Supplementary Materials for "Experimental Evaluation of Individualized Treatment Rules"

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A Supplementary Appendix for "Experimental Evaluation of Individualized Treatment Rules"

A.1 Estimation and Inference for Fixed ITRs with No Budget Constraint

A.1.1 The Population Average Value

For a fixed ITR with no budget constraint, the following unbiased estimator of the population average value (Eqn (1)), based on the experimental data $\mathcal{Z}$, is used in the literature (e.g., Qian and Murphy, 2011),

$$\hat{\lambda}_f(\mathcal{Z}) \;=\; \frac{1}{n_1}\sum_{i=1}^{n} Y_i T_i f(\mathbf{X}_i) + \frac{1}{n_0}\sum_{i=1}^{n} Y_i(1-T_i)(1-f(\mathbf{X}_i)). \tag{A1}$$

Under Neyman's repeated sampling framework, it is straightforward to derive the unbiasedness and variance of this estimator where the uncertainty is based solely on the random sampling of units and the randomization of treatment alone. The results are summarized as the following theorem.

Theorem A1 (Unbiasedness and Variance of the Population Average Value Estimator) *Under Assumptions 1,2, and 3, the expectation and variance of the population average value estimator defined in Eqn* (A1) *are given by,*

$$\mathbb{E}\{\hat{\lambda}_f(\mathcal{Z})\} - \lambda_f \;=\; 0, \quad \mathbb{V}\{\hat{\lambda}_f(\mathcal{Z})\} \;=\; \frac{\mathbb{E}(S_{f1}^2)}{n_1} + \frac{\mathbb{E}(S_{f0}^2)}{n_0}$$

where $S_{ft}^2 = \sum_{i=1}^n (Y_{fi}(t) - \overline{Y_f(t)})^2/(n-1)$ *with* $Y_{fi}(t) = \mathbf{1}\{f(\mathbf{X}_i)=1\}Y_i(t)$ *and* $\overline{Y_f(t)} = \sum_{i=1}^n Y_{fi}(t)/n$ *for* $t = \{0,1\}$.

Proof is straightforward and hence omitted.

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A.1.2 The Population Average Prescriptive Effect (PAPE)

To estimate the PAPE with no budget constraint (Eqn (2)), we propose the following estimator,

$$\begin{aligned}\hat{\tau}_f(\mathcal{Z}) &= \frac{n}{n-1}\left[\frac{1}{n_1}\sum_{i=1}^n Y_i T_i f(\mathbf{X}_i) + \frac{1}{n_0}\sum_{i=1}^n Y_i(1-T_i)(1-f(\mathbf{X}_i))\right. \\ &\qquad \left. -\frac{\hat{p}_f}{n_1}\sum_{i=1}^n Y_i T_i - \frac{1-\hat{p}_f}{n_0}\sum_{i=1}^n Y_i(1-T_i)\right] \qquad \text{(A2)}\end{aligned}$$

where $\hat{p}_f = \sum_{i=1}^n f(\mathbf{X}_i)/n$ is a sample estimate of p_f, and the term $n/(n-1)$ is due to the finite sample degree-of-freedom correction resulting from the need to estimate p_f. The following theorem proves the unbiasedness of this estimator and derives its exact variance.

Theorem A2 (Unbiasedness and Exact Variance of the PAPE Estimator) *Under Assumptions 1, 2, and 3, the expectation and variance of the PAPE estimator defined Eqn* (A2) *are given by,*

$$\begin{aligned}\mathbb{E}\{\hat{\tau}_f(\mathcal{Z})\} &= \tau_f \\ \mathbb{V}\{\hat{\tau}_f(\mathcal{Z})\} &= \frac{n^2}{(n-1)^2}\left[\frac{\mathbb{E}(\widetilde{S}_{f1}^2)}{n_1} + \frac{\mathbb{E}(\widetilde{S}_{f0}^2)}{n_0} + \frac{1}{n^2}\left\{\tau_f^2 - np_f(1-p_f)\tau^2 + 2(n-1)(2p_f-1)\tau_f\tau\right\}\right]\end{aligned}$$

where $\widetilde{S}_{ft}^2 = \sum_{i=1}^n (\widetilde{Y}_{fi}(t) - \overline{\widetilde{Y}_f(t)})^2/(n-1)$ *with* $\widetilde{Y}_{fi}(t) = (f(\mathbf{X}_i) - \hat{p}_f)Y_i(t)$, *and* $\overline{\widetilde{Y}_f(t)} = \sum_{i=1}^n \widetilde{Y}_{fi}(t)/n$ *for* $t = \{0, 1\}$.

Note that $\mathbb{E}(\widetilde{S}_{ft}^2)$ does not equal $\mathbb{V}(\widetilde{Y}_{fi}(t))$ because the proportion of treated units p_f is estimated. The additional term in the variance accounts for this estimation uncertainty of p_f. The variance of the proposed estimator can be consistently estimated by replacing the unknown terms, i.e., p_f, τ_f, τ, $\mathbb{E}(\widetilde{S}_{ft}^2)$, with their unbiased estimates, i.e., $\hat{p}_f$, $\hat{\tau}_f$,

$$\hat{\tau} = \frac{1}{n_1}\sum_{i=1}^n T_i Y_i - \frac{1}{n_0}\sum_{i=1}^n (1-T_i)Y_i, \quad \text{and} \quad \widehat{\mathbb{E}(\widetilde{S}_{ft}^2)} = \frac{1}{n_t-1}\sum_{i=1}^n \mathbf{1}\{T_i = t\}(\widetilde{Y}_{fi} - \overline{\widetilde{Y}_{ft}})^2,$$

where $\widetilde{Y}_{fi} = (f(\mathbf{X}_i) - \hat{p}_f)Y_i$ and $\overline{\widetilde{Y}_{ft}} = \sum_{i=1}^n \mathbf{1}\{T_i = t\}\widetilde{Y}_{fi}/n_t$.

To prove Theorem A2, we first consider the sample average prescription effect (SAPE),

$$\tau_f^s = \frac{1}{n}\sum_{i=1}^n \left\{Y_i(f(\mathbf{X}_i)) - \hat{p}_f Y_i(1) - (1-\hat{p}_f)Y_i(0)\right\}. \qquad \text{(A3)}$$

and its unbiased estimator,

$$\hat{\tau}_f^s = \frac{1}{n_1}\sum_{i=1}^n Y_i T_i f(\mathbf{X}_i) + \frac{1}{n_0}\sum_{i=1}^n Y_i(1-T_i)(1-f(\mathbf{X}_i)) - \frac{\hat{p}_f}{n_1}\sum_{i=1}^n Y_i T_i - \frac{1-\hat{p}_f}{n_0}\sum_{i=1}^n Y_i(1-T_i) \quad \text{(A4)}$$

This estimator differs from the estimator of the PAPE by a small factor, i.e., $\hat{\tau}_f^s = (n-1)/n\hat{\tau}_f$. The following lemma derives the expectation and variance in the Neyman framework. Thus, it only requires the randomization-based finite sample inference and does not need Assumption 2.

Lemma 1 (Unbiasedness and Exact Variance of the Estimator for the SAPE) *Under Assumptions 1, 2, and 3, the expectation and variance of the estimator of the PAPE given in Eqn* (A4) *for estimating the SAPE defined in Eqn* (A3) *are given by,*

$$\begin{aligned}\mathbb{E}(\hat{\tau}_f^s \mid \mathcal{O}_n) &= \tau_f^s \\ \mathbb{V}(\hat{\tau}_f^s \mid \mathcal{O}_n) &= \frac{1}{n}\left(\frac{n_0}{n_1}\widetilde{S}_{f1}^2 + \frac{n_1}{n_0}\widetilde{S}_{f0}^2 + 2\widetilde{S}_{f01}\right)\end{aligned}$$

where $\mathcal{O}_n = \{Y_i(1), Y_i(0), \mathbf{X}_i\}_{i=1}^n$ *and*

$$\widetilde{S}_{f01} = \frac{1}{n-1}\sum_{i=1}^n(\widetilde{Y}_{fi}(0) - \overline{\widetilde{Y}_{fi}(0)})(\widetilde{Y}_{fi}(1) - \overline{\widetilde{Y}_{fi}(1)}).$$

Proof We begin by computing the expectation with respect to the experimental treatment assignment, i.e., T_i,

$$\begin{aligned}\mathbb{E}(\hat{\tau}_f^s \mid \mathcal{O}_n) &= \mathbb{E}\left\{\frac{1}{n_1}\sum_{i=1}^n f(\mathbf{X}_i)T_iY_i(1) + \frac{1}{n_0}\sum_{i=1}^n(1-f(\mathbf{X}_i))(1-T_i)Y_i(0)\right. \\ &\qquad \left. -\frac{\hat{p}_f}{n_1}\sum_{i=1}^n T_iY_i(1) - \frac{1-\hat{p}_f}{n_0}\sum_{i=1}^n(1-T_i)Y_i(0) \;\middle|\; \mathcal{O}_n\right\} \\ &= \frac{1}{n}\sum_{i=1}^n Y_i(1)f(\mathbf{X}_i) + \frac{1}{n}\sum_{i=1}^n Y_i(0)(1-f(\mathbf{X}_i)) - \frac{\hat{p}_f}{n}\sum_{i=1}^n Y_i(1) - \frac{1-\hat{p}_f}{n}\sum_{i=1}^n Y_i(0) \\ &= \tau_f^s\end{aligned}$$

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

$$\hat{\tau}_f^s = \tau_f^s + \sum_{i=1}^n D_i(f(\mathbf{X}_i) - \hat{p}_f)\left(\frac{Y_i(1)}{n_1} + \frac{Y_i(0)}{n_0}\right)$$

where $D_i = T_i - n_1/n$. Thus, noting $\mathbb{E}(D_i) = 0$, $\mathbb{E}(D_i^2) = n_0n_1/n^2$, and $\mathbb{E}(D_iD_j) = -n_0n_1/\{n^2(n-1)\}$ for $i \neq j$, after some algebra, we have,

$$\begin{aligned}\mathbb{V}(\hat{\tau}_f^s \mid \mathcal{O}_n) &= \mathbb{V}(\hat{\tau}_f^s - \tau_f^s \mid \mathcal{O}_n) = \mathbb{E}\left[\left\{\sum_{i=1}^n D_i\left(\frac{\widetilde{Y}_{fi}(1)}{n_1} + \frac{\widetilde{Y}_{fi}(0)}{n_0}\right)\right\}^2 \;\middle|\; \mathcal{O}_n\right] \\ &= \frac{1}{n}\left(\frac{n_0}{n_1}\widetilde{S}_{f1}^2 + \frac{n_1}{n_0}\widetilde{S}_{f0}^2 + 2\widetilde{S}_{f01}\right)\end{aligned}$$

□

Now, we prove Theorem A2. Using Lemma 1 and the law of iterated expectation, we have,

$$\mathbb{E}(\hat{\tau}_f^s) = \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^n\{Y_i(f(\mathbf{X}_i)) - \hat{p}_fY_i(1) - (1-\hat{p}_f)Y_i(0)\}\right].$$

We compute the following expectation for $t = 0, 1$,

$$\mathbb{E}\left(\sum_{i=1}^n \hat{p}_fY_i(t)\right) = \mathbb{E}\left(\sum_{i=1}^n \frac{\sum_{j=1}^n f(\mathbf{X}_j)}{n}Y_i(t)\right) = \frac{1}{n}\mathbb{E}\left\{\sum_{i=1}^n f(\mathbf{X}_i)Y_i(t) + \sum_{i=1}^n\sum_{j\neq i} f(\mathbf{X}_j)Y_i(t)\right\}$$

$$= \mathbb{E}\{f(\mathbf{X}_i)Y_i(t)\} + (n-1)p_f\mathbb{E}(Y_i(t)).$$

Putting them together yields the following bias expression,

$$\begin{aligned}
\mathbb{E}(\hat{\tau}_f^s) &= \mathbb{E}\left[\{Y_i(f(\mathbf{X}_i)) - \frac{1}{n}f(\mathbf{X}_i)\tau_i - \frac{n-1}{n}p_f\tau_i - Y_i(0)]\right] \\
&= \tau_f - \frac{1}{n}\mathbb{E}\left[\{f(\mathbf{X}_i)Y_i(1) - (1-f(\mathbf{X}_i))Y_i(0)\} - \{p_fY_i(1) - (1-p_f)Y_i(0)\}\right] \\
&= \tau_f - \frac{1}{n}\text{Cov}(f(\mathbf{X}_i), \tau_i).
\end{aligned}$$

where $\tau_i = Y_i(1) - Y_i(0)$. We can further rewrite the bias as,

$$\begin{aligned}
-\frac{1}{n}\text{Cov}(f(\mathbf{X}_i), \tau_i) &= \frac{1}{n}p_f\{\mathbb{E}(\tau_i \mid f(\mathbf{X}_i)=1) - \tau\} \\
&= \frac{1}{n}p_f(1-p_f)\{\mathbb{E}(\tau_i \mid f(\mathbf{X}_i)=1) - \mathbb{E}(\tau_i \mid f(\mathbf{X}_i)=0)\} \\
&= \frac{\tau_f}{n}. \qquad \text{(A5)}
\end{aligned}$$

where $\tau = \mathbb{E}(Y_i(1) - Y_i(0))$. This implies the estimator for the PAPE is unbiased, i.e., $\mathbb{E}(\hat{\tau}_f) = \tau_f$.

To derive the variance, Lemma 1 implies,

$$\mathbb{V}(\hat{\tau}_f) = \frac{n^2}{(n-1)^2}\left[\mathbb{V}\left(\frac{1}{n}\sum_{i=1}^n\{\widetilde{Y}_{fi}(1) - \widetilde{Y}_{fi}(0)\}\right) + \mathbb{E}\left\{\frac{1}{n}\left(\frac{n_0}{n_1}\widetilde{S}_{f1}^2 + \frac{n_1}{n_0}\widetilde{S}_{f0}^2 + 2\widetilde{S}_{f01}\right)\right\}\right]. \qquad \text{(A6)}$$

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

$$\mathbb{V}\left(\frac{1}{n}\sum_{i=1}^n\{\widetilde{Y}_{fi}(1) - \widetilde{Y}_{fi}(0)\}\right) = \text{Cov}(\widetilde{Y}_{fi}(1) - \widetilde{Y}_{fi}(0), \widetilde{Y}_{fi}(1) - \widetilde{Y}_{fi}(0)) + \frac{1}{n}\mathbb{E}(\widetilde{S}_{f1}^2 + \widetilde{S}_{f0}^2 - 2\widetilde{S}_{f01}), \qquad \text{(A7)}$$

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

$$\begin{aligned}
&\text{Cov}(\widetilde{Y}_{fi}(1) - \widetilde{Y}_{fi}(0), \widetilde{Y}_{fi}(1) - \widetilde{Y}_{fi}(0)) \\
=\ &\text{Cov}\left(\left\{f(\mathbf{X}_i) - \frac{1}{n}\sum_{i'=1}^n f(\mathbf{X}_{i'})\right\}\tau_i, \left\{f(\mathbf{X}_j) - \frac{1}{n}\sum_{j'=1}^n f(\mathbf{X}_{j'})\right\}\tau_j\right) \\
=\ &-2\text{Cov}\left(\frac{n-1}{n}f(\mathbf{X}_i)\tau_i, \frac{1}{n}f(\mathbf{X}_i)\tau_j\right) + \sum_{i' \neq i,j}\text{Cov}\left(\frac{1}{n}f(\mathbf{X}_{i'})\tau_i, \frac{1}{n}f(\mathbf{X}_{i'})\tau_j\right) \\
&+2\sum_{i' \neq i,j}\text{Cov}\left(\frac{1}{n}f(\mathbf{X}_j)\tau_i, \frac{1}{n}f(\mathbf{X}_{i'})\tau_j\right) + \text{Cov}\left(\frac{1}{n}f(\mathbf{X}_j)\tau_i, \frac{1}{n}f(\mathbf{X}_i)\tau_j\right) \\
=\ &-\frac{2(n-1)\tau}{n^2}\text{Cov}\left(f(\mathbf{X}_i), f(\mathbf{X}_i)\tau_i\right) + \frac{(n-2)\tau^2}{n^2}\mathbb{V}(f(\mathbf{X}_i)) \\
&+\frac{2(n-2)\tau}{n^2}p_f\text{Cov}\left(f(\mathbf{X}_i), \tau_i\right) + \frac{1}{n^2}\left\{\text{Cov}^2\left(f(\mathbf{X}_i), \tau_i\right) + 2p_f\tau\text{Cov}\left(f(\mathbf{X}_i), \tau_i\right)\right\} \\
=\ &\frac{1}{n^2}\text{Cov}^2\left(f(\mathbf{X}_i), \tau_i\right) + \frac{(n-2)\tau^2}{n^2}p_f(1-p_f) + \frac{2(n-1)\tau}{n^2}\text{Cov}\left(f(\mathbf{X}_i), (p_f - f(\mathbf{X}_i))\tau_i\right) \\
=\ &\frac{1}{n^2}\left[\tau_f^2 + (n-2)p_f(1-p_f)\tau^2 + 2(n-1)\tau\left\{p_f\tau_f - (1-p_f)\mathbb{E}(f(\mathbf{X}_i)\tau_i)\right\}\right]
\end{aligned}$$

Individual	T_i	$f(\mathbf{X}_i)$	Y_i	$Y_i(0)$	$Y_i(1)$
A	1	1	2	0	2
B	1	0	3	1	3
C	0	0	−1	−1	−1
D	0	1	1	1	0
E	1	0	3	0	3

Table A1: A Numerical Example for Binary Treatment Assignment and Outcomes

$$= \frac{1}{n^2}\left[\tau_f^2 + (n-2)p_f(1-p_f)\tau^2 + 2(n-1)\tau\left\{\tau_f(2p_f-1) - (1-p_f)p_f\tau\right\}\right]$$
$$= \frac{1}{n^2}\left\{\tau_f^2 - np_f(1-p_f)\tau^2 + 2(n-1)(2p_f-1)\tau_f\tau\right\},$$

where the third equality follows from the formula for the covariance of products of two random variables (Bohrnstedt and Goldberger, 1969). Finally, combining this result with equations (A6) and (A7) yields,

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

□

A potential complication with this estimator in practice is that its estimate (along with the variance) would change under an additive transformation, i.e., $Y_i(t) \to Y_i(t) + \delta$ for $t = 0, 1$ and a given constant δ. This issue is not due to the specific construction of the proposed estimator. It instead reflects the fundamental issue of many prescription effects including the population average value and PAPE that they cannot be defined solely in terms of multiples of $Y_i(1) - Y_i(0)$ (see Appendix A.1.3 for a numerical example). One solution is to center the outcome variable such that $\sum_{i=1}^n Y_i T_i / n_1 + \sum_{i=1}^n Y_i(1-T_i)/n_0 = 0$ holds. This solution is motivated by the fact that when the condition holds in the population (i.e. $\mathbb{E}(Y_i(1) + Y_i(0)) = 0$), the variance of the PAPE estimator is minimized.

A.1.3 A Numerical Example Showing the Lack of Additive Invariance for the Population Average Value

Consider an ITR $f : \mathcal{X} \to \{0, 1\}$, and we would like to know its population average value. Table A1 shows an numerical example with the observed outcome Y_i, the ITR $f(X_i)$, the actual assignment T_i, and the potential outcomes $Y_i(0), Y_i(1)$. Then, in this example, we have $n_1 = 3$ (A,B,E), $n_0 = 2$ (C,D), and the population average value estimator would be:

$$\hat{\lambda}_f(\mathcal{Z}) = \frac{1}{n_1}\sum_{i=1}^n Y_i T_i f(\mathbf{X}_i) + \frac{1}{n_0}\sum_{i=1}^n Y_i(1-T_i)(1-f(\mathbf{X}_i))$$
$$= \frac{1}{3}(1\cdot 2 + 0\cdot 3 + 0\cdot 3) + \frac{1}{2}(1\cdot -1 + 0\cdot 1)$$
$$= \frac{1}{6}$$

Now let us consider an additive transformation $Y_i(t) \to Y_i(t) + 1 := Y_i'(t)$ for $t = 0, 1$, where every outcome value is raised by 1. Then, its population average value estimator is now:

$$\begin{aligned}\hat{\lambda}_f'(\mathcal{Z}) &= \frac{1}{n_1}\sum_{i=1}^{n} Y_i' T_i f(\mathbf{X}_i) + \frac{1}{n_0}\sum_{i=1}^{n} Y_i'(1-T_i)(1-f(\mathbf{X}_i)) \\ &= \frac{1}{3}(1\cdot 3 + 0\cdot 4 + 0\cdot 4) + \frac{1}{2}(1\cdot 0 + 0\cdot 2) \\ &= 1\end{aligned}$$

Note that the difference $\hat{\lambda}_f'(\mathcal{Z}) - \hat{\lambda}_f(\mathcal{Z}) = \frac{5}{6} \neq 1$ does not equal to the amount of additive transformation. The problem arises because they are not multiples of $Y_i(1) - Y_i(0)$ but rather they depend on what the actual assignments of the ITR.

A.2 Proof of Theorem 1

We begin by deriving the variance. The derivation proceeds in the same fashion as the one for Theorem A2. The main difference lies in the derivation of the covariance term, which we detail below. First, we note that,

$$\begin{aligned}\Pr(f(\mathbf{X}_i, \hat{c}_p(f)) = 1) &= \int_{-\infty}^{\infty} \Pr(f(\mathbf{X}_i, c) = 1 \mid \hat{c}_p(f) = c) P(\hat{c}_p(f) = c) \mathrm{d}c \\ &= \int_{-\infty}^{\infty} \frac{\lfloor np \rfloor}{n} P(\hat{c}_p(f) = c) \mathrm{d}c \\ &= \frac{\lfloor np \rfloor}{n},\end{aligned}$$

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

$$\begin{aligned}& \mathrm{Cov}(\widetilde{Y}_i(1) - \widetilde{Y}_i(0), \widetilde{Y}_j(1) - \widetilde{Y}_j(0)) \\ = \ & \mathrm{Cov}\left\{(f(\mathbf{X}_i, \hat{c}_p(f)) - p)\,\tau_i, (f(\mathbf{X}_j, \hat{c}_p(f)) - p)\,\tau_j\right\} \\ = \ & \mathrm{Cov}\left\{f(\mathbf{X}_i, \hat{c}_p(f))\tau_i, f(\mathbf{X}_j, \hat{c}_p(f))\tau_j\right\} - 2p\mathrm{Cov}\left(\tau_i, f(\mathbf{X}_j, \hat{c}_p(f))\tau_j\right) \\ = \ & \frac{n\lfloor np \rfloor(\lfloor np \rfloor - 1) - \lfloor np \rfloor^2(n-1)}{n^2(n-1)} \mathbb{E}(\tau_i \mid f(\mathbf{X}_i, \hat{c}_p(f)) = 1)^2 - 2p\mathrm{Cov}\left(\tau_i, f(\mathbf{X}_j, \hat{c}_p(f))\tau_j\right) \\ = \ & \frac{\lfloor np \rfloor(\lfloor np \rfloor - n)}{n^2(n-1)} \kappa_1(\hat{c}_p(f))^2 + \frac{2p\lfloor np \rfloor(n - \lfloor np \rfloor)}{n^2(n-1)} \left(\kappa_1(\hat{c}_p(f))^2 - \kappa_1(\hat{c}_p(f))\kappa_0(\hat{c}_p(f))\right) \\ = \ & (2p-1)\frac{\lfloor np \rfloor(n - \lfloor np \rfloor)}{n^2(n-1)} \kappa_1(\hat{c}_p(f))^2 - \frac{2p\lfloor np \rfloor(n - \lfloor np \rfloor)}{n^2(n-1)} \kappa_1(\hat{c}_p(f))\kappa_0(\hat{c}_p(f)) \\ = \ & \frac{\lfloor np \rfloor(n - \lfloor np \rfloor)}{n^2(n-1)} \left\{(2p-1)\kappa_1(\hat{c}_p(f))^2 - 2p\kappa_1(\hat{c}_p(f))\kappa_0(\hat{c}_p(f))\right\}.\end{aligned}$$

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

Next, we derive the upper bound of bias. Using the same technique as the proof of Theorem A2, we can rewrite the expectation of the proposed estimator as,

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

Now, define $F(c) = \mathbb{P}(s(\mathbf{X}_i) \leq c)$. Without loss of generality, assume $\hat{c}_p(f) > c_p$ (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,

$$\begin{aligned} |\mathbb{E}(\hat{\tau}_f(\hat{c}_p(f))) - \tau_f(c_p)| &= \left|\mathbb{E}\left[\frac{1}{n}\sum_{i=1}^n \{Y_i\left(f(\mathbf{X}_i, \hat{c}_p(f))\right) - Y_i\left(f(\mathbf{X}_i, c_p)\right)\}\right]\right| \\ &= \left|\mathbb{E}_{\hat{c}_p(f)}\left[\int_{c_p}^{\hat{c}_p(f)} \mathbb{E}(\tau_i \mid s(\mathbf{X}_i) = c)\mathrm{d}F(c)\right]\right| \\ &= \left|\mathbb{E}_{F(\hat{c}_p(f))}\left[\int_{F(c_p)}^{F(\hat{c}_p(f))} \mathbb{E}(\tau_i \mid s(\mathbf{X}_i) = F^{-1}(x))\mathrm{d}x\right]\right| \\ &\leq \mathbb{E}_{F(\hat{c}_p(f))}\left[|F(\hat{c}_p(f)) - (1-p)| \times \max_{c\in[c_p, \hat{c}_p(f)]} |\mathbb{E}(\tau_i \mid s(\mathbf{X}_i) = c)|\right]. \end{aligned}$$

By the definition of $\hat{c}_p(f)$, $F(\hat{c}_p(f))$ is the $(n - \lfloor np \rfloor)$th order statistic of n independent uniform random variables, and thus follows the Beta distribution with the shape and scale parameters equal to $n - \lfloor np \rfloor$ and $\lfloor np \rfloor + 1$, respectively. For the special case where $p = 1$, we define the 0th order statistic of n uniform random variables to be 0, and by extension also define the "beta distribution" with shape parameter ≤ 0 to be $H(x)$ where $H(x)$ is the Heaviside step function. Therefore, we have,

$$\mathbb{P}(|F(\hat{c}_p(f)) - p| > \epsilon) = 1 - B(1-p+\epsilon, n - \lfloor np \rfloor, \lfloor np \rfloor + 1) + B(1-p-\epsilon, n - \lfloor np \rfloor, \lfloor np \rfloor + 1), \quad \text{(A8)}$$

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

$$B(\epsilon, \alpha, \beta) = \int_0^\epsilon t^{\alpha-1}(1-t)^{\beta-1}\mathrm{d}t.$$

Combining with the result above, the desired result follows. □

A.3 Estimation and Inference of the Population Average Prescriptive Difference of Fixed ITRs

Theorem A3 (Bias and Variance of the PAPD Estimator with a Budget Constraint) *Under Assumptions 1, 2, and 3, the bias of the proposed estimator of the PAPD with a budget constraint p defined in Eqn (8) can be bounded as follows,*

$$\begin{aligned} \mathbb{P}_{\hat{c}_p(f),\hat{c}_p(g)}(|\mathbb{E}\{\widehat{\Delta}_p(f,g,\mathcal{Z}) - \Delta_p(f,g) \mid \hat{c}_p(f), \hat{c}_p(g)\}| \geq \epsilon) &\leq 1 - 2B(1-p+\gamma_p(\epsilon), n - \lfloor np \rfloor, \lfloor np \rfloor + 1) \\ &\quad + 2B(1-p-\gamma_p(\epsilon), n - \lfloor np \rfloor, \lfloor np \rfloor + 1), \end{aligned}$$

where any given constant $\epsilon > 0$, $B(\epsilon, \alpha, \beta)$ is the incomplete beta function (if $\alpha = 0$ and $\beta > 0$, we set $B(\epsilon, \alpha, \beta) := H(\epsilon)$ for all ϵ where $H(\epsilon)$ is the Heaviside step function), and

$$\gamma_p(\epsilon) = \frac{\epsilon}{\max_{c\in[c_p(f)-\epsilon,\ c_p(f)+\epsilon],\ d\in[c_p(g)-\epsilon,\ c_p(g)+\epsilon]}\{\mathbb{E}(\tau_i \mid s_f(\mathbf{X}_i) = c), \mathbb{E}(\tau_i \mid s_g(\mathbf{X}_i) = d)\}}.$$

The variance of the estimator is,

$$\mathbb{V}(\widehat{\Delta}_p(f,g,\mathcal{Z})) = \frac{\mathbb{E}(S_{fgp1}^2)}{n_1} + \frac{\mathbb{E}(S_{fgp0}^2)}{n_0} + \frac{\lfloor np \rfloor(\lfloor np \rfloor - n)}{n^2(n-1)}(\kappa_{f1}(p)^2 + \kappa_{g1}(p)^2)$$

$$-2\left(\Pr(f(\mathbf{X}_i,\hat{c}_p(f)) = g(\mathbf{X}_i,\hat{c}_p(g)) = 1) - \frac{\lfloor np \rfloor^2}{n^2}\right)\kappa_{f1}(p)\kappa_{g1}(p),$$

where $S^2_{fgpt} = \sum_{i=1}^n (Y_{fgpi}(t) - \overline{Y_{fgp}(t)})^2/(n-1)$ *with* $Y_{fgpi}(t) = \{f(\mathbf{X}_i,\hat{c}_p(f)) - g(\mathbf{X}_i,\hat{c}_p(g))\}\, Y_i(t)$ *and* $\overline{Y_{fgp}(t)} = \sum_{i=1}^n Y_{fgpi}(t)/n$ *for* $t = 0, 1$.

To estimate the variance, it is tempting to replace all the unknown parameters with their sample analogues. However, unlike the case of the variance of the PAPE estimator under a budget constraint (see Theorem 1), there is no useful identity for the joint probability $\Pr(f(\mathbf{X}_i,\hat{c}_p(f)) = g(\mathbf{X}_i,\hat{c}_p(g)) = 1)$ under general g. Thus, an empirical analogue of $\hat{c}_p(f)$ and $\hat{c}_p(g)$ is not a good estimate because it is solely based on one realization. Thus, we use the following conservative bound,

$$\begin{aligned}
& -\left(\Pr(f(\mathbf{X}_i,\hat{c}_p(f)) = g(\mathbf{X}_i,\hat{c}_p(g)) = 1) - \frac{\lfloor np \rfloor^2}{n^2}\right)\kappa_{f1}(p)\kappa_{g1}(p) \\
\leq\; & \frac{\lfloor np \rfloor \max\{\lfloor np \rfloor, n - \lfloor np \rfloor\}}{n^2(n-1)}|\kappa_{f1}(p)\kappa_{g1}(p)|,
\end{aligned}$$

where the inequality follows because the maximum is achieved when the scoring rules of f and g, i.e., $s_f(\mathbf{X}_i)$ and $s_g(\mathbf{X}_i)$, are perfectly correlated. We use this upper bound in our simulation and empirical studies. In Section 5, we find that this upper bound estimate of the variance produces only a small conservative bias.

Proof The proof of the bounds for the expectation 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.

$$\begin{aligned}
& \operatorname{Cov}(Y_i^*(1) - Y_i^*(0), Y_j^*(1) - Y_j^*(0)) \\
=\; & \operatorname{Cov}\left(\{f(\mathbf{X}_i,\hat{c}_p(f)) - g(\mathbf{X}_i,\hat{c}_p(g))\}\,\tau_i, \{f(\mathbf{X}_j,\hat{c}_p(f)) - g(\mathbf{X}_j,\hat{c}_p(g))\}\,\tau_j\right) \\
=\; & \operatorname{Cov}(f(\mathbf{X}_i,\hat{c}_p(f))\tau_i, f(\mathbf{X}_j,\hat{c}_p(f))\tau_j) + \operatorname{Cov}(g(\mathbf{X}_i,\hat{c}_p(g))\tau_i, g(\mathbf{X}_j,\hat{c}_p(g))\tau_j) \\
& -2\operatorname{Cov}(f(\mathbf{X}_i,\hat{c}_p(f))\tau_i, g(\mathbf{X}_j,\hat{c}_p(g))\tau_j) \\
=\; & \frac{\lfloor np \rfloor(\lfloor np \rfloor - n)}{n^2(n-1)}\left(\kappa_{f1}(p)^2 + \kappa_{g1}(p)^2\right) - 2\operatorname{Cov}(f(\mathbf{X}_i,\hat{c}_p(f))\tau_i, g(\mathbf{X}_j,\hat{c}_p(g))\tau_j) \\
=\; & \frac{\lfloor np \rfloor(\lfloor np \rfloor - n)}{n^2(n-1)}\left(\kappa_{f1}(p)^2 + \kappa_{g1}(p)^2\right) \\
& -2\left(\Pr(f(\mathbf{X}_i,\hat{c}_p(f)) = g(\mathbf{X}_i,\hat{c}_p(g)) = 1) - \frac{\lfloor np \rfloor^2}{n^2}\right)\kappa_{f1}(p)\kappa_{g1}(p)
\end{aligned}$$

□

A.4 Proof of Theorem 2

The derivation of the variance expression in Theorem 2 proceeds in the same fashion as Theorem A2 (see Appendix A.2) with the only non-trivial change being the calculation of the covariance term. Note $\Pr(f(\mathbf{X}_i,\hat{c}_{\frac{k}{n}}(f)) = 1) = k/n$ for $t = 0, 1$ and $n_f = Z \sim \text{Binom}(n, p_f)$. Then, we have:

$$\operatorname{Cov}(Y_i^*(1) - Y_i^*(0), Y_j^*(1) - Y_j^*(0))$$

$$
\begin{aligned}
&= \operatorname{Cov}\left[\left\{\frac{1}{n}\left(\sum_{k=1}^{n_f} f(\mathbf{X}_i, \hat{c}_{k/n}(f)) + \sum_{k=n_f+1}^{n} f(\mathbf{X}_i, \hat{c}_{n_f/n}(f))\right) - \frac{1}{2}\right\}\tau_i,\right. \\
&\qquad\qquad \left.\left\{\frac{1}{n}\left(\sum_{k=1}^{n_f} f(\mathbf{X}_j, \hat{c}_{k/n}(f)) + \sum_{k=n_f+1}^{n} f(\mathbf{X}_j, \hat{c}_{n_f/n}(f))\right) - \frac{1}{2}\right\}\tau_j\right] \\
&= \mathbb{E}\left\{\operatorname{Cov}\left[\left\{\frac{1}{n}\left(\sum_{k=1}^{Z} f(\mathbf{X}_i, \hat{c}_{k/n}(f)) + \sum_{k=Z+1}^{n} f(\mathbf{X}_i, \hat{c}_{Z/n}(f))\right) - \frac{1}{2}\right\}\tau_i,\right.\right. \\
&\qquad\qquad \left.\left.\left\{\frac{1}{n}\left(\sum_{k=1}^{Z} f(\mathbf{X}_j, \hat{c}_{k/n}(f)) + \sum_{k=Z+1}^{n} f(\mathbf{X}_j, \hat{c}_{Z/n}(f))\right) - \frac{1}{2}\right\}\tau_j \;\middle|\; Z\right]\right\} \\
&\quad + \operatorname{Cov}\left\{\mathbb{E}\left[\left\{\frac{1}{n}\left(\sum_{k=1}^{Z} f(\mathbf{X}_i, \hat{c}_{k/n}(f)) + \sum_{k=Z+1}^{n} f(\mathbf{X}_i, \hat{c}_{Z/n}(f))\right) - \frac{1}{2}\right\}\tau_i \;\middle|\; Z\right],\right. \\
&\qquad\qquad \left.\mathbb{E}\left[\left\{\frac{1}{n}\left(\sum_{k=1}^{Z} f(\mathbf{X}_j, \hat{c}_{k/n}(f)) + \sum_{k=Z+1}^{n} f(\mathbf{X}_j, \hat{c}_{Z/n}(f))\right) - \frac{1}{2}\right\}\tau_j \;\middle|\; Z\right]\right\} \\
&= \mathbb{E}\left[-\frac{1}{n}\left\{\sum_{k=1}^{Z} \frac{k(n-k)}{n^2(n-1)}\kappa_{f1}(k/n)\kappa_{f0}(k/n) + \frac{Z(n-Z)^2}{n^2(n-1)}\kappa_{f1}(Z/n)\kappa_{f0}(Z/n)\right\}\right. \\
&\quad - \frac{2}{n^4(n-1)}\sum_{k=1}^{Z-1}\sum_{k'=k+1}^{Z} k(n-k')\kappa_{f1}(k/n)\kappa_{f1}(k'/n) \\
&\quad - \frac{Z^2(n-Z)^2}{n^4(n-1)}\kappa_{f1}(Z/n)^2 - \frac{2(n-Z)^2}{n^4(n-1)}\sum_{k=1}^{Z} k\kappa_{f1}(Z/n)\kappa_{f1}(k/n) \\
&\quad \left. + \frac{1}{n^4}\sum_{k=1}^{Z} k(n-k)\kappa_{f1}(k/n)^2\right] + \mathbb{V}\left(\sum_{i=1}^{Z}\frac{i}{n}\kappa_{f1}(i/n) + \frac{(n-Z)Z}{n}\kappa_{f1}(Z/n)\right),
\end{aligned}
$$

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

For the bias, we can rewrite Γ_f as,

$$
\Gamma_f = \int_0^{p_f} \mathbb{E}\{Y_i(f(\mathbf{X}_i, c_p))\}\mathrm{d}p + (1 - p_f)\mathbb{E}\{Y_i(f(\mathbf{X}_i, c^*))\} - \frac{1}{2}\mathbb{E}\{Y_i(1) + Y_i(0)\},
$$

and similarly its estimator $\widehat{\Gamma}_f$ as,

$$
\mathbb{E}(\widehat{\Gamma}_f) = \mathbb{E}\left\{\int_0^{\hat{p}_f} Y_i(f(\mathbf{X}_i, c_p))\mathrm{d}p\right\} + \mathbb{E}\{(1 - \hat{p}_f)Y_i(f(\mathbf{X}_i, c^*))\} - \frac{1}{2}\mathbb{E}\{Y_i(1) + Y_i(0)\}.
$$

Therefore, the bias of the estimator is, using a derivation similar to Appendix A.2:

$$
\begin{aligned}
\left|\mathbb{E}(\widehat{\Gamma}_f) - \Gamma_f\right| &\leq \mathbb{E}\left[|p_f - \hat{p}_f| \max_{c \in \{\min\{\hat{p}_f, p_f\}, \max\{\hat{p}_f, p_f\}\}} \mathbb{E}\{Y_i(f(\mathbf{X}_i, c)) - Y_i(f(\mathbf{X}_i, c^*))\}|\right. \\
&\qquad \left. + |\mathbb{E}\{Y_i(f(\mathbf{X}_i, c^*))\} - \mathbb{E}\{Y_i(f(\mathbf{X}_i, \hat{c}_{p_f}))\}|\right] \\
&\leq (\epsilon + 1)\max_{c \in [c^* - \epsilon, c^* + \epsilon]} |\mathbb{E}[Y_i(f(\mathbf{X}_i, c)) - Y_i(f(\mathbf{X}_i, c^*))]| \\
&\leq (\epsilon + 1)\epsilon \max_{c \in [c^* - \epsilon, c^* + \epsilon]} |\mathbb{E}(\tau_i \mid s(\mathbf{X}_i) = c)|.
\end{aligned}
$$

Now, taking the bound $\epsilon(1+\epsilon) \leq 2\epsilon$ for $0 \leq \epsilon \leq 1$ in Eqn (A8) of Appendix A.2, we have the desired result. □

A.5 Evaluation of an Estimated ITR with No Budget Constraint

Formally, we define an machine learning algorithm F to be a deterministic map from the space of observable data $\mathcal{Z} = \{\mathcal{X}, \mathcal{T}, \mathcal{Y}\}$ to the space of ITRs $\mathcal{F}$,

$$F : \mathcal{Z} \longrightarrow \mathcal{F}.$$

We emphasize that no restriction is placed on the machine learning algorithm F or ITR f.

To extend the population average value (Eqn (1)), we consider the average performance of an estimated ITR across training data sets of fixed size. First, for any given values of pre-treatment variables $\mathbf{X}_i = \mathbf{x}$, we define the average treatment proportion under the estimated ITR obtained by applying the machine learning algorithm F to training data $\mathcal{Z}^{tr}$ of size $n-m$,

$$\bar{f}_F(\mathbf{x}) \;=\; \mathbb{E}\{\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{x}) \mid \mathbf{X}_i = \mathbf{x}\} \;=\; \Pr(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{x}) = 1 \mid \mathbf{X}_i = \mathbf{x})$$

where the expectation is taken over the random sampling of training data $\mathcal{Z}^{tr}$. Although $\bar{f}_F$ depends on the training data size, we suppress it to ease notational burden.

Then, the population average value of an estimated ITR can be defined as,

$$\lambda_F \;=\; \mathbb{E}\left\{\bar{f}_F(\mathbf{X}_i)Y_i(1) + (1-\bar{f}_F(\mathbf{X}_i))Y_i(0)\right\} \tag{A9}$$

where the expectation is taken over the population distribution of $\{\mathbf{X}_i, Y_i(1), Y_i(0)\}$. In contrast to the population average value of a fixed ITR, this estimand accounts for the estimation uncertainty of the ITR by averaging over the random sampling of training sets.

To generalize the PAPE (Eqn (2)), we first define the population proportion of units assigned to the treatment condition under the estimated ITR as follows,

$$p_F \;=\; \mathbb{E}\{\Pr(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i) = 1 \mid \mathbf{X}_i)\} \;=\; \mathbb{E}\{\bar{f}_F(\mathbf{X}_i)\}$$

where the expectation is taken with respect to the sampling of training data of size $n-m$ and the population distribution of $\mathbf{X}_i$. Then, the PAPE of an estimated ITR is given by,

$$\tau_F \;=\; \mathbb{E}\{\lambda_F - p_F Y_i(1) - (1-p_F)Y_i(0)\}, \tag{A10}$$

where λ_F is the population average value of the estimated ITR defined in Eqn (A9).

A.5.1 The Population Average Value

We begin by considering the following cross-validation estimator of the population average value for an estimated ITR (Eqn (A9)),

$$\hat{\lambda}_F \;=\; \frac{1}{K}\sum_{k=1}^{K} \hat{\lambda}_{\hat{f}_{-k}}(\mathcal{Z}_k). \tag{A11}$$

The following theorem proves the unbiasedness of this estimator and derives its exact variance expression under the Neyman's repeated sampling framework.

Theorem A4 (Unbiasedness and Exact Variance of the Cross-Validation Population Average Value Estimator) *Under Assumptions 1, 2, and 3, the expectation and variance of the cross-validation Population Average Value estimator defined in Eqn* (A11) *are given by,*

$$\begin{aligned}\mathbb{E}(\hat{\lambda}_F) &= \lambda_F \\ \mathbb{V}(\hat{\lambda}_F) &= \frac{\mathbb{E}(S^2_{\hat{f}1})}{m_1} + \frac{\mathbb{E}(S^2_{\hat{f}0})}{m_0} + \mathbb{E}\left\{\mathrm{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i), \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j) \mid \mathbf{X}_i, \mathbf{X}_j)\tau_i\tau_j\right\} - \frac{K-1}{K}\mathbb{E}(S^2_F)\end{aligned}$$

for $i \neq j$ *where* $S^2_{\hat{f}t} = \sum_{i=1}^m \left(Y_{\hat{f}i}(t) - \overline{Y_{\hat{f}}(t)}\right)^2/(m-1)$, $S^2_F = \sum_{k=1}^K \left\{\hat{\lambda}_{\hat{f}_{-k}}(\mathcal{Z}_k) - \overline{\hat{\lambda}_{\hat{f}_{-k}}(\mathcal{Z}_k)}\right\}^2/(K-1)$, *and* $\tau_i = Y_i(1) - Y_i(0)$ *with* $Y_{\hat{f}i}(t) = \mathbf{1}\{\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i) = t\}Y_i(t)$, $\overline{Y_{\hat{f}}(t)} = \sum_{i=1}^m Y_{\hat{f}i}(t)/m$, *and* $\overline{\hat{\lambda}_{\hat{f}_{-k}}(\mathcal{Z}_k)} = \sum_{k=1}^K \hat{\lambda}_{\hat{f}_{-k}}(\mathcal{Z}_k)/K$ *for* $t = \{0, 1\}$.

The proof of unbiasedness is similar to that of Appendix A.1.2 and thus is omitted. To derive the variance, we first introduce the following useful lemma, adapted from Nadeau and Bengio (2000).

Lemma 2

$$\begin{aligned}\mathbb{E}(S^2_F) &= \mathbb{V}(\hat{\lambda}_{\hat{f}_{-k}}(\mathcal{Z}_k)) - \mathrm{Cov}(\hat{\lambda}_{\hat{f}_{-k}}(\mathcal{Z}_k), \hat{\lambda}_{\hat{f}_{-\ell}}(\mathcal{Z}_\ell)), \\ \mathbb{V}(\hat{\lambda}_F) &= \frac{\mathbb{V}(\hat{\lambda}_{\hat{f}_{-k}}(\mathcal{Z}_k))}{K} + \frac{K-1}{K}\mathrm{Cov}(\hat{\lambda}_{\hat{f}_{-k}}(\mathcal{Z}_k), \hat{\lambda}_{\hat{f}_{-\ell}}(\mathcal{Z}_\ell)).\end{aligned}$$

where $k \neq \ell$.

The lemma implies,

$$\mathbb{V}(\hat{\lambda}_F) = \mathbb{V}(\hat{\lambda}_{f_{-k}}(\mathcal{Z}_k)) - \frac{K-1}{K}\mathbb{E}(S^2_F). \tag{A12}$$

We then follow the same process of derivation as in Appendix A.1.2 while replacing $Y_i^*(t)$ with $Y_{\hat{f}i}(t)$ for $t \in \{0, 1\}$. The only difference lies in the covariance term, which can be expanded as follows,

$$\begin{aligned}\mathrm{Cov}(Y_{\hat{f}i}(1) - Y_{\hat{f}i}(0), Y_{\hat{f}j}(1) - Y_{\hat{f}j}(0)) &= \mathrm{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i)\tau_i + Y_i(0), \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j)\tau_j + Y_j(0)) \\ &= \mathrm{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i)\tau_i, \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j)\tau_j) \\ &= \mathbb{E}\left[\mathrm{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i)\tau_i, \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j)\tau_j \mid \mathbf{X}_i, \mathbf{X}_j, \tau_i, \tau_j)\right] \\ &= \mathbb{E}\left[\mathrm{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i), \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j) \mid \mathbf{X}_i, \mathbf{X}_j)\tau_i\tau_j\right].\end{aligned}$$

So the full variance expression is:

$$\begin{aligned}\mathbb{V}(\hat{\lambda}_F) &= \mathbb{V}(\hat{\lambda}_{f_{-k}}(\mathcal{Z}_k)) - \frac{K-1}{K}\mathbb{E}(S^2_F) \\ &= \frac{\mathbb{E}(S^2_{\hat{f}1})}{m_1} + \frac{\mathbb{E}(S^2_{\hat{f}0})}{m_0} + \mathbb{E}\left[\mathrm{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i), \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j) \mid \mathbf{X}_i, \mathbf{X}_j)\tau_i\tau_j\right] - \frac{K-1}{K}\mathbb{E}(S^2_F)\end{aligned}$$

□

When compared to the case of a fixed ITR with the sample size of m (see Theorem A1 in Appendix A.1.1), the variance has two additional terms. The covariance term accounts for the estimation uncertainty about the ITR, and is typically positive because two units, for which an estimated ITR makes the same treatment assignment recommendation, are likely to have causal effects with the same sign. The second term is due to the efficiency gain resulting from the K-fold cross-validation rather than evaluating an estimated ITR once.

The cross-validation estimate of $\mathbb{E}(S^2_{\hat{f}t})$ is straightforward and is given by,

$$\widehat{\mathbb{E}(S^2_{\hat{f}t})} \;=\; \frac{1}{K(m_t-1)}\sum_{k=1}^{K}\sum_{i=1}^{m}\mathbf{1}\{T_i^{(k)}=t\}\left\{Y_{\hat{f}i}^{(k)}(t)-\overline{Y_{\hat{f}t}^{(k)}}\right\}^2,$$

where $Y_{\hat{f}i}^{(k)}(t)=\mathbf{1}\{\hat{f}_{-k}(\mathbf{X}_i^{(k)})=t\}Y_i^{(k)}(t)$ and $\overline{Y_{\hat{f}t}^{(k)}}=\sum_{i=1}^{m}\mathbf{1}\{T_i^{(k)}=t\}Y_{\hat{f}i}^{(k)}(t)/m_t$. In contrast, the estimation of this cross-validation variance requires care. In particular, although it is tempting to estimate $\mathbb{E}(S_F^2)$ using the realization of S_F^2, this estimate is highly variable especially when K is small. As a result, it often yields a negative overall variance estimate. We address this problem by first noting that Lemma 2 implies,

$$\mathbb{V}(\hat{\lambda}_{\hat{f}_{-k}}(\mathcal{Z}_k)) \;=\; \frac{\mathbb{E}(S^2_{\hat{f}1})}{m_1}+\frac{\mathbb{E}(S^2_{\hat{f}0})}{m_0}+\mathbb{E}\left\{\mathrm{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i),\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j)\mid \mathbf{X}_i,\mathbf{X}_j)\tau_i\tau_j\right\} \;\geq\; \mathbb{E}(S_F^2).$$

Then, this inequality suggests the following consistent estimator of $\mathbb{E}(S_F^2)$,

$$\widehat{\mathbb{E}(S_F^2)} \;=\; \min\left(S_F^2, \widehat{\mathbb{V}(\hat{\lambda}_{\hat{f}_{-k}}(\mathcal{Z}_k))}\right).$$

Although this yields a conservative estimate of $\mathbb{V}(\hat{\lambda}_F)$ in finite samples, the bias appears to be small in practice (see Section 5.2).

Finally, for the estimation of the covariance term, since $\hat{f}_{\mathcal{Z}^{tr}}$ is binary, we have,

$$\begin{aligned}&\mathrm{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i),\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j)\mid \mathbf{X}_i,\mathbf{X}_j)\\ =\;&\Pr(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i)=\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j)=1\mid \mathbf{X}_i,\mathbf{X}_j)-\Pr(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i)=1\mid \mathbf{X}_i)\Pr(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j)=1\mid \mathbf{X}_j),\end{aligned}$$

for $i\neq j$. An unbiased cross-validation estimator of this covariance (given $\mathbf{X}_i$ and $\mathbf{X}_j$) is,

$$\widehat{\mathrm{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i),\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j)\mid \mathbf{X}_i,\mathbf{X}_j)} \;=\; \frac{1}{K}\sum_{k=1}^{K}\hat{f}_{-k}(\mathbf{X}_i)\hat{f}_{-k}(\mathbf{X}_j)-\frac{1}{K}\sum_{k=1}^{K}\hat{f}_{-k}(\mathbf{X}_i)\frac{1}{K}\sum_{k=1}^{K}\hat{f}_{-k}(\mathbf{X}_j).$$

Thus, we have the following cross-validation estimator of the required term,

$$\begin{aligned}&\mathbb{E}\left\{\widehat{\mathrm{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i),\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j)}\mid \mathbf{X}_i,\mathbf{X}_j)Y_i(s)Y_j(t)\right\}\\ =\;&\frac{\sum_{i=1}^{n}\sum_{j\neq i}\mathbf{1}\{T_i=s,T_j=t\}Y_iY_j\cdot\widehat{\mathrm{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i),\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j)\mid \mathbf{X}_i,\mathbf{X}_j)}}{\sum_{i=1}^{n}\sum_{j\neq i}\mathbf{1}\{T_i=s,T_j=t\}}.\end{aligned}$$

for $s,t\in\{0,1\}$. However, since this naive calculation is computationally expensive, we rewrite it as follows to reduce the computational time from $O(n^2K)$ to $O(nK)$,

$$\frac{\sum_{k=1}^{K}\left(\sum_{i=1}^{n}\mathbf{1}\{T_i=s\}Y_i\hat{f}_{-k}(\mathbf{X}_i)\right)\left(\sum_{i=1}^{n}\mathbf{1}\{T_i=t\}Y_i\hat{f}_{-k}(\mathbf{X}_i)\right)-\sum_{i=1}^{n}\mathbf{1}\{T_i=s,T_i=t\}Y_i^2\hat{f}_{-k}(\mathbf{X}_i)}{K\left[\left(\sum_{i=1}^{n}\mathbf{1}\{T_i=s\}\right)\left(\sum_{i=1}^{n}\mathbf{1}\{T_i=t\}\right)-\sum_{i=1}^{n}\mathbf{1}\{T_i=s,T_i=t\}\right]}$$

$$
- \frac{(\sum_{i=1}^n \sum_{k=1}^K \mathbf{1}\{T_i = s\} Y_i \hat{f}_{-k}(\mathbf{X}_i))(\sum_{i=1}^n \sum_{k=1}^K \mathbf{1}\{T_i = t\} Y_i \hat{f}_{-k}(\mathbf{X}_i))}{K^2 \left[(\sum_{i=1}^n \mathbf{1}\{T_i = s\})(\sum_{i=1}^n \mathbf{1}\{T_i = t\}) - \sum_{i=1}^n \mathbf{1}\{T_i = s, T_i = t\}\right]}
+ \frac{\sum_{i=1}^n \sum_{k=1}^K \mathbf{1}\{T_i = s, T_i = t\} Y_i^2 \hat{f}_{-k}(\mathbf{X}_i)}{K^2 \left[(\sum_{i=1}^n \mathbf{1}\{T_i = s\})(\sum_{i=1}^n \mathbf{1}\{T_i = t\}) - \sum_{i=1}^n \mathbf{1}\{T_i = s, T_i = t\}\right]}.
$$

A.5.2 The Population Average Prescriptive Effect (PAPE)

Next, we propose the following cross-validation estimator of the PAPE for an estimated ITR (Eqn (A10)),

$$
\hat{\tau}_F = \frac{1}{K} \sum_{k=1}^K \hat{\tau}_{\hat{f}_{-k}}(\mathcal{Z}_k) \tag{A13}
$$

where $\hat{\tau}_f(\cdot)$ is defined in Eqn (A2). The next theorem shows the unbiasedness of this estimator and derives its variance.

Theorem A5 (Unbiasedness and Exact Variance of the Cross-Validation PAPE Estimator) *Under Assumptions 1, 2, and 3, the expectation and variance of the cross-validation PAPE estimator defined in Eqn* (A13) *are given by,*

$$
\begin{aligned}
\mathbb{E}(\hat{\tau}_F) &= \tau_F \\
\mathbb{V}(\hat{\tau}_F) &= \frac{m^2}{(m-1)^2} \Bigg[\frac{\mathbb{E}(\widetilde{S}_{\hat{f}1}^2)}{m_1} + \frac{\mathbb{E}(\widetilde{S}_{\hat{f}0}^2)}{m_0} + \frac{1}{m^2} \left\{ \tau_F^2 - m p_F (1 - p_F) \tau^2 + 2(m-1)(2p_F - 1)\tau \tau_F \right\} \\
&\quad + \frac{1}{m^2} \mathbb{E} \Big\{ \left\{ (m-3)(m-2)\tau^2 + (m^2 - 2m + 2)\tau_i \tau_j - 2(m-2)^2 \tau \tau_i \right\} \\
&\quad \times \mathrm{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i), \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j) \mid \mathbf{X}_i, \mathbf{X}_j) \Big\} \Bigg] - \frac{K-1}{K} \mathbb{E}(\widetilde{S}_F^2)
\end{aligned}
$$

for $i \neq j$, where $\widetilde{S}_{\hat{f}t}^2 = \sum_{i=1}^m (\widetilde{Y}_{\hat{f}i}(t) - \overline{\widetilde{Y}_{\hat{f}}(t)})^2/(m-1)$, $\widetilde{S}_F^2 = \sum_{k=1}^K (\hat{\tau}_{\hat{f}_{-k}}(\mathcal{Z}_k) - \overline{\hat{\tau}_{\hat{f}_{-k}}(\mathcal{Z}_k)})^2/(K-1)$ with $\widetilde{Y}_{\hat{f}i}(t) = (\hat{f}_{-k}(\mathbf{X}_i) - \hat{p}_{\hat{f}_{-k}}) Y_i(t)$, $\overline{\widetilde{Y}_{\hat{f}}(t)} = \sum_{i=1}^m \widetilde{Y}_{\hat{f}i}(t)/m$, and $\overline{\hat{\tau}_{\hat{f}_{-k}}(\mathcal{Z}_k)} = \sum_{k=1}^K \hat{\tau}_{\hat{f}_{-k}}(\mathcal{Z}_k)/K$, for $t = \{0, 1\}$.

Proof The proof of unbiasedness is similar to that of Appendix A.1.2 and thus is omitted. The derivation of the variance is similar to that of Appendix A.5.1. The key difference is the calculation of the following covariance term, which needs care due to the randomness of $\hat{f}_{\mathcal{Z}^{tr}}$,

$$
\begin{aligned}
&\mathrm{Cov}(Y_i^*(1) - Y_i^*(0), Y_j^*(1) - Y_j^*(0)) \\
&= \mathrm{Cov}\left\{ \left(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i) - \frac{1}{m} \sum_{i'=1}^m \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_{i'}) \right) \tau_i, \left(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j) - \frac{1}{m} \sum_{j'=1}^m \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_{j'}) \right) \tau_j \right\},
\end{aligned}
$$

where $i \neq j$. There are seven terms that need to be carefully expanded,

$$
\begin{aligned}
&\frac{m-2}{m^2} \mathrm{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_k)\tau_i, \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_k)\tau_j) + \frac{(m-2)(m-3)}{m^2} \mathrm{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_k)\tau_i, \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_\ell)\tau_j) \\
&+ \frac{(m-1)^2}{m^2} \mathrm{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i)\tau_i, \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j)\tau_j) + \frac{1}{m^2} \mathrm{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j)\tau_i, \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i)\tau_j)
\end{aligned}
$$

$$
\begin{aligned}
&- \frac{2(m-1)}{m^2}\operatorname{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i)\tau_i, \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i)\tau_j) + \frac{2(m-2)}{m^2}\operatorname{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j)\tau_i, \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_k)\tau_j) \\
&- \frac{2(m-2)(m-1)}{m^2}\operatorname{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i)\tau_i, \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_k)\tau_j),
\end{aligned}
$$

where i, j, k, ℓ represent indices that do not take an identical value at the same time (e.g., $i \neq j$). Then, we rewrite the above terms using the properties of covariance as follows,

$$
\begin{aligned}
&\frac{(m-2)\tau^2}{m^2}\mathbb{V}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i)) + \frac{(m-2)(m-3)\tau^2}{m^2}\operatorname{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i), \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j)) \\
&+ \frac{(m-1)^2}{m^2}\left[\mathbb{E}\left\{\operatorname{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i), \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j) \mid \mathbf{X}_i, \mathbf{X}_j)\tau_i\tau_j\right\} + \operatorname{Cov}(\bar{f}_F(\mathbf{X}_i)\tau_i, \bar{f}_F(\mathbf{X}_j)\tau_j)\right] \\
&+ \frac{1}{m^2}\left[\mathbb{E}\left\{\operatorname{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i), \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j) \mid \mathbf{X}_i, \mathbf{X}_j)\tau_i\tau_j\right\} + \operatorname{Cov}(\bar{f}_F(\mathbf{X}_j)\tau_i, \bar{f}_F(\mathbf{X}_i)\tau_j)\right] \\
&- \frac{2(m-1)\tau}{m^2}(1-p_F)\mathbb{E}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i)\tau_i) \\
&+ \frac{2(m-2)\tau}{m^2}\left[\mathbb{E}\left\{\operatorname{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i), \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j) \mid \mathbf{X}_i, \mathbf{X}_j)\tau_i] + p_F\operatorname{Cov}(\bar{f}_F(\mathbf{X}_i), \tau_i)\right\}\right] \\
&- \frac{2(m-2)(m-1)\tau}{m^2}\left[\mathbb{E}\left\{\operatorname{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i), \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j) \mid \mathbf{X}_i, \mathbf{X}_j)\tau_i\right\} + \operatorname{Cov}(\bar{f}_F(\mathbf{X}_i)\tau_i, \bar{f}_F(\mathbf{X}_j))\right] \\
={}& \frac{(m-2)\tau^2}{m^2}p_F(1-p_F) + \frac{(m-2)(m-3)\tau^2}{m^2}\operatorname{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i), \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j)) \\
&+ \frac{m^2-2m+2}{m^2}\mathbb{E}\left\{\operatorname{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i), \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j) \mid \mathbf{X}_i, \mathbf{X}_j)\tau_i\tau_j\right\} + \frac{1}{m^2}(\tau_F^2 + 2\tau p_F\tau_F) \\
&- \frac{2(m-1)\tau^2}{m^2}p_F(1-p_F) - \frac{2(m-1)\tau\tau_F}{m^2}(1-p_F) + \frac{2(m-2)\tau}{m^2}p_F\tau_F \\
&- \frac{2(m-2)^2\tau}{m^2}\mathbb{E}\left\{\operatorname{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i), \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_k) \mid \mathbf{X}_i, \mathbf{X}_j)\tau_i\right\} \\
={}& \frac{1}{m^2}\left(\tau_F^2 - mp_F(1-p_F)\tau^2 + 2(m-1)(2p_F-1)\tau\tau_F\right) \\
&+ \mathbb{E}\left[\frac{(m-2)(m-3)\tau^2}{m^2}\operatorname{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i), \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j) \mid \mathbf{X}_i, \mathbf{X}_j)\right. \\
&\qquad - \frac{2(m-2)^2\tau}{m^2}\operatorname{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i), \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j) \mid \mathbf{X}_i, \mathbf{X}_j)\tau_i. \\
&\qquad\quad \left. + \frac{m^2-2m+2}{m^2}\operatorname{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i), \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j) \mid \mathbf{X}_i, \mathbf{X}_j)\tau_i\tau_j\right],
\end{aligned}
$$

for $i \neq j$, where we used the results from Appendix A.1.2 as well as $\mathbb{V}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i)) = p_F(1-p_F)$ and $\tau_F = \operatorname{Cov}(\bar{f}_F(\mathbf{X}_i), \tau_i) = \operatorname{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i), \tau_i)$. □

Like the case of the population average value, the variance has two extra terms when compared to the case of a fixed ITR (see Theorem A2 in Appendix A.1.2). The estimation of the variance is similar to that for the population average value.

A.6 Proof of Theorem 3

We begin by deriving the variance. The derivation proceeds in the same fashion as the one for Theorem A5 (see Appendix A.5.2). The only non-trivial change is the derivation of the covariance term, which we detail below. First, similar to the proof of Theorem 1 (see Appendix A.2), we note the following relation:

$$\begin{aligned}
\Pr(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i, \hat{c}_p) = 1) &= \mathbb{E}\left(\int_{-\infty}^{\infty} \Pr(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i, c) = 1 \mid \mathcal{Z}^{tr}, \hat{c}_p = c) P(\hat{c}_p = c \mid \mathcal{Z}^{tr}) \mathrm{d}c\right) \\
&= \mathbb{E}\left(\int_{-\infty}^{\infty} \frac{\lfloor mp \rfloor}{m} P(\hat{c}_p = c \mid \mathcal{Z}^{tr}) \mathrm{d}c\right) \\
&= \frac{\lfloor mp \rfloor}{m},
\end{aligned}$$

where the second equality follows from the fact that conditioned on a fixed training set $\mathcal{Z}^{tr}$ and conditioned on $\hat{c}_p = c$, exactly $\lfloor mp \rfloor$ out of m units will be assigned to the treatment condition. Given this result, we can compute the covariance as follows,

$$\begin{aligned}
& \mathrm{Cov}(\widetilde{Y}_i(1) - \widetilde{Y}_i(0), \widetilde{Y}_j(1) - \widetilde{Y}_j(0)) \\
= \;& \mathrm{Cov}\left\{\left(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i, \hat{c}_p) - p\right)\tau_i, \left(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j, \hat{c}_p) - p\right)\tau_j\right\} \\
= \;& \mathrm{Cov}\left(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i, \hat{c}_p)\tau_i, \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j, \hat{c}_p)\tau_j\right) - 2p\mathrm{Cov}\left(\tau_i, \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j, \hat{c}_p)\tau_j\right) \\
= \;& \frac{m\lfloor mp \rfloor(\lfloor mp \rfloor - 1) - \lfloor mp \rfloor^2(m-1)}{m^2(m-1)} \mathbb{E}(\tau_i \mid \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i, \hat{c}_p) = 1)^2 - 2p\mathrm{Cov}\left(\tau_i, \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j, \hat{c}_p)\tau_j\right) \\
= \;& \frac{\lfloor mp \rfloor(\lfloor mp \rfloor - m)}{m^2(m-1)} \kappa_{F1}(p)^2 + \frac{2p\lfloor mp \rfloor(m - \lfloor mp \rfloor)}{m^2(m-1)} \left(\kappa_{F1}(p)^2 - \kappa_{F1}(p)\kappa_{F0}(p)\right) \\
= \;& (2p-1)\frac{\lfloor mp \rfloor(m - \lfloor mp \rfloor)}{m^2(m-1)} \kappa_{F1}(p)^2 - \frac{2p\lfloor mp \rfloor(m - \lfloor mp \rfloor)}{m^2(m-1)} \kappa_{F1}(p)\kappa_{F0}(p) \\
= \;& \frac{\lfloor mp \rfloor(m - \lfloor mp \rfloor)}{m^2(m-1)} \left\{(2p-1)\kappa_{F1}(p)^2 - 2p\kappa_1(p)\kappa_{F0}(p)\right\}
\end{aligned}$$

Combining this covariance result with the expression for the marginal variances yields the desired variance expression for $\hat{\tau}_{Fp}$.

Next, we derive the upper bound of bias. Using the same technique as the proof of Theorem A2, we can rewrite the expectation of the proposed estimator as,

$$\mathbb{E}(\hat{\tau}_{Fp}) = \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}\left\{Y_i\left(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i, \hat{c}_p)\right) - pY_i(1) - (1-p)Y_i(0)\right\}\right]$$

Now, define $F(c) = \mathbb{P}(s(\mathbf{X}_i) \leq c)$. 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,

$$\begin{aligned}
\left|\mathbb{E}(\hat{\tau}_{Fp}) - \tau_{Fp}\right| &= \left|\mathbb{E}\left\{\mathbb{E}(\hat{\tau}_{Fp} - \tau_{Fp} \mid \mathcal{Z}^{tr})\right\}\right| \\
&\leq \mathbb{E}\left\{\left|\mathbb{E}(\hat{\tau}_{Fp} - \tau_{Fp} \mid \mathcal{Z}^{tr})\right|\right\} \\
&= \mathbb{E}\left\{\left|\mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}\left\{Y_i\left(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i, \hat{c}_p)\right) - Y_i\left(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i, c_p)\right)\right\} \;\middle|\; \mathcal{Z}^{tr}\right]\right|\right\} \\
&= \mathbb{E}\left\{\left|\mathbb{E}\left[\int_{c_p}^{\hat{c}_p} \mathbb{E}(\tau_i \mid \hat{s}_{\mathcal{Z}^{tr}}(\mathbf{X}_i) = c, \mathcal{Z}^{tr}) \mathrm{d}F(c)\right]\right|\right\}
\end{aligned}$$

$$
\begin{aligned}
&= \mathbb{E}\left\{\left|\mathbb{E}\left[\int_{F(c_p)}^{F(\hat{c}_p)} \mathbb{E}(\tau_i \mid \hat{s}_{\mathcal{Z}^{tr}}(\mathbf{X}_i) = F^{-1}(x), \mathcal{Z}^{tr})\mathrm{d}x\right]\right|\right\} \\
&\leq \mathbb{E}\left[|F(\hat{c}_p) - 1 - p| \times \max_{c\in[c_p,\hat{c}_p]} \left|\mathbb{E}(\tau_i \mid \hat{s}_{\mathcal{Z}^{tr}}(\mathbf{X}_i) = c, \mathcal{Z}^{tr})\right|\right].
\end{aligned}
$$

By the definition of $\hat{c}_p$, $F(\hat{c}_p)$ is the $m - \lfloor mp \rfloor$th order statistic of n independent uniform random variables. This statistic does not depend on the training set $\mathcal{Z}^{tr}$ as the test samples are independent. Thus, $F(\hat{c}_p)$ follows the Beta distribution with the shape and scale parameters equal to $m - \lfloor mp \rfloor$ and $\lfloor mp \rfloor + 1$, respectively. Therefore, we have,

$$
\mathbb{P}(|F(\hat{c}_p) - p| > \epsilon) = 1 - B(1-p+\epsilon, m-\lfloor mp \rfloor, \lfloor mp \rfloor + 1) + B(1-p-\epsilon, m-\lfloor mp \rfloor, \lfloor mp \rfloor + 1), \quad \text{(A14)}
$$

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

$$
B(\epsilon, \alpha, \beta) = \int_0^{\epsilon} t^{\alpha-1}(1-t)^{\beta-1}\mathrm{d}t.
$$

Combining with the result above, the desired result follows. □

A.7 The Population Average Prescriptive Difference of Estimated ITRs under a Budget Constraint

We consider the estimation and inference for the PAPD of an estimated ITR. The cross-validation estimator of this quantity is given by,

$$
\widehat{\Delta}_p(F, G) = \frac{1}{K}\sum_{k=1}^{K} \widehat{\Delta}_p(\hat{f}_{-k}, \hat{g}_{-k}, \mathcal{Z}_k), \quad \text{(A15)}
$$

where $\widehat{\Delta}_p(\hat{f}_{-k}, \hat{g}_{-k}, \mathcal{Z}_k)$ is defined in Eqn (8). For completeness, we present the algorithm for estimating the PAPD under this setting below.

Algorithm A1 Comparing Two Individualized Treatment Rules (ITR) using the Same Experimental Data via Cross-Validation

Input: Data $\mathcal{Z} = \{\mathbf{X}_i, T_i, Y_i\}_{i=1}^n$, Machine learning algorithms F and G, Evaluation metric $\tau_{f,g}$, Number of folds K

Output: Estimated evaluation metric $\hat{\tau}_{FG}$, Estiamted variance of $\hat{\tau}_{FG}$)

Split data into K random subsets of equal size $(\mathcal{Z}_1, \cdots, \mathcal{Z}_k)$
$k \leftarrow 1$
while $k \leq K$ **do**
    $\mathcal{Z}_{-k} = [\mathcal{Z}_1, \cdots, \mathcal{Z}_{k-1}, \mathcal{Z}_{k+1}, \cdots, \mathcal{Z}_K]$
    $\hat{f}_{-k} = F(\mathcal{Z}_{-k})$ ▷ Estimate ITR f by applying F to $\mathcal{Z}_{-k}$
    $\hat{g}_{-k} = G(\mathcal{Z}_{-k})$ ▷ Estimate ITR g by applying G to $\mathcal{Z}_{-k}$
    $\hat{\tau}_k = \hat{\tau}_{\hat{f}_{-k}, \hat{g}_{-k}}(\mathcal{Z}_k)$ ▷ Evaluate estimated ITR $\hat{f}$ using $\mathcal{Z}_k$
    $k \leftarrow k + 1$
end while
return $\hat{\tau}_{FG} = \frac{1}{K}\sum_{k=1}^{K} \hat{\tau}_k$, $\widehat{\mathbb{V}(\hat{\tau}_{FG})} = w(\hat{f}_{-1}, \cdots, \hat{f}_{-k}, \hat{g}_{-1}, \cdots, \hat{g}_{-k}, \mathcal{Z}_1, \cdots, \mathcal{Z}_K)$

Although the bias of the proposed estimator is not zero, we derive its upper bound as done in Theorem 3.

Theorem A6 (Bias and Variance of the Cross-validation PAPD Estimator with a Budget Constraint) *Under Assumptions 1, 2, and 3, the bias of the cross-validation PAPD estimator with a budget constraint p defined in Eqn* (A15) *can be bounded as follows,*

$$\begin{aligned}
&\mathbb{E}_{\mathcal{Z}^{tr}}[\mathbb{P}_{c_p(\hat{f}_{\mathcal{Z}^{tr}}),c_p(\hat{g}_{\mathcal{Z}^{tr}})}(|\mathbb{E}\{\widehat{\Delta}_p(F,G)-\Delta_p(F,G)\mid c_p(\hat{f}_{\mathcal{Z}^{tr}}),c_p(\hat{g}_{\mathcal{Z}^{tr}})\}|\geq\epsilon)]\\
&\leq\ 1-2B(1-p+\gamma_p(\epsilon),n-\lfloor np\rfloor,\lfloor np\rfloor+1)+2B(1-p-\gamma_p(\epsilon),n-\lfloor np\rfloor,\lfloor np\rfloor+1),
\end{aligned}$$

where any given constant $\epsilon>0$, $B(\epsilon,\alpha,\beta)$ is the incomplete beta function (if $\alpha=0$ and $\beta>0$, we set $B(\epsilon,\alpha,\beta):=H(\epsilon)$ for all ϵ where $H(\epsilon)$ is the Heaviside step function), and

$$\gamma_p(\epsilon)=\frac{\epsilon}{\mathbb{E}_{\mathcal{Z}^{tr}}[\max_{c\in[c_p(\hat{f}_{\mathcal{Z}^{tr}})-\epsilon,c_p(\hat{f}_{\mathcal{Z}^{tr}})+\epsilon],d\in[c_p(\hat{g}_{\mathcal{Z}^{tr}})-\epsilon,c_g(\hat{g}_{\mathcal{Z}^{tr}})+\epsilon]}\{\mathbb{E}(\tau_i\mid\hat{s}_{\hat{f}_{\mathcal{Z}^{tr}}}(\mathbf{X}_i)=c),\mathbb{E}(\tau_i\mid\hat{s}_{\hat{g}_{\mathcal{Z}^{tr}}}(\mathbf{X}_i)=d)\}]}.$$

The variance of the estimator is,

$$\begin{aligned}
\mathbb{V}(\widehat{\Delta}_p(F,G))\ =\ &\frac{\mathbb{E}(S^2_{\hat{f}\hat{g}1})}{n_1}+\frac{\mathbb{E}(S^2_{\hat{f}\hat{g}0})}{n_0}+\frac{\lfloor np\rfloor(\lfloor np\rfloor-n)}{n^2(n-1)}(\kappa_{F1}(p)^2+\kappa_{G1}(p)^2)\\
&-2\left(\Pr(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i,\hat{c}_p(\hat{f}_{\mathcal{Z}^{tr}}))=\hat{g}_{\mathcal{Z}^{tr}}(\mathbf{X}_i,\hat{c}_p(\hat{f}_{\mathcal{Z}^{tr}}))=1)-\frac{\lfloor np\rfloor^2}{n^2}\right)\kappa_{F1}(p)\kappa_{G1}(p)\\
&-\frac{K-1}{K}\mathbb{E}(S^2_{FG}),
\end{aligned}$$

where $S^2_{\hat{f}\hat{g}t}=\sum_{i=1}^n(\widetilde{Y}_{\hat{f}\hat{g}i}(t)-\overline{\widetilde{Y}_{\hat{f}\hat{g}}(t)})^2/(n-1)$, $S^2_{FG}=\sum_{k=1}^K(\widehat{\Delta}_p(\hat{f}_{-k},\hat{g}_{-k},\mathcal{Z}_k))-\overline{\widehat{\Delta}_p(\hat{f}_{-k},\hat{g}_{-k},\mathcal{Z}_k)})^2/(K-1)$, $\kappa_{Ft}(p)=\mathbb{E}(\tau_i\mid\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i,\hat{c}_p(\hat{f}_{\mathcal{Z}^{tr}}))=t)$, and $\kappa_{Gt}(p)=\mathbb{E}(\tau_i\mid\hat{g}_{\mathcal{Z}^{tr}}(\mathbf{X}_i,\hat{c}_p(g))=t)$ with $Y_{\hat{f}\hat{g}i}(t)=\left\{\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i,\hat{c}_p(\hat{f}_{\mathcal{Z}^{tr}}))-\hat{g}_{\mathcal{Z}^{tr}}(\mathbf{X}_i,\hat{c}_p(\hat{g}_{\mathcal{Z}^{tr}}))\right\}Y_i(t)$, $\overline{Y(t)}=\sum_{i=1}^n Y_{\hat{f}\hat{g}i}(t)/n$, and $\overline{\widehat{\Delta}_p(\hat{f}_{-k},\hat{g}_{-k},\mathcal{Z}_k)}=\sum_{k=1}^K\widehat{\Delta}_p(\hat{f}_{-k},\hat{g}_{-k},\mathcal{Z}_k)/K$ for $t=0,1$.

Proof is similar to that of Theorem 3, and hence is omitted. To estimate the variance, it is tempting to replace all unknowns with their sample analogues. However, the empirical analogue for the joint probability $\Pr(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i,\hat{c}_p(\hat{f}_{\mathcal{Z}^{tr}}))=\hat{g}_{\mathcal{Z}^{tr}}(\mathbf{X}_i,\hat{c}_p(\hat{g}_{\mathcal{Z}^{tr}}))=1)$ under general $\hat{f}_{\mathcal{Z}^{tr}},\hat{g}_{\mathcal{Z}^{tr}}$ is not a good estimate because it is solely based on one realization. Thus, we use the following conservative bound,

$$\begin{aligned}
&-\left(\Pr(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i,\hat{c}_p(\hat{f}_{\mathcal{Z}^{tr}}))=\hat{g}_{\mathcal{Z}^{tr}}(\mathbf{X}_i,\hat{c}_p(\hat{f}_{\mathcal{Z}^{tr}}))=1)-\frac{\lfloor np\rfloor^2}{n^2}\right)\kappa_{F1}(p)\kappa_{G1}(p)\\
&\leq\frac{\lfloor np\rfloor\max\{\lfloor np\rfloor,n-\lfloor np\rfloor\}}{n^2(n-1)}|\kappa_{F1}(p)\kappa_{G1}(p)|,
\end{aligned}$$

where the inequality follows because the maximum is achieved when the scoring rules of $\hat{f}_{\mathcal{Z}^{tr}}$ and $\hat{g}_{\mathcal{Z}^{tr}}$ are perfectly negatively correlated. We use this upper bound in our simulation and empirical studies. In Section 5, we find that this upper bound estimate of the variance produces only a small conservative bias.

A.8 An Additional Empirical Application

In this section, we describe an additional empirical application based on the canvassing experiment (Broockman and Kalla, 2016). This study was also re-analyzed by Künzel *et al.* (2018). The original authors find little heterogeneity in treatment effect. Our analysis below confirms this finding.

	BCF			Causal Forest			R-Learner		
	est.	s.e.	treated	est.	s.e.	treated	est.	s.e.	treated
No budget constraint	−0.104	0.128	48.4%	−0.349	0.137	47.5%	0	0	100%
20% Budget constraint	−0.02	0.121	20%	−0.120	0.107	20%	0	0.104	20%

Table A2: The Estimated Population Average Prescription Effect (PAPE) for Bayesian Causal Forest (BCF), Causal Forest, and R-Learner 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%.

A.8.1 The Experiment and Setup

We analyze the transgender canvas study of Broockman and Kalla (2016). This is an experiment that randomly assigned a door-to-door canvassing treatment to over 1,200 households (with a total of over 1,800 members) in Florida to estimate the treatment effect on support for a transgender rights law. The placebo group received a conversation on recycling, while the treatment group received a conversation about transgender issues. The support is measured at various time points after the intervention (i.e., 3 days, 3 weeks, 6 weeks, 3 months) using an online survey. The treatment effect heterogeneity is important in this scenario as canvassing is both costly and time-consuming. An ITR may allow canvassers to contact only those who are positively influenced by the message.

We follow the pre-experiment analysis plan by the original authors, and select a total of 26 baseline covariates including political inclination, gender, race, and opinions on social issues. Our treatment variable is whether or not the individual received the conversation about transgender issues (as opposed to the recycling message). Since the randomization was conducted on the household level, we randomly select one individual from each household for our analysis. We focus on the primary target (support for the transgender law) at the 3 day time point after the intervention, which is measured on a discrete scale with 7 possible values $\{-3, -2, -1, 0, 1, 2, 3\}$, with positive values indicating support.

The resulting dataset consists of 409 observations. We randomly select approximately 70% of the sample (i.e., 287 observations) as the training data and the reminder of the sample (i.e., 122 observations) as the evaluation data. We center the outcome variable using the mean in the training data to minimize variance, as discussed in Section 2. We train three machine learning models designed to measure heterogeneous treatment effects: Causal Forests, Bayesian Causal Forests (Hahn *et al.*, 2020), and R-Learner (Nie and Wager, 2017). All tuning was done through the 5-fold cross validation procedure on the training set using the PAPE as the evaluation metric. For Causal Forest, we set `tune.parameters = TRUE`. For Bayesian Causal Forests (BCF), tuning was done using a burn-in sample for MCMC sampling. For R-Learner, we utilized the lasso loss function and the default cross-validation for the regularization parameter. We then create an ITR as $\mathbf{1}\{\hat{\tau}(\mathbf{x}) > 0\}$ where $\hat{\tau}(\mathbf{x})$ is the estimated conditional average treatment effect obtained from each fitted model. We will evaluate these ITRs using the evaluation sample.

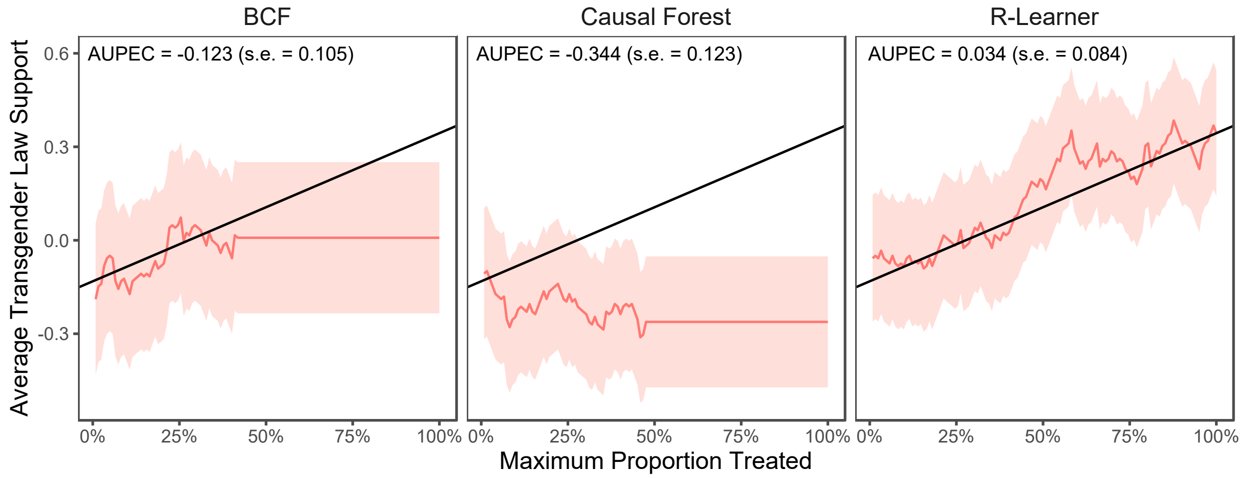

Figure A1: Estimated Area Under the Prescriptive Effect Curve (AUPEC). A solid red line in each plot represents the Population Average Prescriptive Effect (PAPE) with pointwise 95% confidence intervals shaded. The area between this line and the black line (representing random treatment) is the AUPEC. The results are presented for the individualized treatment rules based on Bayesian Causal Forest (BCF), Causal Forest, and R-Learner.

A.8.2 Results

Table A2 presents the results. We find that without a budget constraint, none of the ITRs based on the machine learning methods significantly improves upon the random treatment rule. In particular, the R-Learner leads to an ITR that treats everyone. Furthermore, we see that the ITR based on Causal Forest performs worse than the random treatment rule by 0.349 (out of a -3 to 3 scale) with a standard error of 0.137. The results are similar when we impose a budget constraint, and none of the resulting ITRs perform statistically significantly better than the random treatment rule. The result based on R-Learner is consistent with the conclusion of the original study indicating that there was no heterogeneity detected using LASSO.

We plot the estimated PAPE (with 95% pointwise confidence interval) as a function of budget constraint in Figure A1. The area between this line and the black horizontal line at zero corresponds to the AUPEC. 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. While BCF and R-Learner fail to create an ITR that is significantly different from the random treatment rule, Causal Forest produces an ITR that is statistically significantly worse than the random treatment rule. The result illustrates a potential danger of using an advanced machine learning algorithm to create an ITR. Indeed, there is no guarantee that the resulting ITR outperforms the random treatment rule.

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