_i)) - \frac{1}{n_f} \sum_{i=1}^{n} \sum_{j=1}^{n} \left\{ \frac{n_f n}{n^2} Y_i(1) f(X_j) + Y_i(0) \frac{n_f n}{n^2} (1 - f(X_j)) \right\} \]

\[= \frac{1}{n} \sum_{i=1}^{n} Y_i(f(X_i)) - \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} (Y_i(1) f(X_j) + Y_i(0) (1 - f(X_j))) \]

Finally, we take the expectation over the sampling of \( \{X_i, Y_i(1), Y_i(0)\} \):

\[\mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} Y_i(f(X_i)) - \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \{Y_i(1) f(X_j) + Y_i(0) (1 - f(X_j))\} \right] \]

\[= \mathbb{E} \{Y_i(f(X_i))\} - p_f \mathbb{E}(Y(1)) - (1 - p_f) \mathbb{E}(Y(0)) - \frac{1}{n^2} \sum_{i=1}^{n} \mathbb{E}\{\text{Cov}(Y_i(1), f(X_i)) + \text{Cov}(Y_i(0), 1 - f(X_i))\} \]

\[= \tau_f - \text{Cov}(Y_i(1) - Y_i(0), f(X_i)) \]

\[= \frac{n - 1}{n} \tau_f \]

where the last equality follows from the relation derived in Appendix [A.1].

For the variance expression, we proceed as follows:

\[\mathbb{V}(\tau^*_f) = \mathbb{V} \left\{ \mathbb{E}(\tau^*_f \mid X_i, Y_i(1), Y_i(0), F_i) \right\} + \mathbb{V} \left\{ \mathbb{E}(\tau^*_f \mid X_i, Y_i(1), Y_i(0), F_i) \right\} \]

\[= \mathbb{V} \left[ \frac{1}{n_f} \sum_{i=1}^{n} \left\{ Y_i(1) f(X_i) + Y_i(0) (1 - f(X_i)) \right\} F_i - \frac{1}{n_r} \sum_{i=1}^{n} \left\{ Y_i(1) \hat{p}_f + Y_i(0) (1 - \hat{p}_f) \right\} (1 - F_i) \right] \]

\[+ \mathbb{V} \left\{ \frac{1}{n_f} \sum_{i=1}^{n} \left\{ Y_i T_i + Y_i (1 - T_i) \right\} (1 - F_i) \mid X_i, Y_i(1), Y_i(0), F_i \right\} \]

For the first term, we further use the law of total variance by conditioning on the sample, and use the same proof strategy as the one used Appendix [A.1] by centering \( F_i \) via the transformation \( D_i = F_i - n_f / n \). For the second term, we use the results of [Neyman (1923)] with the following notation,

\[S_t^2 = \frac{1}{n - 1} \sum_{i=1}^{n} (Y_i(t) - \overline{Y(t)})^2, \quad S_{01} = \frac{1}{n - 1} \sum_{i=1}^{n} (Y_i(0) - \overline{Y(0)})(Y_i(1) - \overline{Y(1)}) \]

for \( t = 0, 1 \). Then, the variance becomes,

\[\mathbb{V}(\tau^*_f) = \mathbb{V} \left\{ \frac{1}{n} \sum_{i=1}^{n} D_i \left( \frac{n}{n_f} Y(f(X_i)) + \frac{n}{n_r} \hat{Y}_i \right) \mid X_i, Y_i(1), Y_i(0) \right\} \]

\[+ \mathbb{V} \left\{ \frac{1}{n} \sum_{i=1}^{n} (Y(f(X_i)) - \hat{Y}_i) \right\} + \mathbb{E} \left[ \frac{1}{n_r} \left\{ \hat{p}^2 f n_r S_1^2 + (1 - \hat{p}_f)^2 n_r S_0^2 - 2 \hat{p}_f (1 - \hat{p}_f) S_{01} \right\} \right] \]

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where $\tilde{Y}_i = \hat{p}_f Y_i(1) + (1 - \hat{p}_f) Y_i(0)$.

Following the same analytical strategy as the one in Appendix A.1, we have,

$$
\mathbb{V}(\tau^*_f) = \frac{\mathbb{E}(S^2_f)}{n_f} + \mathbb{E}(S^2_n) + \mathbb{E} \left[ \frac{1}{n_r} \left\{ \hat{p}^2 n_{r0} S^2_1 + \frac{(1 - \hat{p}_f)^2 n_{r1} S^2_0}{n_{r0}} - 2 \hat{p}_f (1 - \hat{p}_f) S_{01} \right\} \right] \\
+ \mathbb{Cov}((f(X_i) - \hat{p}_f Y_i(1)) - (f(X_i) - \hat{p}_f Y_i(0)), (f(X_i) - \hat{p}_f Y_i(1) - (f(X_i) - \hat{p}_f) Y_i(0))
$$

where $S^2_n = \frac{1}{n-1} \sum_{i=1}^{n} (\tilde{Y}_i - \bar{Y})^2$ and the last equality follows from $\mathbb{E}(S^2_n) = \mathbb{E}(\hat{p}_f S^2_1 + (1 - \hat{p}_f^2) S^2_0 + 2 \hat{p}_f (1 - \hat{p}_f) S_{01})$.

\section*{A.6 Details of the Comparison between Ex-ante and Ex-Post Evaluations}

\subsection*{A.6.1 Difference of the Variances}

To compute the difference of the variance, we begin by defining the following,

\begin{align*}
A_i &= \hat{p}_f Y_i(1) - \hat{p}_f Y(1), \quad B_i = (1 - \hat{p}_f) Y_i(0) - (1 - \hat{p}_f) Y(0) \\
C_i &= f(X_i) Y_i(1) - f(X) Y(1), \quad D_i = (1 - f(X)) Y_i(0) - (1 - f(X)) Y(0)
\end{align*}

Then, a simple algebraic manipulation yields,

\begin{align*}
\mathbb{V}(\tau_f) &= \frac{n^2}{(n-1)^2} \mathbb{E} \left( \sum_{i=1}^{n} A_i^2 + C_i^2 - 2 A_i C_i + B_i^2 + D_i^2 - 2 B_i D_i \right) + \xi \\
\mathbb{V}(\tau^*_f) &= \frac{n^2}{(n-1)^2} \mathbb{E} \left( \sum_{i=1}^{n} \frac{A_i^2}{n_{r0}(n-1)} + \frac{B_i^2}{n_{r1}(n-1)} + \frac{C_i^2 + D_i^2 + 2 C_i D_i}{n_f (n-1)} \right) + \xi
\end{align*}

where $\xi = \frac{1}{n} \left\{ \tau_f^2 - n p_f (1 - p_f) \tau^2 + 2(n - 1)(2p_f - 1) \tau_f \right\}$.

Given these expressions, the difference is given by,

\begin{align*}
\mathbb{V}(\tau^*_f) - \mathbb{V}(\tau_f) &= \frac{n^2}{(n-1)^2} \mathbb{E} \left( \sum_{i=1}^{n} \frac{A_i^2 (n_1 - n_0)}{n_0 n_1 (n-1)} + \frac{B_i^2 (n_0 - n_{r1})}{n_{r1} n_0 (n-1)} + \frac{D_i^2 (n_0 - n_f)}{n_f n_0 (n-1)} \\
&\quad + \frac{2 C_i D_i}{n_f (n-1)} + \frac{2 A_i C_i}{n_1 (n-1)} + \frac{2 B_i D_i}{n_0 (n-1)} \right)
\end{align*}

Under the assumption that $n_1 = n_0 = n_f = n_r = n/2$ and $n_{r0} = n_{r1} = n/4$, we have,

\begin{align*}
\mathbb{V}(\tau^*_f) - \mathbb{V}(\tau_f) &= \frac{2n}{(n-1)^2} \mathbb{E} \left( \sum_{i=1}^{n} \frac{A_i^2 + B_i^2}{n-1} + \frac{2 C_i D_i + 2 A_i C_i + 2 B_i D_i}{n-1} \right)
\end{align*}
\[
\begin{align*}
&= \frac{2n}{(n-1)^2} \left[ \mathbb{E} \left\{ p_f^2 s_i^2 + (1 - p_f)^2 s_0^2 \right\} + 2 \text{Cov}(f(X_i)Y_i(1), (1 - f(X_i))Y_i(0)) \\
&\quad + 2p_f \text{Cov}(f(X_i)Y_i(1), Y_i(1)) + 2(1 - p_f) \text{Cov}((1 - f(X_i))Y_i(0), Y_i(0)) \right]
\end{align*}
\]

Finally, note the following,

\[
\begin{align*}
\text{Cov}(f(X_i)Y_i(1), (1 - f(X_i))Y_i(0)) &= \mathbb{E}\{f(X_i)Y_i(1)(f(X_i) - 1)Y_i(0)\} - \mathbb{E}\{f(X_i)Y_i(1)\}\mathbb{E}\{(1 - f(X_i))Y_i(0)\} \\
&= -\text{Pr}(f(X_i) = 1)\mathbb{E}(Y_i(1) | f(X_i) = 1)\text{Pr}(f(X_i) = 0)\mathbb{E}(Y_i(0) | f(X_i) = 0) \\
&= -p_f(1 - p_f)\mathbb{E}(Y_i(0) | f(X_i) = 0)\mathbb{E}(Y_i(1) | f(X_i) = 1)
\end{align*}
\]

and

\[
\begin{align*}
p_f \text{Cov}(f(X_i)Y_i(1), Y_i(1)) &= p_f^2 \left\{ \mathbb{E}(Y_i^2(1) | f(X_i) = 1) - \mathbb{E}(Y_i(1))\mathbb{E}(Y_i(1) | f(X_i) = 1) \right\} \\
(1 - p_f) \text{Cov}(f(X_i)Y_i(0), Y_i(0)) &= (1 - p_f)^2 \left\{ \mathbb{E}(Y_i^2(0) | f(X_i) = 0) - \mathbb{E}(Y_i(0))\mathbb{E}(Y_i(0) | f(X_i) = 0) \right\}
\end{align*}
\]

Hence, we have,

\[
\begin{align*}
\mathbb{V}(\hat{\tau}_f^*) - \mathbb{V}(\hat{\tau}_f) &= \frac{2n}{(n-1)^2} \left[ p_f^2 \mathbb{V}(Y_i(1)) + (1 - p_f)^2 \mathbb{V}(Y_i(0)) - 2p_f(1 - p_f)\mathbb{E}(Y_i(0) | f(X_i) = 0)\mathbb{E}(Y_i(1) | f(X_i) = 1) \\
&\quad + 2p_f^2 \left\{ \mathbb{E}(Y_i^2(1) | f(X_i) = 1) - \mathbb{E}(Y_i(1))\mathbb{E}(Y_i(1) | f(X_i) = 1) \right\} \\
&\quad + 2(1 - p_f)^2 \left\{ \mathbb{E}(Y_i^2(0) | f(X_i) = 0) - \mathbb{E}(Y_i(0))\mathbb{E}(Y_i(0) | f(X_i) = 0) \right\} \right]
\end{align*}
\]

\[
\begin{align*}
&= \frac{2n}{(n-1)^2} \left[ p_f^2 \mathbb{V}(Y_i(1)) + (1 - p_f)^2 \mathbb{V}(Y_i(0)) - 2p_f(1 - p_f)\mathbb{E}(Y_i(0) | f(X_i) = 0)\mathbb{E}(Y_i(1) | f(X_i) = 1) \\
&\quad + 2p_f^2 \left\{ \mathbb{V}(Y_i(1) | f(X_i) = 1) \right\} \\
&\quad + (1 - p_f)^2 \left\{ \mathbb{E}(Y_i(1) | f(X_i) = 1) - \mathbb{E}(Y_i(1))\mathbb{E}(Y_i(1) | f(X_i) = 1) \right\} \\
&\quad + 2(1 - p_f)^2 \left\{ \mathbb{V}(Y_i(0) | f(X_i) = 0) \right\} \\
&\quad + p_f \left\{ \mathbb{E}(Y_i(0) | f(X_i) = 0) - \mathbb{E}(Y_i(0))\mathbb{E}(Y_i(0) | f(X_i) = 1) \right\} \mathbb{E}(Y_i(0) | f(X_i) = 1) \right]\end{align*}
\]

A.6.2 Comparison under the Simplifying Assumption

Define \( M_{st} = \mathbb{E}(Y_i(s) | f(X_i) = t) \) for \( s, t \in \{0, 1\} \). Then, we can rewrite the variance difference as,

\[
\begin{align*}
\mathbb{V}(\hat{\tau}_f^*) - \mathbb{V}(\hat{\tau}_f) &= \frac{2n}{(n-1)^2} \left[ p_f^2 \mathbb{V}(Y_i(1)) + (1 - p_f)^2 \mathbb{V}(Y_i(0)) - 2p_f(1 - p_f)M_{11}M_{00} \\
&\quad + 2p_f^2 \left\{ \mathbb{V}(Y_i(1) | f(X_i) = 1) \right\} + (1 - p_f)(M_{11} - M_{00})M_{11} \\
&\quad + 2(1 - p_f)^2 \left\{ \mathbb{V}(Y_i(0) | f(X_i) = 0) \right\} + p_f(M_{00} - M_{01})M_{00} \right]
\end{align*}
\]

Now consider a constant shift of the outcome variable, i.e., \( Y_i(t) + \delta \) for \( t = 0, 1 \). Then, the variance difference becomes,

\[
\mathbb{V}(\hat{\tau}_f^*) - \mathbb{V}(\hat{\tau}_f)
\]

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Therefore, we can bound the variance difference from below as follows,

\begin{align*}
&= \frac{2n}{(n-1)^2} \left[ p_f^2 \mathbb{V}(Y_i(1)) + (1-p_f)^2 \mathbb{V}(Y_i(0)) - 2p_f(1 - p_f)(M_{11} + \delta)(M_{00} + \delta) \\
&\quad + 2p_f^2 \{ \mathbb{V}(Y_i(1) \mid f(X_i) = 1) + (1-p_f)(M_{11} - M_{10})(M_{11} + \delta) \} \\
&\quad + 2(1 - p_f)^2 \{ \mathbb{V}(Y_i(0) \mid f(X_i) = 0) + p_f(M_{00} - M_{01})(M_{00} + \delta) \} \right] \\
&= \frac{2n}{(n-1)^2} \left[ p_f^2 \mathbb{V}(Y_i(1)) + (1-p_f)^2 \mathbb{V}(Y_i(0)) - 2p_f(1 - p_f)M_{11}M_{00} \\
&\quad + 2p_f^2 \{ \mathbb{V}(Y_i(1) \mid f(X_i) = 1) + (1-p_f)(M_{11} - M_{10})M_{11} \} \\
&\quad + 2(1 - p_f)^2 \{ \mathbb{V}(Y_i(0) \mid f(X_i) = 0) + p_f(M_{00} - M_{01})M_{00} \} \\
&\quad - 2p_f(1 - p_f)\delta^2 + 2p_f(1 - p_f)\delta \{ p_f(M_{11} - M_{10}) + (1 - p_f)(M_{00} - M_{01}) - M_{11} - M_{00} \} \right] \\
&= \frac{2n}{(n-1)^2} \left[ p_f^2 \mathbb{V}(Y_i(1)) + (1-p_f)^2 \mathbb{V}(Y_i(0)) - 2p_f(1 - p_f)M_{11}M_{00} \\
&\quad + 2p_f^2 \{ \mathbb{V}(Y_i(1) \mid f(X_i) = 1) + (1-p_f)(M_{11} - M_{10})M_{11} \} \\
&\quad + 2(1 - p_f)^2 \{ \mathbb{V}(Y_i(0) \mid f(X_i) = 0) + p_f(M_{00} - M_{01})M_{00} \} \\
&\quad - 2p_f(1 - p_f)\delta^2 - 2p_f(1 - p_f)\delta \{ p_f(M_{00} + M_{10}) + (1 - p_f)(M_{11} + M_{01}) \} \right]
\end{align*}

Thus, we observe that the variance difference decreases by,

\[ 2p_f(1 - p_f)\delta^2 + 2p_f(1 - p_f)\delta \{ p_f(M_{00} + M_{10}) + (1 - p_f)(M_{11} + M_{01}) \} \]

Note that since the \textit{ex-ante} estimator is completely unaffected by this change, the constant shift increases the variance of the \textit{ex-post} evaluation estimator by the same amount. Under the simplifying assumption, we have,

\[ M_{11} + M_{01} = M_{00} + M_{10} = 0 \]

Therefore, we can bound the variance difference from below as follows,

\begin{align*}
\mathbb{V}(\hat{\tau}_f) - \mathbb{V}(\hat{\tau}_f) &= \frac{2n}{(n-1)^2} \left[ p_f^2 \mathbb{V}(Y_i(1)) + (1-p_f)^2 \mathbb{V}(Y_i(0)) - 2p_f(1 - p_f)M_{11}M_{00} \\
&\quad + 2p_f^2 \{ \mathbb{V}(Y_i(1) \mid f(X_i) = 1) + (1-p_f)(M_{11} - M_{10})M_{11} \} \\
&\quad + 2(1 - p_f)^2 \{ \mathbb{V}(Y_i(0) \mid f(X_i) = 0) + p_f(M_{00} - M_{01})M_{00} \} \right] \\
&= \frac{2n}{(n-1)^2} \left[ p_f^2 \mathbb{V}(Y_i(1)) + (1-p_f)^2 \mathbb{V}(Y_i(0)) - 2p_f(1 - p_f)M_{11}M_{00} \\
&\quad + 2p_f^2 \{ \mathbb{V}(Y_i(1) \mid f(X_i) = 1) + (1-p_f)(M_{11} + M_{00})M_{11} \} \\
&\quad + 2(1 - p_f)^2 \{ \mathbb{V}(Y_i(0) \mid f(X_i) = 0) + p_f(M_{00} + M_{11})M_{00} \} \right] \\
&= \frac{2n}{(n-1)^2} \left[ p_f^2 \mathbb{V}(Y_i(1)) + (1-p_f)^2 \mathbb{V}(Y_i(0)) + 2p_f^2 \mathbb{V}(Y_i(1) \mid f(X_i) = 1) + 2(1 - p_f)^2 \mathbb{V}(Y_i(0) \mid f(X_i) = 0) \\
&\quad + 2p_f(1 - p_f) \left[ (1 - p_f)M_{00}^2 + p_fM_{11}^2 \right] \right] \\
&\geq 0
\end{align*}

A.7 Additional Empirical Results
Figure A1: Estimated Prescriptive Effect Curves for the Individualized Treatment Rules based on BART, Causal Forest, and LASSO. Each row presents the results for a different outcome. For each plot, the estimated Area Under Prescriptive Effect Curve (AUPEC) and its standard error are shown. The solid lines represent the random assignment rule.