Supplementary Material for "Individualized treatment rules under stochastic treatment cost constraints"

This Supplementary Material is organized as follows. Section S1 contains technical conditions to ensure that the statistical parameter of interest, the average treatment effect, is pathwise differentiable and that our proposed estimator is asymptotically efficient. We discuss a particular technical condition that may be difficult to verify in Section S2. In Section S3, we describe a modified version of our proposed estimator with improved performance in small to moderate samples. We present proofs of theoretical results in Section S4. In Section S5, we present the results of a simulation under an idealized setting. These results may provide guidance on interpreting the simulation results in Section 5.

As noted in the main text, the methods proposed in this work build upon tools used in Qiu et al. [34]; as such, the involved technical details bear similarity. To orient readers and facilitate comparisons, we have organized these supplementary materials for these papers similarly and shared portions of technical details when appropriate.

S1 Technical conditions for pathwise differentiability of parameter and asymptotic linearity of proposed estimator

In this section, we list the additional technical conditions required by Theorems 3 and 4 in Section 4 that we omit in the main text. Before doing this, we define pointwise

$$
\begin{aligned}
D_{n,\mathrm{FR}}(o) &:= D(\hat{P}_n, \rho_n, \tau_0, \mu_n^C)(o) - D(\hat{P}_n, \rho^{\mathrm{FR}}, 0, \mu_0^C)(o) \ , \\
D_{n,\mathrm{RD}}(o) &:= D(\hat{P}_n, \rho_n, \tau_0, \mu_n^C)(o) - D(\hat{P}_n, \rho_n^{\mathrm{RD}}, 0, \mu_0^C)(o) \\
&\qquad - \alpha \frac{\Psi_{\rho_n^{\mathrm{RD}}}(\hat{P}_n)}{\kappa - \phi_n} D_1(\hat{P}_n, \mu_n^C)(o) - \frac{\Psi_{\rho_n^{\mathrm{RD}}}(\hat{P}_n)}{P_n \hat{\Delta}_n^C} D_2(\hat{P}_n, \hat{\mu}_n^C)(o) \ , \\
D_{n,\mathrm{TP}}(o) &:= D(\hat{P}_n, \rho_n, \tau_0, \mu_n^C)(o) - G_{\mathrm{TP}}(\hat{P}_n)(o) \ .
\end{aligned}
$$

Condition B2 (Nonzero continuous density of $\xi_0(V)$ around η_0)**.** If $\eta_0 > -\infty$, then the distribution of $\xi_0(V)$ has positive, finite and continuous Lebesgue density in a neighborhood of η_0.

Since Condition B2 is most plausible when covariates are continuous, in this case, it is also plausible to expect the distribution of $\xi_0(V)$ to be continuous and thus Condition B2 holds.

Condition B3 (Smooth treatment cost function or lack of constraint)**.** If $\eta_0 > -\infty$, then the function $\eta \mapsto \mathrm{E}_0\left[I\left(\xi_0(V) > \eta\right)\Delta_0^C(W)\right]$ is continuously differentiable with nonzero derivative in a neighborhood of η_0; if $\eta_0 = -\infty$ and $\kappa < \infty$, then $\mathrm{E}_0\left[\Delta_0^C(W)\right] < \kappa - \alpha\phi_0$.

Condition B3 requires different conditions in separate cases. There are three cases in terms of the sufficiency of the budget to treat every individual: (i) there is an infinite budget and no constraint is present ($\kappa = \infty$); (ii) the budget is insufficient ($\eta_0 > -\infty$); and (iii) the budget is finite but sufficient ($\eta_0 = -\infty$ and $\kappa < \infty$). Condition B3 makes no assumption for Case (i). In Case (ii), we require a function $\eta \mapsto \mathrm{E}_0\left[I\left(\xi_0(V) > \eta\right)\Delta_0^C(W)\right]$ to be locally continuously differentiable. Since $\Delta_0^C > 0$ by Condition A4, this function is nonincreasing and thus only continuous differentiability is required. For each η, this function is an integral of additional cost Δ_0^C over the set $\{v : \xi_0(v) > 0\}$ and has a similar nature to survival functions. When covariates are continuous, it is plausible to assume that $\Delta_0^C(W)$ is continuous and thus $\eta \mapsto \mathrm{E}_0\left[I\left(\xi_0(V) > \eta\right)\Delta_0^C(W)\right]$ is continuously differentiable. In Case (iii), we require that the budget has a surplus. When it is unknown *a priori* whether the budget is sufficient to treat every individual, namely in Case (ii) or (iii), it is highly unlikely that the budget exactly suffices with no surplus. Therefore, Condition B3 is mild.

Condition B4 (Bounded additional treatment cost)**.** Δ_0^C is bounded.

Condition B5 (Active constraint)**.** If $\mathcal{R} = \mathrm{RD}$, then it holds that $(\kappa - \alpha\phi_0)/\,\mathrm{E}_0\left[\Delta_0^C(W)\right] < 1$.

Condition B5 requires that, when the rule ρ^{RD} that assigns treatment completely at random while respecting the budget constraint is the reference rule of interest, it should not correspond to the trivial rule $v \mapsto 1$ that assigns treatment to every individual. The rule ρ^{RD} equals $v \mapsto 1$ only when the budget is sufficient to treat every individual. Since, as a separate reference rule from given fixed rules ρ^{FR}, the reference rule ρ^{RD} is only interesting when the budget constraint is active, Condition B5 often holds automatically.

Condition B6 (Sufficient rates for nuisance estimators)**.**

$$\begin{aligned}\|\mu_n^T - \mu_0^T\|_{2,P_0}\Big\{&\|\mu_n^Y - \mu_0^Y\|_{2,P_0} + \|\hat{\mu}_n^Y - \mu_0^Y\|_{2,P_0}\\ &+ \|\mu_n^C - \mu_0^C\|_{2,P_0} + \|\hat{\mu}_n^C - \mu_0^C\|_{2,P_0}\Big\} = \mathrm{o}_p(n^{-1/2})\ .\end{aligned}$$

Condition B6 holds if all above nuisance estimators converge at a rate faster than $n^{-1/4}$, which may be much slower than the parametric rate $n^{-1/2}$ and thus allows for the use of flexible nonparametric estimators. This condition also holds if μ_n^Y, $\hat{\mu}_n^Y$, μ_n^C and $\hat{\mu}_n^C$ each converges slower than $n^{-1/4}$, as long as the estimated propensity score μ_n^T converges sufficiently fast to compensate.

Condition B7 (Consistency of estimated influence function)**.** The following terms are all $\mathrm{o}_p(1)$:

$$\|D_1(\hat{P}_n, \hat{\mu}_n^C) - D_1(P_0, \mu_0^C)\|_{2,P_0} \ , \quad \|D_2(\hat{P}_n, \mu_n^C) - D_2(P_0, \mu_0^C)\|_{2,P_0} \ , \quad \|D_{n,\mathcal{R}} - D_{\mathcal{R}}(P_0)\|_{2,P_0} \ ,$$
$$\|[D(\hat{P}_n, \rho_n, \tau_0, \mu_n^C) - D(\hat{P}_n, \rho_n^{\mathrm{RD}}, 0, \mu_0^C)] - [D(P_0, \rho_0, \tau_0, \mu_0^C) - D(P_0, \rho_0^{\mathrm{RD}}, 0, \mu_0^C)]\|_{2,P_0} \ .$$

Condition B8 (Consistency of strong positivity)**.** With probability tending to one over the sample used to obtain μ_n^T, it holds that $\int I\{\epsilon_T < \mu_n^T(w) < 1 - \epsilon_T\} dP_0(w) = 1$.

Condition B9 (Consistency of strictly more costly treatment)**.** With probability tending to one over the sample used to obtain Δ_n^C and δ_n^C, it holds that $\int I(\Delta_n^C(w) > \delta_C) dP_0(w) = 1$ and $\int I(\delta_n^C(v) > \delta_C) dP_0(v) = 1$.

Condition B10 (Fast rate of estimated optimal ITR)**.** As sample size n tends to infinity, it holds that

$$\int \{\rho_n(v) - \rho_0(v)\} \left\{\delta_0^Y(v) - \tau_0 \delta_0^C(v)\right\} dP_0(v) = \mathrm{o}_p(n^{-1/2}) \ .$$

Condition B10 may, at first sight, appear to be difficult to verify and is discussed in detail in Section S2. As shown in Theorem S1 of Section S2, Condition B10 may require faster rates on nuisance estimators than Condition B6. For example, convergence in the L^2-sense at a rate $\mathrm{o}_p(n^{-1/4})$ is sufficient for Condition B6, but a rate $\mathrm{o}_p(n^{-3/8})$ is needed in order to use Theorem S1 to show that Condition B10 holds.

Condition B11 (Donsker condition)**.** $\{o \mapsto d_{n,k}(v) D_2(\hat{P}_n, \mu_n^C)(o) : k \in [0,1]\}$ is a subset of a fixed P_0-Donsker class with probability tending to 1. Additionally, each of $D_1(\hat{P}_n, \mu_n^C)$, $D(\hat{P}_n, \rho_n, \tau_0, \mu_n^C) - D(\hat{P}_n, \rho_n^{\mathrm{RD}}, 0, \mu_0^C)$ and $D_{n,\mathcal{R}}$ belongs to a (possibly different) fixed P_0-Donsker class with probability tending to 1.

Condition B12 (Glivenko-Cantelli condition)**.** $\|\xi_n - \xi_0\|_{1,P_0} = \mathrm{o}_p(1)$ and $\|\Delta_n^C - \Delta_0^C\|_{1,P_0} = \mathrm{o}_p(1)$. Moreover, (i) if $\eta_0 > -\infty$, then, for any η sufficiently close to η_0, $w \mapsto I(\xi_n(v) > \eta) \Delta_n^C(w)$ belongs to a P_0-Glivenko-Cantelli class with probability tending to 1; (ii) otherwise, if $\eta_0 = -\infty$, then, for any $\eta < 0$ with sufficiently large $|\eta|$, $w \mapsto I(\xi_n(v) > \eta) \Delta_n^C(w)$ belongs to a P_0-Glivenko-Cantelli class with probability tending to 1.

The Donsker condition B11 and the Glivenko-Cantelli condition B12 impose restrictions on the flexibility of the methods used to estimate nuisance functions. We refer readers to, for example, van der Vaart and Wellner [50], for a more thorough introduction to such conditions.

All above conditions are similar to those in Qiu et al. [34] except that Conditions B9 and B4 are additional in this paper because the assumption of more costly treatment was not needed and a boundedness condition similar to B4 was automatically satisfied with a binary cost.

S2 Sufficient condition for fast convergence rate of estimated optimal rule

Condition B10, which is required by Theorem 4, may seem unintuitive and difficult to verify. In Theorem S1 below, we present sufficient conditions for Condition B10 that are similar to those in Qiu et al. [34].

Throughout the rest of the Supplement, for two quantities $a, b \in \mathbb{R}$, we use $a \lesssim b$ to denote $a \leq \mathcal{C} b$ for some constant $\mathcal{C} > 0$ that may depend on P_0.

Theorem S1 (Sufficient condition for Condition B10)**.** *Assume that* $\int I(\xi_n(v) = \tau_n) dP_0(v) = \mathrm{O}_p(n^{-1/2})$*. Further assume that each of* $o \mapsto I(\xi_n(v) > \eta_n)$ *and* $o \mapsto I(\xi_n(v) > \eta_n)\delta_0^C(v)$ *belongs to a (possibly different) fixed* P_0*-Donsker class with probability tending to 1. Suppose also that the distribution of* $\xi_0(V)$ *(*$V \sim P_0$*) has nonzero finite continuous Lebesgue density in a neighborhood of* η_0 *and a neighborhood of* τ_0*. Under Condition B4, the following statements hold.*

- *If* $\|\delta_n^Y - \delta_0^Y\|_{q,P_0} = \mathrm{o}_p(1)$ *for some* $q \geq 1$*, then*

$$|P_0\{(\rho_n - \rho_0)(\delta_0^Y - \tau_0 \delta_0^C)\}| \lesssim \|\delta_n^Y - \delta_0^Y\|_{q,P_0}^{2q/(q+1)} + \mathrm{O}_p(n^{-1}).$$

- *If* $\|\delta_n^Y - \delta_0^Y\|_{\infty,P_0} = \mathrm{o}_p(1)$*, then*

$$|P_0\{(\rho_n - \rho_0)(\delta_0^Y - \tau_0 \delta_0^C)\}| \lesssim \|\delta_n^Y - \delta_0^Y\|_{\infty,P_0}^2 + \mathrm{O}_p(n^{-1}).$$

The proof of Theorem S1 is very similar to Theorem 5 in Qiu et al. [34] and can be found in Section S4.5.

S3 Modified procedure with cross-fitting

In this section, we describe our proposed procedure to estimate the ATE with cross-fitting, which is mentioned in Remark 6. We use Λ to denote a user-specified fixed number of folds to split the data. Common choices of Λ used in practice include 5, 10 and 20.

1. Use the empirical distribution $\hat{P}_{W,n}$ of W as an estimate of the true marginal distribution of W. Compute estimates μ_n^Y, μ_n^C and μ_n^T of μ_0^Y, μ_n^C and μ_0^T, respectively using flexible regression methods.

2. Estimate an optimal individualized treatment rule for each observation:

   (a) Create folds: split the set of observation indices $\{1, 2, \dots, n\}$ into Λ mutually exclusive and exhaustive folds of (approximately) equal size. Denote these sets by S_λ, $\lambda = 1, 2, \dots, \Lambda$. Define $S_{-\lambda} := \cup_{\lambda' \neq \lambda} S_{\lambda'}$. For each $i = 1, 2, \dots, n$, let $\lambda(i)$ be the index of the fold containing i; in other words, $\lambda(i)$ is the unique value of λ such that $i \in S_\lambda$.

   (b) Estimate $\xi_0(V_i)$ using sample splitting: for each $\lambda = 1, 2, \dots, \Lambda$, compute estimates $\delta^Y_{n,S_{-\lambda}}$ and $\delta^C_{n,S_{-\lambda}}$ of δ_0^Y and $\Delta^C_{0,b}$ using flexible regression methods based on data $\{O_i : i \in S_{-\lambda}\}$. For each $i = 1, 2, \dots, n$, let $\xi_{n,i} := \delta^Y_{n,S_{-\lambda(i)}}(V_i)/\delta^C_{n,S_{-\lambda(i)}}(V_i)$ be the sample splitting estimate of $\xi_0(V_i)$.

   (c) Estimate ϕ_0 with a one-step correction estimator

   $$\phi_n := \frac{1}{n}\sum_{i=1}^{n}\{\mu_n^C(0, W_i) + \frac{1 - T_i}{1 - \mu_n^T(W_i)}[C_i - \mu_n^C(0, W_i)]\}.$$

   (d) Let $\Gamma_n : \tau \mapsto \frac{1}{n}\sum_{i:\xi_{n,i}>\tau} \Delta_n^C(1, W_i)$ and $\gamma_n : \tau \mapsto \frac{1}{n}\sum_{i:\xi_{n,i}=\tau} \Delta_n^C(W_i)$. For any $k \in [0, \infty)$, define $\eta_n(k) := \inf\{\tau : \Gamma_n(\tau) \leq k - \alpha\phi_n\}$, $\tau_n(k) := \max\{\eta_n(k), 0\}$, and, for $i = 1, 2, \dots, n$,

   $$d_{n,k,i} := \begin{cases} \frac{k - \alpha\phi_n - \Gamma_n(\eta_n(k))}{\gamma_n(\eta_n(k))}, & \text{if } \xi_{n,i} = \eta_n(k) \text{ and } \gamma_n(\eta_n(k)) > 0, \\ I\{\xi_{n,i} > \eta_n(k)\}, & \text{otherwise.} \end{cases}$$

   (e) Compute k_n, which is used to define an estimate of ρ_0 for which the plug-in estimator is asymptotically linear.

   - If $\tau_n(\kappa) > 0$ *and* there is a solution in $k \in [0, \infty)$ to

   $$\frac{1}{n}\sum_{i=1}^{n} d_{n,k,i}\left[\Delta_n^C(W_i) + \frac{1}{T_i + \mu_n^T(W_i) - 1}[C_i - \mu_n^C(T_i, W_i)]\right] + \alpha\phi_n = \kappa, \tag{S1}$$

then take k_n to be this solution.

- otherwise, set $k_n = \kappa$.

(f) For each $i = 1, 2, \ldots, n$, estimate $\rho_0(V_i)$ with

$$\rho_{n,i} := \begin{cases} \frac{k_n - \alpha\phi_n - \Gamma_n(\tau_n(k_n))}{\gamma_n(\tau_n(k_n))}, & \text{if } \xi_{n,i} = \tau_n(k_n), \text{ and } \gamma_n(\tau_n(k_n)) > 0, \\ I\{\xi_{n,i} > \tau_n(k_n)\}, & \text{otherwise.} \end{cases}$$

3. Obtain an estimate $\rho_n^{\mathcal{R}}$ of the reference ITR $\rho_0^{\mathcal{R}}$ as follows:

- For $\mathcal{R} = \text{FR}$, take $\rho_n^{\mathcal{R}}$ to be ρ^{FR}.
- For $\mathcal{R} = \text{RD}$,
  (a) obtain a targeted estimate $\hat{\mu}_n^C$ of μ_0^C: run an ordinary least-squared regression using observations $i = 1, 2, \ldots, n$ with outcome C_i, offset $\mu_n^C(T_i, W_i)$, no intercept and covariate $1/(T_i + \mu_n^T(W_i) - 1)$. Take $\hat{\mu}_n^C$ to be the fitted mean model;
  (b) take $\rho_n^{\mathcal{R}}$ to be the constant function $o \mapsto \min\{1, (\kappa - \alpha\phi_n)/\hat{P}_{W,n}\hat{\Delta}_n^C\}$, where we define pointwise $\hat{\Delta}_n^C : w \mapsto \hat{\mu}_n^C(1, w) - \hat{\mu}_n^C(0, w)$.
- For $\mathcal{R} = \text{TP}$, take $\rho_n^{\mathcal{R}}$ to be μ_n^T.

4. Estimate ATE of ρ_0 relative to the reference ITR $\rho_0^{\mathcal{R}}$ with a targeted minimum-loss based estimator (TMLE) ψ_n:

   (a) obtain a targeted estimate $\hat{\mu}_n^Y$ of μ_0^Y: run an ordinary least-squares linear regression using observations $i = 1, 2, \ldots, n$ with outcome Y_i, offset $\mu_n^Y(T_i, W_i)$, no intercept and covariate $[\rho_{n,i} - \rho_n^{\mathcal{R}}(O_i)]/[T_i + \mu_n^T(W_i) - 1]$. Take $\hat{\mu}_n^Y$ to be the fitted mean function.

   (b) with $\hat{P}_n$ being any distribution with components $\hat{\mu}_n^Y$ and $\hat{P}_{W,n}$, set $\psi_n := \frac{1}{n}\sum_{i=1}^n \rho_{n,i}\hat{\Delta}_n^Y(W_i) - \Psi_{\rho_n^{\mathcal{R}}}(\hat{P}_n)$ where $\hat{\Delta}_n^Y : w \mapsto \hat{\mu}_n^Y(1, w) - \hat{\mu}_n^Y(0, w)$.

S4 Proof of theorems

S4.1 Identification results (Theorem 1 and 2)

Theorem 1 is a simple corollary of the standard G-formula [36]. We provide a complete proof below.

Proof of Theorem 1. Note that

$$\mathbb{E}[Y(1) \mid W] = \mathbb{E}[Y(1) \mid T=1, W] = \mathrm{E}_0[Y \mid T=1, W] = \mu_0^Y(1, W).$$

Similarly, $\mathbb{E}[Y(0) \mid W] = \mathrm{E}_0[Y \mid T=0, W] = \mu_0^Y(0, W)$. Hence, $\mathbb{E}[Y(1) - Y(0) \mid W] = \Delta_0^Y(W)$. By the law of total expectation, this yields that $\mathbb{E}[Y(1) - Y(0) \mid V] = \mathrm{E}_0[\Delta_0^Y(W) \mid V] = \delta_0^Y(V)$. It then follows that

$$\begin{aligned}
\mathbb{E}[Y(\rho) - Y(\rho_0^{\mathcal{R}})] &= \mathbb{E}[\{\rho(V) - \rho_0^{\mathcal{R}}(W)\}\{Y(1) - Y(0)\}] \\
&= \mathrm{E}_0[\{\rho(V) - \rho_0^{\mathcal{R}}(W)\}\, \mathbb{E}[Y(1) - Y(0) \mid W]] \\
&= \mathrm{E}_0[\{\rho(V) - \rho_0^{\mathcal{R}}(W)\}\Delta_0^Y(W)].
\end{aligned}$$

The results for the treatment cost can be proved similarly. □

We next prove Theorem 2.

Proof of Theorem 2. Let ρ be any ITR that satisfies the constraint that $\mathrm{E}_0[\rho(V)\delta_0^C(V)] + \alpha\phi_0 \leq \kappa$. We will show that $\mathrm{E}_0[\rho_0(V)\delta_0^Y(V)] \geq \mathrm{E}_0[\rho(V)\delta_0^Y(V)]$, implying that ρ_0 is a solution to (2).

Observe that

$$\begin{aligned}
&\mathrm{E}_0[\rho_0(V)\delta_0^Y(V)] - \mathrm{E}_0[\rho(V)\delta_0^Y(V)] \\
&= \mathrm{E}_0[\{\rho_0(V) - \rho(V)\}\delta_0^Y(V)] \\
&= \mathrm{E}_0[\{\rho_0(V) - \rho(V)\}\delta_0^Y(V) I(\xi_0(V) > \tau_0)] + \mathrm{E}_0[\{\rho_0(V) - \rho(V)\}\delta_0^Y(V) I(\xi_0(V) < \tau_0)] \\
&\qquad + \mathrm{E}_0[\{\rho_0(V) - \rho(V)\}\delta_0^Y(V) I(\xi_0(V) = \tau_0)] \\
&= \mathrm{E}_0[\{\rho_0(V) - \rho(V)\}\xi_0(V)\delta_0^C(V) I(\xi_0(V) > \tau_0)] + \mathrm{E}_0[\{\rho_0(V) - \rho(V)\}\xi_0(V)\delta_0^C(V) I(\xi_0(V) < \tau_0)] \\
&\qquad + \mathrm{E}_0[\{\rho_0(V) - \rho(V)\}\xi_0(V)\delta_0^C(V) I(\xi_0(V) = \tau_0)].
\end{aligned}$$

Note that $\rho_0(v) = 1 \geq \rho(v)$ if $\xi_0(v) > \tau_0$ and $\rho_0(v) = 0 \leq \rho(v)$ if $\xi_0(v) < \tau_0$. Combining this observation with the fact that $\tau_0 \geq 0$, the above shows that

$$\begin{aligned}
&\mathrm{E}_0[\rho_0(V)\delta_0^Y(V)] - \mathrm{E}_0[\rho(V)\delta_0^Y(V)] \\
&\geq \tau_0\, \mathrm{E}_0[\{\rho_0(V) - \rho(V)\}\delta_0^C(V) I(\xi_0(V) > \tau_0)] + \tau_0\, \mathrm{E}_0[\{\rho_0(V) - \rho(V)\}\delta_0^C(V) I(\xi_0(V) < \tau_0)]
\end{aligned}$$

$$
\begin{aligned}
&\quad + \tau_0 \, \mathrm{E}_0[\{\rho_0(V) - \rho(V)\}\delta_0^C(V) I(\xi_0(V) = \tau_0)] \\
&= \tau_0 \, \mathrm{E}_0[\{\rho_0(V) - \rho(V)\}\delta_0^C(V)].
\end{aligned}
$$

If $\tau_0 = 0$, then $\mathrm{E}_0[\rho_0(V)\delta_0^Y(V)] - \mathrm{E}_0[\rho(V)\delta_0^Y(V)] \geq 0$, as desired; otherwise, $\tau_0 > 0$ and $\mathrm{E}_0[\rho(V)\delta_0^C(V)] \leq \kappa - \alpha\phi_0 = \mathrm{E}_0[\rho_0(V)\delta_0^C(V)]$, and so it follows that $\mathrm{E}_0[\rho_0(V)\delta_0^Y(V)] \geq \mathrm{E}_0[\rho(V)\delta_0^Y(V)]$. Therefore, we conclude that ρ_0 is a solution to (2). $\square$

S4.2 Pathwise differentiability of ATE parameter (Theorem 3)

We follow existing literature on semiparametric efficiency theory closely to prove pathwise differentiability of our estimands and asymptotic efficiency of our estimators under nonparametric models. We refer readers to, for example, Pfanzagl [30, 31], Bolthausen et al. [4], for a more thorough introduction to semiparametric efficiency.

To derive the canonical gradient of the ATE parameters, let $\mathcal{H} \subseteq L_0^2(P_0)$ be the set of score functions with range contained in $[-1, 1]$ and we study the behavior of the parameters under perturbations in an arbitrary direction $H \in \mathcal{H}$. We note that the $L_0^2(P_0)$-closure of $\mathcal{H}$ is indeed $L_0^2(P_0)$.

We define $H_W : w \mapsto \mathrm{E}_0[H(O) \mid W = w]$, $H_T : (t \mid w) \mapsto \mathrm{E}_0[H(O) \mid T = t, W = w]$ and $P_{H,\epsilon}$ via its Radon-Nikodym derivative with respect to P_0:

$$
\frac{dP_{H,\epsilon}}{dP_0} : o \mapsto [1 + \epsilon H(o) - \epsilon H_T(t \mid w) - \epsilon H_W(w)] \, [1 + \epsilon H_T(t \mid w)] \, [1 + \epsilon H_W(w)] \tag{S2}
$$

for any ϵ in a sufficiently small neighborhood of 0 such that the right-hand side is positive for all $o \in \mathcal{W} \times \{0, 1\} \times \{0, 1\} \times \mathbb{R}$. It is straightforward to verify that the score function for ϵ at $\epsilon = 0$ is indeed H. For the rest of this section, we may drop H from the notation and use P_ϵ as a shorthand notation for $P_{H,\epsilon}$ when no confusion should arise.

We will see that each parameter evaluated at P_ϵ depends on the following marginal or conditional distributions in a clean way: the marginal distribution $P_{W,\epsilon}$ of W, the marginal distribution $P_{T,W,\epsilon}$ of (T, W), the conditional distribution $P_{T,\epsilon}$ of T given W, the conditional distribution $P_{C,\epsilon}$ of C given (T, W), and the conditional distribution $P_{Y,\epsilon}$ of Y given (T, W). We now derive their closed-form expressions. Let $H_C : (c \mid t, w) \mapsto \mathrm{E}_0[H(O) \mid C = c, T = t, W = w] - H_T(t \mid w) - H_W(w)$, and $H_Y : (y \mid t, w) \mapsto$

$\mathrm{E}_0[H(O) \mid Y=y, T=t, W=w] - H_T(t \mid w) - H_W(w)$. We can then show that

$$\begin{aligned}
\frac{dP_{W,\epsilon}}{dP_{W,0}} &: w \mapsto 1 + \epsilon H_W(w), \\
\frac{dP_{T,W,\epsilon}}{dP_{T,W,0}} &: (t,w) \mapsto 1 + \epsilon H_T(t \mid w) + \epsilon H_W(w), \\
\frac{dP_{T,\epsilon}}{dP_{T,0}}(\cdot \mid w) &: t \mapsto 1 + \epsilon H_T(t \mid w), \\
\frac{dP_{C,\epsilon}}{dP_{C,0}}(\cdot \mid t,w) &: c \mapsto 1 + \epsilon H_C(c \mid t,w), \\
\frac{dP_{Y,\epsilon}}{dP_{Y,0}}(\cdot \mid t,w) &: y \mapsto 1 + \epsilon H_Y(y \mid t,w).
\end{aligned} \tag{S3}$$

Moreover, $\mathrm{E}_0[H_W(W)] = 0$, $\mathrm{E}_0[H_T(T \mid W) \mid W] = 0$ P_0-a.s., $\mathrm{E}_0[H_C(C \mid T,W) \mid T,W] = 0$ P_0-a.s., and $\mathrm{E}_0[H_Y(Y \mid T,W) \mid T,W] = 0$ P_0-a.s.

We finally introduce some additional notations that are used for the rest of the section. We use $\mathcal{C}$ to denote a generic positive constant that may vary line by line. Let S_0 be the survival function of the distribution of $\xi_0(V)$ when $V \sim P_0$. We also use the notation $\lesssim$ defined in Section S2. For a generic function $f : \mathbb{R} \to \mathbb{R}$, we will use the big- and little-oh notations, namely $\mathrm{O}(f(\epsilon))$ and $\mathrm{o}(f(\epsilon))$, respectively, to denote the behavior of $f(\epsilon)$ as $\epsilon \to 0$. Finally, for a general function or quantity f_P that depends on a distribution P, we use f_ϵ to denote f_{P_ϵ}. For example, we may write μ^Y_ϵ as a shorthand for $\mu^Y_{P_\epsilon}$. We will also write expectations under P_ϵ as E_ϵ.

The derivation of the canonical gradients of $P \mapsto \Psi_{\rho^{\mathrm{FR}}}(P)$ can be found in the Supplement of Qiu et al. [34]. We now derive the canonical gradients of $P \mapsto \Psi_{\rho_P^{\mathrm{TP}}}(P)$, $P \mapsto \Psi_{\rho_P^{\mathrm{RD}}}(P)$ and $P \mapsto \Psi_{\rho_P}(P)$, which are different from the parameters in Qiu et al. [34].

S4.2.1 Canonical gradient of $P \mapsto \Psi_{\rho_P^{\mathrm{TP}}}(P)$ (Theorem 3)

Fix a score $H \in \mathcal{H}$. Note that, for all $P \in \mathcal{M}$, $\Psi_{\rho_P^{\mathrm{TP}}}(P) = \int \mu_P^T(w) \Delta_P^Y(w) P_W(dw)$. Combining this, (S3) and the chain rule yields that

$$\begin{aligned}
&\frac{d}{d\epsilon} \Psi_{\rho_\epsilon^{\mathrm{TP}}}(P_\epsilon) \bigg|_{\epsilon=0} \\
&= \int \frac{d}{d\epsilon} \left[\mu_\epsilon^T(w) \Delta_\epsilon^Y(w) P_{W,\epsilon}(dw) \right] \bigg|_{\epsilon=0} \\
&= \int \left(\frac{d}{d\epsilon} \mu_\epsilon^T(w) \bigg|_{\epsilon=0} \right) \Delta_0^Y(w) P_{W,0}(dw) + \int \mu_0^T(w) \left(\frac{d}{d\epsilon} \Delta_\epsilon^Y(w) \bigg|_{\epsilon=0} \right) P_{W,0}(dw) \\
&\quad + \int \mu_0^T(w) \Delta_0^Y(w) \, \frac{d}{d\epsilon} P_{W,\epsilon}(dw) \bigg|_{\epsilon=0}
\end{aligned}$$

$$
\begin{aligned}
&= \iint (t - \mu_0^T(w)) H_T(t \mid w) \Delta_0^Y(w) P_{T,0}(dt \mid w) P_{W,0}(dw) \\
&\quad + \iiint \mu_0^T(w) \left(\frac{I(t=1)}{\mu_P^T(w)} - \frac{I(t=0)}{1-\mu_P^T(w)} \right) (y - \mu_0^Y(t,w)) H_Y(y \mid t, w) P_{Y,0}(dy \mid t, w) P_{T,0}(dt \mid w) P_{W,0}(dw) \\
&\quad + \int (\mu_0^T(w) \Delta_0^Y(w) - \Psi_{\rho_0^{\mathrm{TP}}}(P_0)) H_W(w) P_{W,0}(dw) \\
&= \int G_{\mathrm{TP}}(P_0)(o) H(o) P_0(do),
\end{aligned}
$$

where we have used the fact that $\mathrm{E}_0[H_Y(Y \mid T, W) \mid T, W] = 0$ P_0-a.s., $\mathrm{E}_0[H_T(T \mid W) \mid W] = 0$ P_0-a.s., and $\mathrm{E}_0[H_W(W)] = 0$. Therefore, the canonical gradient of $P \mapsto \Psi_{\rho_P^{\mathrm{TP}}}(P)$ at P_0 is $G_{\mathrm{TP}}(P_0)$.

S4.2.2 Canonical gradient of $P \mapsto \Psi_{\rho_P^{\mathrm{RD}}}(P)$

Let H be a score function in $\mathcal{H}$. We aim to show that

$$
\left. \frac{d}{d\epsilon} \Psi_{\rho_\epsilon^{\mathrm{RD}}}(P_\epsilon) \right|_{\epsilon=0} = \int G_{\mathrm{RD}}(P_0)(o) H(o) P_0(do), \tag{S4}
$$

which shows that $P \mapsto \Psi_{\rho_P^{\mathrm{RD}}}(P)$ is pathwise differentiable with canonical gradient $G_{\mathrm{RD}}(P_0)$ at P_0.

By similar arguments to those in Section 3.4 of Kennedy [16], we can show that

$$
\left. \frac{d}{d\epsilon} P_\epsilon \mu_\epsilon^C(0, \cdot) \right|_{\epsilon=0} = \int \left\{ \frac{1-t}{1-\mu_0^T(w)} [c - \mu_0^C(0, w)] + \mu_0^C(0, w) - P_0 \mu_0^C(0, \cdot) \right\} H(o) P_0(do), \tag{S5}
$$

$$
\left. \frac{d}{d\epsilon} P_\epsilon \Delta_\epsilon^C \right|_{\epsilon=0} = \int \left\{ \frac{1}{t + \mu_0^T(w) - 1} [c - \mu_0^C(t, w)] + \Delta_0^C(w) - P_0 \Delta_0^C \right\} H(o) P_0(do). \tag{S6}
$$

Consequently, $P_\epsilon \mu_\epsilon^C(0, \cdot) = P_0 \mu_0^C(0, \cdot) + \mathrm{O}(\epsilon)$ and $P_\epsilon \Delta_\epsilon^C = P_0 \Delta_0^C + \mathrm{O}(\epsilon)$. It follows that, for all ϵ in a sufficiently small neighborhood of zero, Condition B5 implies that $(\kappa - \alpha P_\epsilon \mu_\epsilon^C(0, \cdot))/P_\epsilon \Delta_\epsilon^C < 1$. Consequently, for each ϵ in this neighborhood, $\Psi_{\rho_\epsilon^{\mathrm{RD}}}(P_\epsilon) = \frac{\kappa - \alpha P_\epsilon \mu_\epsilon^C(0,\cdot)}{P_\epsilon \Delta_\epsilon^C} \Psi_{v \mapsto 1}(P_\epsilon)$, where we have used that $P_\epsilon \Delta_\epsilon^Y = \Psi_{v \mapsto 1}(P_\epsilon)$. It follows that the derivative $\frac{d}{d\epsilon} P_\epsilon \mu_\epsilon^C(0, \cdot)\big|_{\epsilon=0}$ is the same as the derivative of $f : \epsilon \mapsto \frac{\kappa - P_\epsilon \mu_\epsilon^C(0,\cdot)}{P_\epsilon \Delta_\epsilon^C} \Psi_{v \mapsto 1}(P_\epsilon)$ at $\epsilon = 0$, provided this derivative exists. Noting that $v \mapsto 1$ is a particular instance of a fixed treatment rule, we may take ρ^{FR} to be $v \mapsto 1$ in the results on pathwise differentiability of $P \mapsto \Psi_{\rho^{\mathrm{FR}}}(P)$ and show that

$$
\left. \frac{d}{d\epsilon} \Psi_{v \mapsto 1}(P_\epsilon) \right|_{\epsilon=0} = \int D(P_0, v \mapsto 1, 0, \mu_0^C)(o) H(o) P_0(do). \tag{S7}
$$

As both the above derivative and the derivatives in (S5) and (S6) exist, by the chain rule, it follows that

$$\frac{d}{d\epsilon}f(\epsilon)\bigg|_{\epsilon=0} = \frac{\kappa - \alpha P_0\mu_0^C(0,\cdot)}{P_0\Delta_0^C}\,\frac{d}{d\epsilon}\Psi_{v\mapsto 1}(P_\epsilon)\bigg|_{\epsilon=0} - \frac{(\kappa - \alpha P_0\mu_0^C(0,\cdot))\Psi_{v\mapsto 1}(P_0)}{(P_0\Delta_0^C)^2}\,\frac{d}{d\epsilon}P_\epsilon\Delta_\epsilon^C\bigg|_{\epsilon=0}$$
$$- \alpha\frac{\Psi_{v\mapsto 1}(P_0)}{P_0\Delta_0^C}\,\frac{d}{d\epsilon}P_\epsilon\mu_\epsilon^C(0,\cdot)\bigg|_{\epsilon=0}.$$

Note that $\phi_P = P\mu_P^C(0,\cdot)$. Plugging (S5), (S6) and (S7) into the above and we can show that the right-hand side of the above is equal to the right-hand side of (S4). As $\frac{d}{d\epsilon}f(\epsilon)\big|_{\epsilon=0} = \frac{d}{d\epsilon}\Psi_{\rho_\epsilon^{\mathrm{RD}}}(P_\epsilon)\Big|_{\epsilon=0}$, we have shown that (S4) holds, and the desired result follows.

S4.2.3 Canonical gradient of $P \mapsto \Psi_{\rho_P}(P)$

Let H be a score function in $\mathcal{H}$. The argument that we use parallels that of Luedtke and van der Laan [20] and Qiu et al. [34], except that it is slightly modified to account for the fact that the resource constraint takes a different form in this paper.

We first note that all of following hold for all ϵ sufficiently close to zero:

$$\sup_w |\Delta_\epsilon^C(w) - \Delta_0^C(w)| \lesssim |\epsilon|, \tag{S8}$$

$$\sup_v |\delta_\epsilon^Y(v) - \delta_0^Y(v)| \lesssim |\epsilon|, \tag{S9}$$

$$\sup_v |\delta_\epsilon^C(v) - \delta_0^C(v)| \lesssim |\epsilon|. \tag{S10}$$

The derivations of these inequalities are straightforward and hence omitted. Under Condition A4, the above inequalities imply that

$$\sup_v |\xi_\epsilon(v) - \xi_0(v)| = \left|\frac{\delta_\epsilon^Y(v)}{\delta_\epsilon^C(v)} - \frac{\delta_0^Y(v)}{\delta_0^C(v)}\right| \lesssim |\epsilon|. \tag{S11}$$

For ϵ sufficiently close to zero, it will be useful to define

$$\Gamma_\epsilon : \eta \mapsto \mathrm{E}_\epsilon[I\{\xi_\epsilon(V) > \eta\}\delta_\epsilon^C(V)]$$

for $\eta \in [-\infty, \infty)$. We also define $\Gamma'_\epsilon : \eta \mapsto \frac{d}{ds}\Gamma_\epsilon(s)|_{s=\eta}$ when the derivative exists.

We first show two lemmas. These two lemmas show that, under a perturbed distribution P_ϵ with magnitude ϵ, the fluctuation in the threshold $\tau_\epsilon - \epsilon_0$ is of order ϵ. This result is crucial in quantifying the convergence rate of two terms in the expansion of $\Psi_{\rho_\epsilon}(P_\epsilon) - \Psi_{\rho_0}(P_0)$, namely terms 1 and 3 in (S12) below. In particular, term 1 is the main challenge in the analysis as it comes from the perturbation in the threshold and is unique in estimation problems involving the evaluation of optimal ITRs. The first studies the convergence of η_ϵ to η_0. Because it may be the case that $\eta_0 = -\infty$, the convergence stated in this result is convergence in the extended real line.

Lemma S1. *Under the conditions of Theorem 3, $\eta_\epsilon \to \eta_0$ as $\epsilon \to 0$.*

Proof of Lemma S1. We separately consider the cases where $\eta_0 > -\infty$ and $\eta_0 = -\infty$.

Suppose that $\eta_0 > -\infty$. For all sufficiently small $\delta > 0$ and sufficiently small $|\epsilon|$, by (S10), (S11) and the fact that the range of H is contained in $[-1, 1]$, we can show that

$$\Gamma_\epsilon(\eta_0 + \delta) + \alpha\phi_\epsilon \leq (1 + \mathcal{C}|\epsilon|)\,\mathrm{E}_0[I\{\xi_\epsilon(V) > \eta_0 + \delta\}\delta_0^C(V)] + \alpha\phi_\epsilon \leq (1 + \mathcal{C}|\epsilon|)\Gamma_0\left(\eta_0 + \delta - \mathcal{C}|\epsilon|\right) + \alpha\phi_\epsilon.$$

Under Condition B3, as long as δ is small enough, the right-hand side converges to $\Gamma_0(\eta_0 + \delta) + \alpha\phi_0$ as $\epsilon \to 0$. Moreover, Conditions B3 and A4 can be combined to show that the derivative of Γ_0 is strictly negative for all $x \in [\eta_0, \eta_0 + \delta]$ for sufficiently small δ, and so $\Gamma_0(\eta_0) > \Gamma_0(\eta_0 + \delta)$. Because $\Gamma_0(\eta_0) + \alpha\phi_0 = \kappa$ by the definition of ρ_0 under Condition B2, it follows that, for all ϵ sufficiently close to zero, $\Gamma_\epsilon(\eta_0 + \delta) + \alpha\phi_\epsilon < \kappa$. By the definition $\eta_\epsilon := \inf\{\eta : \Gamma_\epsilon(\eta) \leq \kappa - \alpha\phi_\epsilon\}$, it follows that, for all ϵ sufficiently close to zero, $\eta_0 + \delta \geq \eta_\epsilon$, that is, $\eta_\epsilon - \eta_0 \leq \delta$.

By similar arguments, we can show that, for all ϵ sufficiently close to zero, $\eta_\epsilon - \eta_0 \geq -\delta$. Indeed,

$$\Gamma_\epsilon(\eta_0 - \delta) + \alpha\phi_\epsilon \geq (1 - \mathcal{C}|\epsilon|)\Gamma_0(\eta_0 - \delta + \mathcal{C}|\epsilon|) + \alpha\phi_\epsilon.$$

The right-hand side converges to $\Gamma_0(\eta_0 - \delta) + \alpha\phi_0$ as $\epsilon \to 0$ provided δ is sufficiently small. The derivative of Γ_0 is strictly negative on $[\eta_0 - \delta, \eta_0]$ provided δ is small enough, and therefore, $\Gamma_0(\eta_0 - \delta) + \alpha\phi_0 > \Gamma_0(\eta_0) + \alpha\phi_0 = \kappa$. Hence, $\Gamma_\epsilon(\eta_0 - \delta) + \alpha\phi_\epsilon > \kappa$. By the definition of η_ϵ, it follows that $\eta_\epsilon - \eta_0 \geq -\delta$.

Combining these two results, we see that, for all ϵ sufficiently close to zero, $|\eta_\epsilon - \eta_0| \leq \delta$. Hence, $\limsup_{\epsilon \to 0} |\eta_\epsilon - \eta_0| \leq \delta$. As $\delta > 0$ is an arbitrary in a neighborhood of zero, it follows that $\limsup_{\epsilon \to 0} |\eta_\epsilon - \eta_0| = 0$. That is, $\eta_\epsilon \to \eta_0$ as $\epsilon \to 0$ in the case that $\eta_0 > -\infty$.

We now study the case where $\eta_0 = -\infty$. If $\kappa = \infty$, then it is trivial that $\eta_\epsilon = -\infty = \eta_0$ for all ϵ, and so the desired result holds. Suppose now that $\kappa < \infty$. Fix a small enough $\delta > 0$ so that the bound in (S11) is valid for all $\epsilon \in [-\delta, \delta]$. Also fix $\epsilon \in [-\delta, \delta]$ and $\eta \in \mathbb{R}$. By (S11) and the bound on the range of

H,

$$\Gamma_\epsilon(\eta) + \alpha\phi_\epsilon \le (1 + \mathcal{C}|\epsilon|)\,\mathrm{E}_0[I\{\xi_\epsilon(V) > \eta\}\Delta^C_{0,b}(V)] + \alpha\phi_\epsilon \le (1 + \mathcal{C}|\epsilon|)\Gamma_0(\eta - \mathcal{C}|\epsilon|) + \alpha\phi_\epsilon.$$

Because Γ_0 is a nonnegative decreasing function, the right-hand side is no greater than $(1 + \mathcal{C}|\epsilon|)\Gamma_0(\eta - \mathcal{C}\delta) + \alpha\phi_\epsilon$. This upper bound tends to $\Gamma_0(\eta - \mathcal{C}\delta) + \alpha\phi_0$ as $\epsilon \to 0$. Hence, $\limsup_{\epsilon\to 0} \Gamma_\epsilon(\eta) + \alpha\phi_\epsilon \le \Gamma_0(\eta-\mathcal{C}\delta)+\alpha\phi_0$. By Condition B3 and the monotonicity of Γ_0, $\Gamma_0(\eta-\mathcal{C}\delta)+\alpha\phi_0 < \kappa$, and so $\Gamma_\epsilon(\eta)+\alpha\phi_\epsilon < \kappa$ for all ϵ sufficiently close to zero. By the definition of η_ϵ, it follows that $\eta_\epsilon \le \eta$ for all ϵ sufficiently close to zero. Since $\eta \in \mathbb{R}$ is arbitrary, the desired result follows. □

The next lemma establishes a rate of convergence of τ_ϵ to τ_0 as $\epsilon \to 0$.

Lemma S2. *Under conditions of Theorem 3, $\tau_\epsilon = \tau_0 + \mathrm{O}(\epsilon)$.*

Proof of Lemma S2. We separately consider the cases where $\eta_0 < 0$ and $\eta_0 \ge 0$.

We start with the easier case where $\eta_0 < 0$. In this case, Lemma S1 shows that $\tau_\epsilon := \max\{\eta_\epsilon, 0\}$ is equal to $\tau_0 = 0$ for all ϵ sufficiently close to zero. Thus, $\tau_\epsilon - \tau_0 = \mathrm{O}(|\epsilon|)$.

Now consider the more difficult case where $\eta_0 \ge 0$. By the Lipschitz property of the function $x \mapsto \max\{x, 0\}$, we can show that $|\max\{\eta_\epsilon, 0\} - \max\{\eta_0, 0\}| \le |\eta_\epsilon - \eta_0|$. As a consequence, to show that $\tau_\epsilon - \tau_0 = \mathrm{O}(\epsilon)$, it suffices to show that $\eta_\epsilon - \eta_0 = \mathrm{O}(\epsilon)$. We next establish this statement.

Fix ϵ in a sufficiently small neighborhood of zero. By the definition $\eta_\epsilon := \inf\{\eta : \Gamma_\epsilon(\eta) \le \kappa - \phi_\epsilon\}$, the bound on the range of H, and (S11), it holds that $\kappa < \Gamma_\epsilon(\eta_\epsilon - |\epsilon|) + \alpha\phi_\epsilon \le [1+\mathcal{C}|\epsilon|]\Gamma_0(\eta_\epsilon - [1+\mathcal{C}]|\epsilon|) + \alpha\phi_\epsilon$. We use a Taylor expansion of Γ_0 about η_0, which is justified by Condition B3 provided $|\epsilon|$ is small enough, and it follows that

$$\kappa < [1 + \mathcal{C}|\epsilon|]\left[\Gamma_0(\eta_0) + \{\eta_\epsilon - \eta_0 - (1 - \mathcal{C})|\epsilon|\}\{\Gamma_0'(\eta_0) + \mathrm{o}(1)\}\right] + \alpha\phi_0 + \mathrm{O}(\epsilon).$$

By Condition B3, $\Gamma_0(\eta_0) + \alpha\phi_0 = \kappa$. Plugging this into the above shows that

$$0 < \mathcal{C}\Gamma_0(\eta_0)|\epsilon| + [1 + \mathcal{C}|\epsilon|]\left[\eta_\epsilon - \eta_0 - (1 - \mathcal{C})|\epsilon|\right]\left[\Gamma_0'(\eta_0) + \mathrm{o}(1)\right] + \mathrm{O}(\epsilon).$$

Note that Condition B3 implies that $\Gamma_0'(\eta_0) \in (-\infty, 0)$. Therefore, the above shows that, for all ϵ sufficiently close to zero, $0 < [\eta_\epsilon - \eta_0]\Gamma_0'(\eta_0) + \mathcal{C}|\epsilon| + \mathrm{o}\,(\eta_\epsilon - \eta_0)$, which implies that there exists an $\mathrm{O}(\epsilon)$ sequence for which $\eta_\epsilon - \eta_0 < \mathrm{O}(\epsilon)$.

A similar argument, which is based on the observation that $\Gamma_\epsilon(\eta_\epsilon + |\epsilon|) + \phi_\epsilon \le \kappa$, can be used to show that there exists an $\mathrm{O}(\epsilon)$ sequence such that $\eta_\epsilon - \eta_0 > \mathrm{O}(\epsilon)$. Combining these two bounds shows that $\eta_\epsilon - \eta_0 = \mathrm{O}(\epsilon)$, as desired. This concludes the proof. $\square$

Our derivation of the canonical gradient is based on the following decomposition:

$$\begin{aligned}
&\Psi_{\rho_\epsilon}(P_\epsilon) - \Psi_{\rho_0}(P_0) \\
&\quad = \Psi_{\rho_\epsilon}(P_\epsilon) - \Psi_{\rho_0}(P_\epsilon) + \Psi_{\rho_0}(P_\epsilon) - \Psi_{\rho_0}(P_0) \\
&\quad = P_\epsilon\{[\rho_\epsilon - \rho_0]\delta_\epsilon^Y\} + \Psi_{\rho_0}(P_\epsilon) - \Psi_{\rho_0}(P_0) \\
&\quad = P_\epsilon\{[\rho_\epsilon - \rho_0](\delta_\epsilon^Y - \tau_0\delta_\epsilon^C)\} + \tau_0 P_\epsilon\{(\rho_\epsilon - \rho_0)\delta_\epsilon^C\} + \Psi_{\rho_0}(P_\epsilon) - \Psi_{\rho_0}(P_0) \\
&\quad = P_\epsilon\{[\rho_\epsilon - \rho_0](\delta_\epsilon^Y - \tau_0\delta_0^C)\} + [\Psi_{\rho_0}(P_\epsilon) - \Psi_{\rho_0}(P_0)] + \tau_0\{P_\epsilon[\delta_\epsilon^C\rho_\epsilon] + \alpha\phi_\epsilon - P_0[\delta_0^C\rho_0] - \alpha\phi_0\} \\
&\qquad - \tau_0 P_\epsilon\{(\delta_\epsilon^C - \Delta_{0,b}^C)\rho_0\} - \tau_0(P_\epsilon - P_0)\{\delta_0^C\rho_0\} - \alpha\tau_0\{\phi_\epsilon - \phi_0\}.
\end{aligned} \tag{S12}$$

We separately study each of the six terms on the right-hand side, which we refer to as term 1 up to term 6.

Study of term 1 in (S12)**:** We will show that this term is $\mathrm{o}(\epsilon)$. By Lemma S2 and (S9),

$$\sup_v |\delta_\epsilon^Y(v) - \tau_\epsilon\delta_\epsilon^C - \delta_0^Y(v) + \tau_0\delta_0^C| \le \sup_v |\delta_\epsilon^Y(v) - \delta_0^Y(v)| + \sup_v |\delta_\epsilon^C(v) - \delta_0^C(v)| + |\tau_\epsilon - \tau_0| \lesssim |\epsilon|.$$

Under Condition B2, $P_0\{\xi_0(V) = \tau_0\} = 0$. We apply a similar argument as that used to prove Lemma 2 in van der Laan and Luedtke [46]:

$$\begin{aligned}
&\left|P_\epsilon\{[\rho_\epsilon - \rho_0](\delta_\epsilon^Y - \tau_0\delta_\epsilon^C)\}\right| \\
&\quad = \left|\int [\rho_\epsilon(v) - \rho_0(v)][\delta_\epsilon^Y(v) - \tau_0\delta_\epsilon^C(v)] P_{W,\epsilon}(dw)\right| \\
&\quad \le \int |\rho_\epsilon(v) - \rho_0(v)| \left|\delta_\epsilon^Y(v) - \tau_0\delta_\epsilon^C(v)\right| P_{W,\epsilon}(dw).
\end{aligned}$$

Because $\rho_\epsilon(v) \ne \rho_0(v)$ implies that either (i) $\xi_\epsilon(v) - \tau_\epsilon$ and $\xi_0(v) - \tau_0$ have different signs or (ii) only one of these quantities is zero, the display continues as

$$\begin{aligned}
&\le \int I\{|\xi_0(v) - \tau_0| \le |\xi_\epsilon(v) - \tau_\epsilon - \xi_0(v) + \tau_0|\} \left|\delta_\epsilon^Y(v) - \tau_0\delta_\epsilon^C(v)\right| P_{W,\epsilon}(dw) \\
&\le \int I\{|\xi_0(v) - \tau_0| \le \mathcal{C}|\epsilon|\} \left(\left|\delta_0^Y(v) - \tau_0\delta_0^C(v)\right| + \mathcal{C}|\epsilon|\right) P_{W,\epsilon}(dw).
\end{aligned}$$

Using the facts that $\inf_v \delta_0^C(v) > 0$ by Condition A4, that $\sup_v \delta_0^C(v) \leq 1$ since probabilities are no more than one, and that $\xi_0(v) := \delta_0^Y(v)/\delta_0^C(v)$, the display continues as

$$\leq \int I\{|\xi_0(v) - \tau_0| \leq \mathcal{C}|\epsilon|\} \left(|\xi_0(v) - \tau_0| + \mathcal{C}|\epsilon|\right) P_{W,\epsilon}(dw)$$

Leveraging the bound on $|\xi_0(v) - \tau_0|$ that appears in the indicator function, we see that

$$\begin{aligned}
&\leq \int I\{|\xi_0(v) - \tau_0| \leq \mathcal{C}|\epsilon|\}(\mathcal{C}|\epsilon| + \mathcal{C}|\epsilon|)P_{W,\epsilon}(dw) \\
&\lesssim |\epsilon| \int I\{|\xi_0(v) - \tau_0| \leq \mathcal{C}|\epsilon|\}P_{W,0}(dw) \\
&= |\epsilon| \int I\{0 < |\xi_0(v) - \tau_0| \leq \mathcal{C}|\epsilon|\}P_{W,0}(dw),
\end{aligned}$$

where the final equality holds by Condition B1. The integral in the final expression is $\mathrm{o}(1)$, and so this expression is $\mathrm{o}(\epsilon)$.

Study of term 2 in (S12)**:** By the result on the pathwise differentiability of $P \mapsto \Psi_{\rho^{\mathrm{FR}}}(P)$, setting ρ^{FR} to be ρ_0, we see that the second term satisfies $\Psi_{\rho_0}(P_\epsilon) - \Psi_{\rho_0}(P_0) = \epsilon \int G_2(o)H(o)P(do) + \mathrm{o}(\epsilon)$, where $G_2 \in L_0^2(P_0)$ is equal to $D(P_0, \rho_0, 0, \mu_0^C)$.

Study of term 3 in (S12)**:** We will show that the third term is identical to zero for any ϵ that is sufficiently close to zero. If $\tau_0 = 0$, then this term is trivially zero. Otherwise, $\tau_0 = \eta_0 > 0$. Lemma S1 shows that, in this case, $\eta_\epsilon > 0$ for ϵ sufficiently close to zero. Hence, $\mathrm{E}_\epsilon[\delta_\epsilon^C(V)\rho_\epsilon(V)] + \alpha\phi_\epsilon = \kappa = \mathrm{E}_0[\delta_0^C(V)\rho_0(V)] + \alpha\phi_0$. Consequently, term 3 equals zero for all ϵ sufficiently close to zero.

Study of term 4 in (S12)**:** We will show that this term can be writes as $\epsilon \int G_4(o)H(o)P_0(do) + \mathrm{o}(\epsilon)$ for an appropriately defined $G_4 \in L_0^2(P_0)$ that does not depend on H. Note that there exists a function $H_W : (w \mid v) \mapsto H_W(w \mid v)$ for which $\int H_W(w \mid v)P_{W,0}(dw \mid v) = 0$, $\sup_{w,v} |H_W(w \mid v)| < \infty$, and, for all v,

$$P_{W,\epsilon}(dw \mid v) = (1 + \epsilon H_W(w \mid v) + \mathrm{o}(\epsilon))P_{W,0}(dw \mid v).$$

The function H_W can be chosen so that the above $\mathrm{o}(\epsilon)$ term indicates little-oh behavior uniformly over

w and v. By the definition of H_C from (S3), we see that

$$\begin{aligned}\delta_\epsilon^C(v) - \delta_0^C(v) &= \iint c\Big\{[1+\epsilon H_C(c \mid 1, w)][1+\epsilon H_W(w \mid v) + \mathrm{o}(\epsilon)] - 1\Big\} P_0(dc \mid 1, w) P_0(dw \mid v) \\ &\quad - \iint c\Big\{[1+\epsilon H_C(c \mid 0, w)][1+\epsilon H_W(w \mid v) + \mathrm{o}(\epsilon)] - 1\Big\} P_0(dc \mid 0, w) P_0(dw \mid v) \\ &= \epsilon \Big\{ \iint c(H_C(c \mid 1, w) + H_W(w \mid v) + \mathrm{o}(1)) P_0(dc \mid 1, w) P_0(dw \mid v) \\ &\quad - \iint c(H_C(c \mid 0, w) + H_W(w \mid v) + \mathrm{o}(1)) P_0(dc \mid 0, w) P_0(dw \mid v) \Big\} + \mathrm{o}(\epsilon),\end{aligned}$$

where the little-oh terms are uniform over w and v. Hence,

$$\begin{aligned}&\frac{d}{d\epsilon} P_\epsilon\{[\delta_\epsilon^C - \delta_0^C]\rho_0\}\Big|_{\epsilon=0} \\ &= \iint \rho_0(v) c\{H_C(c \mid 1, w) + H_W(w \mid v)\} P_0(dc \mid 1, w) P_0(dw) \\ &\quad - \iint \rho_0(v) c\{H_C(c \mid 0, w) + H_W(w \mid v)\} P_0(dc \mid 0, w) P_0(dw) \\ &= \mathrm{E}_0\left[\rho_0(V)\left(\frac{1}{T + \mu_0^T(W) - 1}\{C - \mu_0^C(T, W)\} H_C(C \mid 1, W) + \{\Delta_0^C(W) - \delta_0^C(V)\} H_W(W \mid V)\right)\right].\end{aligned}$$

Since $\mathrm{E}_0[H_C(C \mid T, W) \mid T, W] = \mathrm{E}_0[H_W(W \mid V) \mid V] = 0$ P_0-a.s., the display continues as

$$= \mathrm{E}_0\left[\rho_0(V)\left(\frac{1}{T + \mu_0^T(W) - 1}\{C - \mu_0^C(T, W)\} + \Delta_0^C(W) - \delta_0^C(V)\right) H(O)\right].$$

As a consequence, term 4 satisfies

$$-\tau_0 P_\epsilon\{[\delta_\epsilon^C - \delta_0^C]\rho_0\} = \epsilon \int G_4(o) H(o) P_0(do) + \mathrm{o}(\epsilon),$$

where

$$G_4 : o \mapsto -\tau_0 \rho_0(v) \left\{\frac{1}{t + \mu_0^T(w) - 1}[c - \mu_0^C(t, w)] + \Delta_0^C(w) - \delta_0^C(v)\right\}.$$

Study of term 5 in (S12)**:** By (S3) and the fact that $P_0\{\delta_0^C \rho_0\} = \kappa - \alpha\phi_0$ whenever $\tau_0 > 0$, we see that $-\tau_0(P_\epsilon - P_0)\{\delta_0^C \rho_0\} = \epsilon \int G_5(o) H_V(v) P_0(do)$, where $G_5 \in L_0^2(P_0)$ is defined as $o \mapsto -\tau_0[\delta_0^C(v)\rho_0(v) - \kappa + \alpha\phi_0]$. Since H_V is defined as $v \mapsto \mathrm{E}_0[H(O) \mid V = v]$, we see that it also holds that $-\tau_0(P_\epsilon - P_0)\{\delta_0^C \rho_0\} = \epsilon \int G_5(o) H(o) P_0(do)$.

Study of term 6 in (S12)**:** We have shown that

$$\phi_\epsilon - \phi_0 = \epsilon \int \left\{ \frac{1-t}{1-\mu_0^T(w)}[c - \mu_0^C(0,w)] + \mu_0^C(0,w) - \phi_0 \right\} H(o) P_0(do) + \mathrm{o}(\epsilon).$$

Therefore, $-\tau_0 \alpha(\phi_\epsilon - \phi_0) = \epsilon \int G_6(o) H(o) P_0(do) + \mathrm{o}(\epsilon)$ where

$$G_6 : o \mapsto -\tau_0 \alpha \left\{ \frac{1-t}{1-\mu_0^T(w)}[c - \mu_0^C(0,w)] + \mu_0^C(0,w) - \phi_0 \right\}.$$

Conclusion of the derivation of the canonical gradient of $P \mapsto \Psi_{\rho_P}(P)$: Combining our results regarding the six terms in (S12), we see that

$$\Psi_{\rho_\epsilon}(P_\epsilon) - \Psi_{\rho_0}(P_0) = \epsilon \int [G_2(o) + G_4(o) + G_5(o) + G_6(o)] H(o) P_0(do) + \mathrm{o}(\epsilon).$$

Dividing both sides by $\epsilon \neq 0$ and taking the limit as $\epsilon \to 0$, we see that $G_2 + G_4 + G_5 + G_6 = G(P_0)$ is the canonical gradient of $P \mapsto \Psi_{\rho_P}(P)$ at P_0.

S4.3 Expansions based on gradients or pseudo-gradients

In this section, we present (approximate) first-order expansions of ATE parameters based on which we construct our proposed targeted minimum-loss based estimators (TMLE) and prove their asymptotic linearity. We refer the readers to Supplement S5 of Qiu et al. [34] for an overview of TMLE based on gradients and pseudo-gradients. The overall idea behind TMLE based on gradients is the following: the empirical mean of the gradient at the estimated distribution can be viewed as the first-order bias of the plug-in estimator; this bias can be removed by solving the estimating equation that equates the first-order bias to zero. The idea behind pseudo-gradients is similar, except that the gradient is replaced by an approximation that we term *pseudo-gradient* so that the corresponding estimating equation is easy to solve with a single regression step.

For any ITR $\rho : \mathcal{W} \to [0,1]$ that utilizes all covariates, we define

$$\begin{aligned} R_\rho(P, P_0) :=& \Psi_\rho(P) - \Psi_\rho(P_0) + P_0 D(P, \rho, 0, \mu^C) \\ =& \mathrm{E}_0 \left[\rho(W) \left\{ \frac{\mu_P^T(W) - \mu_0^T(W)}{\mu_P^T(W)} (\mu_P^Y(1,W) - \mu_0^Y(1,W)) \right.\right. \\ & \left.\left. + \frac{\mu_P^T(W) - \mu_0^T(W)}{1 - \mu_P^T(W)} (\mu_P^Y(0,W) - \mu_0^Y(0,W)) \right\} \right]. \end{aligned}$$

For any ITR $\rho : \mathcal{V} \to [0,1]$ that only utilizes V, for convenience, we define $R_\rho(P, P_0) := R_{w \mapsto \rho(V(w))}(P, P_0)$.

For $\Psi_{\rho^{\mathrm{FR}}}$ and $\Psi_{\rho_P^{\mathrm{TP}}}$, it is straightforward to show that the following expansions hold:

$$
\begin{aligned}
&\Psi_{\rho^{\mathrm{FR}}}(P) - \Psi_{\rho^{\mathrm{FR}}}(P_0) = -P_0 G_{\mathrm{FR}}(P) + R_{\rho^{\mathrm{FR}}}(P, P_0), \\
&\Psi_{\rho_P^{\mathrm{TP}}}(P) - \Psi_{\rho_{P_0}^{\mathrm{TP}}}(P_0) = -P_0 G_{\mathrm{TP}}(P) + P_0 \left\{ \frac{\mu_P^T(\cdot) - \mu_0^T(\cdot)}{1 - \mu_P^T(\cdot)} (\mu_P^Y(0, \cdot) - \mu_0^Y(0, \cdot)) \right\}.
\end{aligned}
$$

For $P \mapsto \Psi_{\rho_P^{\mathrm{RD}}}(P)$, we expand this parameter sequentially as follows:

$$
\begin{aligned}
&\Psi_{\rho_P^{\mathrm{RD}}}(P) - \Psi_{\rho_{P_0}^{\mathrm{RD}}}(P_0) = P_0 D(P, \rho_P^{\mathrm{RD}}, 0, \mu_P^C) + R_{\rho_P^{\mathrm{RD}}}(P, P_0) + (\rho_P^{\mathrm{RD}} - \rho_0^{\mathrm{RD}}) P_0 \Delta_0^Y, \\
&\rho_P^{\mathrm{RD}} - \rho_0^{\mathrm{RD}} = \frac{\kappa - \phi_P}{P \Delta_P^C} - \frac{\kappa - \phi_0}{P_0 \Delta_0^C}, \\
&(\kappa - \alpha\phi_P) - (\kappa - \alpha\phi_0) = \alpha \left\{ P_0 D_1(P, \mu^C) + P_0 \left\{ (\mu^C(0, \cdot) - \mu^C(1, \cdot)) \frac{\mu_P^T - \mu_0^T}{1 - \mu_P^T} \right\} \right\}, \\
&P \Delta_P^C - P_0 \Delta_0^C = -P_0 D_2(P, \mu_P^C) + P_0 \left\{ (\mu_P^C(1, \cdot) - \mu_0^C(1, \cdot)) \frac{\mu_P^T - \mu_0^T}{\mu_P^T} + (\mu_P^C(0, \cdot) - \mu_0^C(0, \cdot)) \frac{\mu_P^T - \mu_0^T}{1 - \mu_P^T} \right\}.
\end{aligned}
$$

For $P \mapsto \Psi_{\rho_P}(P)$, straightforward but tedious calculation shows that the following expansion holds:

$$
\begin{aligned}
\Psi_{\rho_P}(P) - \Psi_{\rho_0}(P_0) = &-P_0 D(P, \rho, \tau_0, \mu^C) \\
&+ R_\rho(P, P_0) + P_0\{(\rho - \rho_0)(\delta_0^Y - \tau_0 \delta_0^C)\} \\
&- \tau_0 \, \mathrm{E}_0 \left[\rho(V) \frac{\mu_P^T(W) - \mu_0^T(W)}{\mu_P^T(W)} \{\mu^C(1, W) - \mu_0^C(1, W)\} \right] \\
&+ \tau_0 \, \mathrm{E}_0 \left[(1 - \rho(V)) \frac{\mu_P^T(W) - \mu_0^T(W)}{1 - \mu_P^T(W)} \{\mu^C(0, W) - \mu_0^C(0, W)\} \right].
\end{aligned}
$$

S4.4 Asymptotic linearity of proposed estimator (Theorem 4)

For convenience, we set $\hat{P}_n$ to have component μ_n^T and $\hat{\mu}_n^C$, even though the plug-in estimator does not explicitly involve these functions. We start with some lemmas that facilitate the proof of the main theorem. In this section, we define $\eta_n := \eta_n(k_n)$ and $\tau_n := \tau_n(k_n)$ to simplify notations.

Our proof is centered around the expansions in Supplement S4.3. We first prove a few lemmas. Lemma S3 is a standard asymptotic linearity result on estimators ϕ_n and $P_n \hat{\Delta}_n^C$ about treatment resource being used for constant ITRs $v \mapsto 0$ and $v \mapsto 1$, respectively; Lemma S4 is a technical convenient tool to convert conditions on norms in Condition B6 between functions; Lemmas S5–S7 are analysis results for estimators that are similar to Lemmas S1–S2 for deterministic perturbations of P_0, and they lead to the crucial Lemma S8 on the negligibility of the remainder $R_\rho(\hat{P}_n, P_0)$ for an arbitrary ITR ρ.

Lemma S3 (Asymptotic linearity of ϕ_n and $P_n\hat{\Delta}_n^C$)**.** *Under the conditions of Theorem 4,*

$$\begin{aligned}\phi_n - \phi_0 &= (P_n - P_0)D_1(P_0, \mu_0^C) + \mathrm{o}_p(n^{-1/2}) = \mathrm{O}_p(n^{-1/2}),\\ P_n\hat{\Delta}_n^C - P_0\Delta_0^C &= (P_n - P_0)D_2(P_0, \mu_0^C) + \mathrm{o}_p(n^{-1/2}) = \mathrm{O}_p(n^{-1/2}).\end{aligned}$$

This result follows from the facts that (i) ϕ_n is a one-step correction estimator of ϕ_0 [30], and (ii) $P_n\hat{\Delta}_n^C$ is a TMLE for $P_0\Delta_0^C$ [44, 49]. Therefore the proof is omitted.

Lemma S4 (Lemma S8 in Qiu et al. [34])**.** *Fix functions $\mu^C : \{0,1\}\times\mathcal{W} \to [0,1]$ and $\mu^Y : \{0,1\}\times\mathcal{W} \to \mathbb{R}$, and suppose that $P_0\mu^Y(0,\cdot)^2 < \infty$ and $P_0\mu^Y(1,\cdot)^2 < \infty$. If Condition A2 holds, then*

$$\begin{aligned}\|\mu^Y(1,\cdot) - \mu_0^Y(1,\cdot)\|_{2,P_0} + \|\mu^Y(0,\cdot) - \mu_0^Y(0,\cdot)\|_{2,P_0} &\simeq \|\mu^Y - \mu_0^Y\|_{2,P_0},\\ \|\mu^C(1,\cdot) - \mu_0^C(1,\cdot)\|_{2,P_0} + \|\mu^C(0,\cdot) - \mu_0^C(0,\cdot)\|_{2,P_0} &\simeq \|\mu^C - \mu_0^C\|_{2,P_0},\end{aligned}$$

where $a \simeq b$ is defined as $a \lesssim b$ and $b \lesssim a$.

The following Lemmas S5–S7 prove consistency of the estimated thresholds used to define the estimated optimal ITR ρ_n.

Lemma S5 (Lemma S5 in Qiu et al. [34])**.** *Let $\epsilon > 0$, $\eta \in \mathbb{R}$, $g : \mathcal{O} \to \mathbb{R}$ be bounded and functions $f_0 : \mathcal{O} \to \mathbb{R}$ and $f : \mathcal{O} \to \mathbb{R}$. Then*

$$\begin{aligned}|P_0([I(f > \eta) - I(f_0 > \eta)]g)| &\le P_0|[I(f > \eta) - I(f_0 > \eta)]g|\\ &\lesssim P_0\{|f(O) - f_0(O)| > \epsilon\} + P_0\{|f_0(O) - \eta| \le \epsilon\}.\end{aligned}$$

If g takes values in $[-1, 1]$, then $\lesssim$ can be replaced by $\le$.

Lemma S6 (Consistency of $\eta_n(\kappa)$)**.** *Under Conditions B2, B3 and B12, $\eta_n(\kappa) \xrightarrow{p} \eta_0$.*

This lemma is a stochastic variant of the deterministic result in Lemma S1 and has a similar proof. Therefore, the arguments are slightly abbreviated here.

Proof of Lemma S6. We separately consider the cases where $\eta_0 > -\infty$ and $\eta_0 = -\infty$.

First consider the case where $\eta_0 > -\infty$. We start by showing that, for any η sufficiently close to η_0, it holds that $\Gamma_n(\eta) - \Gamma_0(\eta) = o_p(1)$. Fix an η in a neighborhood of η_0. By the triangle inequality,

$$\begin{aligned}|\Gamma_n(\eta) - \Gamma_0(\eta)| \leq& |P_0[I\{\xi_n(V(\cdot)) > \eta\} - I(\xi_0(V(\cdot)) > \eta)]\Delta_0^C| \\ &+ |P_0 I\{\xi_n(V(\cdot)) > \eta\}[\Delta_n^C - \Delta_0^C]| \\ &+ |(P_n - P_0) I\{\xi_n(V(\cdot)) > \eta\}\Delta_n^C|. \end{aligned} \tag{S13}$$

We will show that the right-hand side is $o_p(1)$. By Condition B12, the third term on the right is $o_p(1)$ for η sufficiently close to η_0. Moreover, because the second term is no greater than $\|\Delta_n^C - \Delta_0^C\|_{1,P_0}$, Condition B12 also implies that this second term is also $o_p(1)$. We will now argue that the first term is $o_p(1)$. By Lemma S5 and Condition B4, for any $\epsilon' > 0$,

$$\begin{aligned}|P_0[I(\xi_n(V(\cdot)) > \eta) - I(\xi_0(V(\cdot)) > \eta)]\Delta_0^C| &\lesssim P_0|I(\xi_n > \eta) - I(\xi_0 > \eta)| \\ &\leq P_0 I(|\xi_n - \xi_0| > \epsilon') + P_0 I(|\xi_0 - \eta| \leq \epsilon') \\ &\leq \frac{\|\xi_n - \xi_0\|_{1,P_0}}{\epsilon'} + P_0 I(|\xi_0 - \eta| \leq \epsilon'),\end{aligned}$$

where the final relation follows from Markov's inequality. We next show that the last line is $o_p(1)$. Fix $\epsilon > 0$. For η that is sufficiently close to η_0 and ϵ' that is sufficiently small, by Condition B2, we see that S_0 is continuous in $[\eta - \epsilon', \eta + \epsilon']$ and hence, for all sufficiently small $\epsilon' > 0$, it holds that $P_0 I(|\xi_0 - \eta| \leq \epsilon') \leq \epsilon/2$. Therefore,

$$\begin{aligned}P_0\left\{|P_0[I(\xi_n > \eta) - I(\xi_0 > \eta)]| > \epsilon\right\} &\leq P_0\left\{\frac{\|\xi_n - \xi_0\|_{1,P_0}}{\epsilon'} + P_0 I(|\xi_0 - \eta| \leq \epsilon') > \epsilon\right\} \\ &\leq P_0\left\{\frac{\|\xi_n - \xi_0\|_{1,P_0}}{\epsilon'} > \epsilon/2\right\}.\end{aligned}$$

Since $\|\xi_n - \xi_0\|_{1,P_0} = o_p(1)$ by Condition B12, the right-hand side of the above display converges to zero as $n \to \infty$. Therefore, $|P_0[I(\xi_n(V(\cdot)) > \eta) - I(\xi_0(V(\cdot)) > \eta)]\Delta_0^C| = o_p(1)$. Recalling (S13), the above results imply that $\Gamma_n(\eta) - \Gamma_0(\eta) = o_p(1)$ for any η that is sufficiently close to η_0.

Fix $\epsilon > 0$. For any ϵ sufficiently small, the above result and Lemma S3 imply that $\Gamma_n(\eta_0 - \epsilon) + \alpha\phi_n = \Gamma_0(\eta_0 - \epsilon) + \alpha\phi_0 + o_p(1)$ and $\Gamma_n(\eta_0 + \epsilon) + \alpha\phi_n = \Gamma_0(\eta_0 + \epsilon) + \alpha\phi_0 + o_p(1)$. By Condition B3, $\Gamma_0(\eta_0 - \epsilon) + \alpha\phi_0 > \kappa > \Gamma_0(\eta_0 + \epsilon) + \alpha\phi_0$ provided ϵ is sufficiently small. It follows that, with probability tending to one, $\Gamma_n(\eta_0 - \epsilon) + \alpha\phi_n > \kappa > \Gamma_n(\eta_0 + \epsilon) + \alpha\phi_n$, and hence $\eta_0 - \epsilon \leq \eta_n(\kappa) \leq \eta_0 + \epsilon$ by the definition of $\eta_n(\kappa)$. Because ϵ is arbitrary, it follows that $\eta_n(\kappa) \xrightarrow{p} \eta_0$.

The case where $\eta_0 = -\infty$ can be proved similarly. If $\kappa = \infty$, then it trivially holds that $\eta_n(\kappa) = -\infty = \eta_0$ for all n and the desired result holds. Otherwise, for any $\eta < 0$ for which $|\eta|$ is sufficiently large, a nearly identical argument to that used above shows that $[\Gamma_n(\eta) + \alpha\phi_n] - [\Gamma_0(\eta) + \alpha\phi_0] = \mathrm{o}_p(1)$. By Condition B3 and monotonicity of Γ_0, it follows that $\Gamma_0(\eta) + \alpha\phi_0 < \kappa$, and so, with probability tending to one, $\Gamma_n(\eta) + \alpha\phi_n < \kappa$ and hence $\eta_n(\kappa) \leq \eta$ by the definition of $\eta_n(\kappa)$. Because η is arbitrary, we have shown that $\eta_n(\kappa) \xrightarrow{p} -\infty = \eta_0$. $\square$

Lemma S7 (Consistency of τ_n and existence of solution to Eq. 5 when $\eta_0 > -\infty$)**.** *Assume that the conditions of Theorem 4 hold. The following statements hold:*

i) if $\eta_0 > -\infty$, then, with probability tending to one, a solution $k_n' \in [0, \infty)$ to (5) exists. Note that we let $k_n = k_n'$ when $\eta_n(\kappa) > 0$ and k_n' exists. Hence, if $\eta_0 > 0$, $\eta_n = \eta_n(k_n) = \eta_n(k_n')$ with probability tending to one;

ii) if a solution k_n' to (5) exists, then with probability tending to one, $P_0\{d_{n,k_n'}\Delta_n^C\} + \alpha\phi_0 = \kappa + \mathrm{O}_p(n^{-1/2})$;

iii) $\tau_n - \tau_0 = \mathrm{o}_p(1)$.

We separately prove i, ii, and iii in the case that $\eta_0 > -\infty$, and then we separately prove iii in the cases where $\eta_0 > 0$, $\eta_0 = 0$ and $\eta_0 < 0$.

Proof of i from Lemma S7. Our strategy for showing the existence of a solution to (5) is as follows. First, we show that the left-hand side of (5) consistently estimates the treatment resource being used uniformly over rules $\{d_{n,k} : k \in [0, \infty]\}$. Next, we show that the left-hand side of (5) is a continuous function in k that takes different signs at $k = 0$ and $k = \infty$ with probability tending to one.

Define $f_{n,k} : o \mapsto d_{n,k}(v)\left[\Delta_n^C(w) + \frac{1}{t+\mu_n^T(w)-1}[c - \mu_n^C(t,w)]\right]$. We first show that

$$\sup_{k\in[0,\infty]} |P_n f_{n,k} - P_0\{d_{n,k}\Delta_0^C\}| = \mathrm{O}_p(n^{-1/2}). \tag{S14}$$

We rely on the fact that, for fixed $d_{n,k}$, $P_n f_{n,k}$ is a one-step estimator of $P_0\{d_{n,k}\Delta_0^C\}$. Note that

$$\begin{aligned}\sup_{k\in[0,\infty]} \left|P_n f_{n,k} - P_0\{d_{n,k}\Delta_0^C\}\right| \leq& \sup_{k\in[0,\infty]} \left|(P_n - P_0) d_{n,k} D_2(\hat{P}_n, \mu_n^C)\right| \\ &+ \sup_{k\in[0,\infty]} \left|P_0\left\{d_{n,k}(V(\cdot))\frac{\mu_n^T(\cdot) - \mu_0^T(\cdot)}{\mu_n^T(\cdot)}[\mu_n^C(1,\cdot) - \mu_0^C(1,\cdot)]\right\}\right|\end{aligned}$$

$$+ \sup_{k\in[0,\infty]} \left| P_0 \left\{ d_{n,k}(V(\cdot)) \frac{\mu_n^T(\cdot) - \mu_0^T(\cdot)}{1-\mu_n^T(\cdot)} [\mu_n^C(0,\cdot) - \mu_0^C(0,\cdot)] \right\} \right|.$$

Conditions B7 and B11 along with Lemma S4 imply that the first term on the right-hand side is $\mathrm{O}_p(n^{-1/2})$. For the second term, we note that the fact that $d_{n,k}(V(w)) \in [0,1]$ for all $w \in \mathcal{W}$ and all $k \in [0,\infty]$ and the Cauchy-Schwarz inequality imply that

$$\begin{aligned} &\sup_{k\in[0,\infty]} \left| P_0 \left\{ d_{n,k}(V(\cdot)) \frac{\mu_n^T(\cdot) - \mu_0^T(\cdot)}{\mu_n^T(\cdot)} [\mu_n^C(1,\cdot) - \mu_0^C(1,\cdot)] \right\} \right| \\ &\leq P_0 \left| \frac{\mu_n^T(\cdot) - \mu_0^T(\cdot)}{\mu_n^T(\cdot)} [\mu_n^C(1,\cdot) - \mu_0^C(1,\cdot)] \right| \lesssim \|\mu_n^T - \mu_0^T\|_{2,P_0} \|\mu_n^C(1,\cdot) - \mu_0^C(1,\cdot)\|_{2,P_0}. \end{aligned}$$

Hence, the second term is $\mathrm{o}_p(n^{-1/2})$ by Condition B6. The third term is also $\mathrm{o}_p(n^{-1/2})$ by an almost identical argument. Combining the previous two displays shows that (S14) holds.

Applying (S14) at $k=0$ shows that $P_n f_{n,0} + \alpha\phi_n = P_0\{d_{n,0}\Delta_0^C\} + \alpha\phi_0 + \mathrm{O}_p(n^{-1/2}) = \alpha\phi_0 + \mathrm{O}_p(n^{-1/2})$. Therefore, $P_n f_{n,0} + \alpha\phi_n < \kappa$ with probability tending to one. Applying this result at $k=\infty$ shows that $P_n f_{n,1} + \alpha\phi_n = P_0\{d_{n,\infty}\Delta_0^C\} + \alpha\phi_0 + \mathrm{O}_p(n^{-1/2}) = P_0\Delta_0^C + \alpha\phi_0 + \mathrm{O}_p(n^{-1/2})$. Combining this fact with the fact that $P_0\Delta_0^C + \alpha\phi_0 > \kappa$ whenever $\eta_0 > -\infty$ shows that $P_n f_{n,1} + \alpha\phi_n > \kappa$ with probability tending to one. Combining these results at $k=0$ and $k=\infty$ with the fact that $k \mapsto P_n f_{n,k}$ is a continuous function shows that, with probability tending to one, there exists a $k_n' \in [0,\infty)$ such that $P_n f_{n,k_n'} = \kappa - \alpha\phi_n$. Lemma S6 then implies $\eta_n = \eta_n(k_n)$ with probability tending to 1. □

Proof of ii from Lemma S7. . By Lemma S3, Eq. S14 and part i of this lemma, we see that $P_0\{d_{n,k_n}\Delta_0^C\} + \alpha\phi_0 = P_n f_{n,k_n} + \alpha\phi_n + \mathrm{O}_p(n^{-1/2}) = \kappa + \mathrm{O}_p(n^{-1/2})$, as desired. □

Proof of iii from Lemma S7 when $\eta_0 > 0$. In this proof, we use P_0^n to denote a probability statement over the draws of $O_1, \ldots, O_n$. Fix $\epsilon > 0$. We will argue by contradiction to show that $P_0^n\{\eta_n \geq \eta_0 + \epsilon\} \to 0$ and $P_0^n\{\eta_n \leq \eta_0 - \epsilon\} \to 0$ as $n \to \infty$, implying the consistency of η_n. The consistency of τ_n then follows. We study these two events separately. First, we suppose that

$$\limsup_n P_0^n\{\eta_n \geq \eta_0 + \epsilon\} > 0. \tag{S15}$$

Then there exists $\delta > 0$ such that, for all n in an infinite sequence $N \subseteq \mathbb{N}$, the probability $P_0^n\{\eta_n \geq \eta_0 + \epsilon\}$

is at least δ. Consequently, for any $n \in N$, the following holds with probability at least δ:

$$\begin{aligned} P_0\{d_{n,k_n}\Delta_0^C\} + \alpha\phi_0 - \kappa &\leq P_0\{I(\xi_n > \eta_0 + \epsilon/2)\Delta_0^C\} + \alpha\phi_0 - \kappa \\ &= P_0\{[I(\xi_n > \eta_0 + \epsilon/2) - I(\xi_0 > \eta_0 + \epsilon/2)]\Delta_0^C\} + \Gamma_0(\eta_0 + \epsilon/2) + \alpha\phi_0 - \kappa. \end{aligned} \tag{S16}$$

We now show that the first term is $\mathrm{o}_p(1)$. For any $x > 0$ and $n \in \mathbb{N}$, by Lemma S5 and Condition B4,

$$\begin{aligned} |P_0\{[I(\xi_n > \eta_0 + \epsilon/2) - I(\xi_0 > \eta_0 + \epsilon/2)]\Delta_0^C\}| &\lesssim P_0 I(|\xi_n - \xi_0| > x) + P_0 I(|\xi_0 - \eta_n + \epsilon/2| \leq x) \\ &\leq \frac{\|\xi_n - \xi_0\|_{1,P_0}}{x} + P_0 I(|\xi_0 - \eta_n + \epsilon/2| \leq x). \end{aligned}$$

Similarly to the proof of Lemma S6, the fact that $\|\xi_n - \xi_0\|_{1,P_0} = \mathrm{o}_p(1)$ (Condition B12) ensures that $P_0\{[I(\xi_n > \eta_0 + \epsilon/2) - I(\xi_0 > \eta_0 + \epsilon/2)]\Delta_0^C = \mathrm{o}_p(1)$. By Condition B3, $\Gamma_0(\eta_0 + \epsilon/2) - \Gamma_0(\eta_0)$ is a negative constant. Because (S16) holds with probability at least $\delta > 0$ for infinitely many n, this shows that $P_0\{d_{n,k_n}\Delta_0^C\} + \alpha\phi_0 - \kappa$ *is not* $\mathrm{o}_p(1)$. This contradicts our result from part ii of this lemma. Therefore, (S15) is false, that is, $\limsup_n P_0^n\{\eta_n \geq \eta_0 + \epsilon\} = 0$.

Now we assume that, for some $\epsilon > 0$, $\limsup_n P_0^n\{\eta_n \leq \eta_0 - \epsilon\} > 0$. Then there exists $\delta > 0$ such that, for all n in an infinite sequence $N \subseteq \mathbb{N}$, $P_0^n\{\eta_n \leq \eta_0 - \epsilon\} \geq \delta$. Now, for any $n \in N$, the following holds with probability at least δ:

$$\begin{aligned} P_0\{d_{n,k_n}\Delta_0^C\} + \alpha\phi_0 - \kappa &\geq P_0\{I(\xi_n > \eta_0 - \epsilon)\Delta_0^C\} + \alpha\phi_0 - \kappa \\ &= P_0\{[I(\xi_n > \eta_0 - \epsilon) - I(\xi_0 > \eta_0 - \epsilon)]\nu_0\} + \Gamma_0(\eta_0 - \epsilon) + \alpha\phi_0 - \kappa. \end{aligned}$$

The rest of the argument is almost identical to the contradiction argument for the previous event, and is therefore omitted.

Since ϵ is arbitrary, combining the results of these two contradiction arguments shows that $|\tau_n - \tau_0| \leq |\eta_n - \eta_0| = \mathrm{o}_p(1)$, as desired. □

Proof of iii from Lemma S7 when $\eta_0 = 0$. If $\eta_0 = 0$, then the construction of η_n implies that η_n takes values from two sequences: $\eta_n(\kappa)$ and $\eta_n(k_n)$ where k_n is a solution to (5). By Lemma S6, $\eta_n(\kappa)$ is consistent for η_0. When a solution to (5) exists and equals k_n, the proof of part iii from Lemma S7 when $\eta_0 > 0$ shows that $\eta_n(k_n)$ is consistent for η_0 and the desired result follows. □

Proof of iii from Lemma S7 when $\eta_0 < 0$. If $\eta_0 < 0$, then by Lemma S6, $\eta_n(\kappa) \leq 0$ with probability tending to one. Hence, with probability tending to one, $\tau_n = 0 = \tau_0$. Therefore, part iii holds. □

The following Lemma S8 show that certain remainders in the expansions in Section S4.3 are $\mathrm{o}_p(n^{-1/2})$.

Lemma S8. *Under Conditions A2, B8 and B6,*

$$\sup_{\rho:\mathcal{W}\to[0,1]} \left| R_\rho(\hat{P}_n, P_0) \right| = \mathrm{o}_p(n^{-1/2}).$$

Proof of Lemma S8. By the boundedness of the range of ρ, we see that

$$\begin{aligned}
&\sup_{\rho:\mathcal{W}\to[0,1]} \left| R_\rho(\hat{P}_n, P_0) \right| \\
&= \sup_{\rho:\mathcal{W}\to[0,1]} P_0 \left| \rho(\cdot) \left[\frac{\mu_n^T(\cdot) - \mu_0^T(\cdot)}{\mu_n^T(\cdot)} \{\hat{\mu}_n^Y(1,\cdot) - \mu_0^Y(1,\cdot)\} + \frac{\mu_n^T(\cdot) - \mu_0^T(\cdot)}{1-\mu_n^T} \{\hat{\mu}_n^Y(0,\cdot) - \mu_0^Y(0,\cdot)\} \right] \right| \\
&\leq P_0 \left| \left[\frac{\mu_n^T(\cdot) - \mu_0^T(\cdot)}{\mu_n^T(\cdot)} \{\hat{\mu}_n^Y(1,\cdot) - \mu_0^Y(1,\cdot)\} + \frac{\mu_n^T(\cdot) - \mu_0^T(\cdot)}{1-\mu_n^T(\cdot)} \{\hat{\mu}_n^Y(0,\cdot) - \mu_0^Y(0,\cdot)\} \right] \right|.
\end{aligned}$$

Using Condition B8 and Lemma S4, the display continues as

$$\begin{aligned}
&\lesssim P_0 \left| (\mu_n^T(\cdot) - \mu_0^T(\cdot))[\hat{\mu}_n^Y(1,\cdot) - \mu_0^Y(1,\cdot)] \right| + P_0 \left| (\mu_n^T(\cdot) - \mu_0^T(\cdot))[\hat{\mu}_n^Y(0,\cdot) - \mu_0^Y(0,\cdot)] \right| \\
&\leq \|\mu_n^T - \mu_0^T\|_{2,P_0} \|\hat{\mu}_n^Y(1,\cdot) - \mu_0^Y(1,\cdot)\|_{2,P_0} + \|\mu_n^T - \mu_0^T\|_{2,P_0} \|\hat{\mu}_n^Y(0,\cdot) - \mu_0^Y(0,\cdot)\|_{2,P_0} \\
&\lesssim \|\mu_n^T - \mu_0^T\|_{2,P_0} \|\hat{\mu}_n^Y - \mu_0^Y\|_{2,P_0}.
\end{aligned}$$

The right-hand side is $\mathrm{o}_p(n^{-1/2})$ by Condition B6. □

We next prove Theorem 4.

Proof of Theorem 4. By the expansion of $P \mapsto \Psi_{\rho_P}(P)$ presented in Section S4.3,

$$\begin{aligned}
&\Psi_{\rho_n}(\hat{P}_n) - \Psi_{\rho_0}(P_0) \\
&\quad = P_0 D(\hat{P}_n, \rho_n, \tau_0, \mu_n^C) + R_{\rho_n}(\hat{P}_n, P_0) + P_0\{(\rho_n - \rho_0)(\delta_0^Y - \tau_0 \delta_0^C)\} \\
&\qquad - \tau_0 P_0 \left\{ \rho_n(\cdot) \frac{\mu_n^T(\cdot) - \mu_0^T(\cdot)}{\mu_n^T(\cdot)} [\mu_n^C(1,\cdot) - \mu_0^C(1,\cdot)] \right\} \\
&\qquad + \tau_0 P_0 \left\{ (1-\rho_n(\cdot)) \frac{\mu_n^T(\cdot) - \mu_0^T(\cdot)}{1-\mu_n^T(\cdot)} [\mu_n^C(0,\cdot) - \mu_0^C(0,\cdot)] \right\} \\
&\quad = (P_n - P_0) D(P_0, \rho_0, \tau_0, \mu_0^C) - P_n D(\hat{P}_n, \rho_n, \tau_0, \mu_n^C)
\end{aligned}$$

$$
\begin{aligned}
&+ (P_n - P_0)\left[D(\hat{P}_n, \rho_n, \tau_0, \mu_n^C) - D(P_0, \rho_0, \tau_0, \mu_0^C)\right] \\
&+ R_{\rho_n}(\hat{P}_n, P_0) + P_0\{(\rho_n - \rho_0)(\delta_0^Y - \tau_0\delta_0^C)\} \\
&- \tau_0 P_0\left\{\rho_n(\cdot)\frac{\mu_n^T(\cdot) - \mu_0^T(\cdot)}{\mu_n^T(\cdot)}[\mu_n^C(1,\cdot) - \mu_0^C(1,\cdot)]\right\} \\
&+ \tau_0 P_0\left\{(1 - \rho_n(\cdot))\frac{\mu_n^T(\cdot) - \mu_0^T(\cdot)}{1 - \mu_n^T(\cdot)}[\mu_n^C(0,\cdot) - \mu_0^C(0,\cdot)]\right\}.
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
\Psi_{\rho^{\mathrm{FR}}}(\hat{P}_n) - \Psi_{\rho^{\mathrm{FR}}}(P_0) &= (P_n - P_0)D(P_0, \rho^{\mathrm{FR}}, 0, \mu_0^C) - P_n D(\hat{P}_n, \rho^{\mathrm{FR}}, 0, \mu_0^C) \\
&\quad + (P_n - P_0)\left[D(\hat{P}_n, \rho^{\mathrm{FR}}, 0, \mu_0^C) - D(P_0, \rho^{\mathrm{FR}}, 0, \mu_0^C)\right] + R_{\rho^{\mathrm{FR}}}(\hat{P}_n, P_0); \\
\Psi_{\rho_n^{\mathrm{RD}}}(\hat{P}_n) - \Psi_{\rho_0^{\mathrm{RD}}}(P_0) &= (P_n - P_0)D(P_0, \rho_0^{\mathrm{RD}}, 0, \mu_0^C) - P_n D(\hat{P}_n, \rho_n^{\mathrm{RD}}, 0, \mu_0^C) \\
&\quad + (P_n - P_0)\left[D(\hat{P}_n, \rho_n^{\mathrm{RD}}, 0, \mu_0^C) - D(P_0, \rho_0^{\mathrm{RD}}, 0, \mu_0^C)\right] \\
&\quad + R_{\rho_n^{\mathrm{RD}}}(\hat{P}_n, P_0) + (\rho_n^{\mathrm{RD}} - \rho_0^{\mathrm{RD}})P_0\Delta_0^Y; \\
\Psi_{\rho_n^{\mathrm{TP}}}(\hat{P}_n) - \Psi_{\rho_0^{\mathrm{TP}}}(P_0) &= (P_n - P_0)G_{\mathrm{TP}}(P_0) - P_n G_{\mathrm{TP}}(\hat{P}_n) + (P_n - P_0)\left[G_{\mathrm{TP}}(\hat{P}_n) - G_{\mathrm{TP}}(P_0)\right] \\
&\quad + R_{\rho_0^{\mathrm{TP}}}(\hat{P}_n, P_0).
\end{aligned}
$$

First, we note the following facts, which will be sufficient to ensure that the remainders and empirical process terms in all of the first-order expansions given above are $\mathrm{o}_p(n^{-1/2})$. By Condition B6, Lemmas S4 and S8, the Cauchy-Schwarz inequality, and boundedness of the range of an ITR, the following terms are all $\mathrm{o}_p(n^{-1/2})$:

$$
\begin{aligned}
&R_\rho(\hat{P}_n, P_0) \text{ for } \rho = \rho_n, \rho^{\mathrm{FR}}, \rho_n^{\mathrm{RD}}, \\
&P_0\left\{\frac{\mu_n^T(\cdot) - \mu_0^T(\cdot)}{1 - \mu_n^T(\cdot)}(\hat{\mu}_P^Y(0,\cdot) - \hat{\mu}_0^Y(0,\cdot))\right\}, \\
&\tau_0 P_0\left\{\rho_n(\cdot)\frac{\mu_n^T(\cdot) - \mu_0^T(\cdot)}{\mu_n^T(\cdot)}[\mu_n^C(1,\cdot) - \mu_0^C(1,\cdot)]\right\}, \\
&\tau_0 P_0\left\{(1 - \rho_n(\cdot))\frac{\mu_n^T(\cdot) - \mu_0^T(\cdot)}{1 - \mu_n^T(\cdot)}[\mu_n^C(0,\cdot) - \mu_0^C(0,\cdot)]\right\}.
\end{aligned}
$$

Moreover, by Condition B10, $P_0\{(\rho_n - \rho_0)(\delta_0^Y - \tau_0\delta_0^C)\} = \mathrm{o}_p(n^{-1/2})$; by Conditions B7 and B11, $(P_n - P_0)\left[D_{n,\mathcal{R}} - D_{\mathcal{R}}(P_0)\right] = \mathrm{o}_p(n^{-1/2})$ for all $\mathcal{R} \in \{\mathrm{FR}, \mathrm{RD}, \mathrm{TP}\}$ and

$$
(P_n - P_0)\left\{[D(\hat{P}_n, \rho_n, \tau_0, \mu_n^C) - D(\hat{P}_n, \rho_n^{\mathrm{RD}}, 0, \mu_0^C)] - [D(P_0, \rho_0, \tau_0, \mu_0^C) - D(P_0, \rho_0^{\mathrm{RD}}, 0, \mu_0^C)]\right\} = \mathrm{o}_p(n^{-1/2}).
$$

Therefore, all relevant remainders and empirical process terms are $\mathrm{o}_p(n^{-1/2})$.

We separately study the three cases where $\mathcal{R} = \mathrm{FR}$, $\mathcal{R} = \mathrm{RD}$, and $\mathcal{R} = \mathrm{TP}$.

Case I: $\mathcal{R} = \mathrm{FR}$. It holds that

$$
\begin{aligned}
\psi_n - \psi_0 &= (P_n - P_0)D_{\mathrm{FR}}(P_0) - P_n D_{n,\mathrm{FR}} + \mathrm{o}_p(n^{-1/2}) \\
&= (P_n - P_0)D_{\mathrm{FR}}(P_0) \\
&\quad + \tau_0 \Bigg\{ \frac{1}{n}\sum_{i=1}^{n} \Bigg\{ \rho_n(V_i) \left[\Delta_n^C(W_i) + \frac{1}{T_i + \mu_n^T(W_i) - 1}[C_i - \mu_n^C(T_i, W_i)] \right] \\
&\qquad + \alpha \left[\mu_n^C(0, W_i) + \frac{1 - T_i}{1 - \mu_n^T(W_i)}[C_i - \mu_n^C(0, W_i)] \right] \Bigg\} - \kappa \Bigg\} + \mathrm{o}_p(n^{-1/2}),
\end{aligned}
$$

where the last step follows from the TMLE construction of $\hat{P}_n$ (Step 4a of our estimator), which implies that

$$
\frac{1}{n}\sum_{i=1}^{n} \left\{ \frac{\rho_n(V_i) - \rho^{\mathrm{FR}}(V)}{T_i + \mu_n^T(W_i) - 1}[Y_i - \hat{\mu}_n^Y(T_i, W_i)] \right\} = 0.
$$

We now show that the second term on the right-hand side is zero with probability tending to one. If $\tau_0 = 0$, then this term is zero. Otherwise, $\tau_0 = \eta_0 > 0$. By Lemma S7, the following holds with probability tending to one:

$$
\frac{1}{n}\sum_{i=1}^{n} \left\{ \rho_n(V_i) \left[\mu_n^C(1, W_i) + \frac{T_i}{\mu_n^T(W_i)}[C_i - \mu_n^C(1, W_i)] \right] + \alpha \left[\mu_n^C(0, W_i) + \frac{1 - T_i}{1 - \mu_n^T(W_i)}[C_i - \mu_n^C(0, W_i)] \right] \right\} = \kappa,
$$

and hence the second term is zero with probability tending to one, as desired. Therefore, $\psi_n - \psi_0 = (P_n - P_0)D_{\mathrm{FR}}(P_0) + \mathrm{o}_p(n^{-1/2})$.

Case II: $\mathcal{R} = \mathrm{RD}$. It holds that

$$
\begin{aligned}
\psi_n - \psi_0 &= (P_n - P_0)\{D(P_0, \rho_0, \tau_0, \mu_0^C) - D(P_0, \rho_0^{\mathrm{RD}}, 0, \mu_0^C)\} \\
&\quad - P_n\{D(\hat{P}_n, \rho_n, \tau_0, \mu_n^C) - D(\hat{P}_n, \rho_n^{\mathrm{RD}}, 0, \mu_0^C)\} \\
&\quad - (\rho_n^{\mathrm{RD}} - \rho_0^{\mathrm{RD}})P_0\Delta_0^Y + \mathrm{o}_p(n^{-1/2}),
\end{aligned}
$$

where we have used ρ_n^{RD} and ρ_0^{RD} to denote the values that the two functions take, respectively. The

TMLE construction of $\hat{P}_n$ (Step 4a of our estimator) implies that

$$\frac{1}{n}\sum_{i=1}^{n}\frac{\rho_n(V_i)-\rho_n^{\mathrm{RD}}(V_i)}{T_i+\mu_n^T(W_i)-1}[Y_i-\hat{\mu}_n^Y(T_i,W_i)]=0,$$

and hence

$$\begin{aligned}
&P_n\{D(\hat{P}_n,\rho_n,\tau_0,\mu_n^C)-D(\hat{P}_n,\rho_n^{\mathrm{RD}},0,\mu_0^C)\}\\
&=-\tau_0\Bigg\{\frac{1}{n}\sum_{i=1}^{n}\Bigg\{\rho_n(V_i)\left[\Delta_n^C(W_i)+\frac{1}{T_i+\mu_n^T(W_i)-1}[C_i-\mu_n^C(T_i,W_i)]\right]\\
&\qquad+\alpha\left[\mu_n^C(0,W_i)+\frac{1-T_i}{1-\mu_n^T(W_i)}[C_i-\mu_n^C(0,W_i)]\right]\Bigg\}-\kappa\Bigg\},
\end{aligned}$$

which is zero with probability tending to one as proved above. By Condition B5, Lemma S3 and the delta method for influence functions, the value that ρ_n^{RD} takes is an asymptotic linear estimator of the value that ρ_0^{RD} takes. Straightforward application of the delta method for influence functions implies that

$$\psi_n-\psi_0=(P_n-P_0)D_{\mathrm{RD}}(P_0)+\mathrm{o}_p(n^{-1/2}).$$

Case 3: $\mathcal{R}=\mathrm{TP}$. It holds that

$$\psi_n-\psi_0=(P_n-P_0)D_{\mathrm{TP}}(P_0)-P_nD_{n,\mathrm{TP}}+\mathrm{o}_p(n^{-1/2}).$$

The TMLE construction of $\hat{P}_n$ (Step 4a of our estimator) implies that

$$\frac{1}{n}\sum_{i=1}^{n}\left\{\frac{\rho_n(V_i)-\mu_n^T(W_i)}{T_i+\mu_n^T(W_i)-1}[Y_i-\hat{\mu}_n^Y(T_i,W_i)]\right\}=0,$$

so

$$\begin{aligned}
P_nD_{n,\mathrm{TP}}=-\tau_0\Bigg\{\frac{1}{n}\sum_{i=1}^{n}\Bigg\{\rho_n(V_i)&\left[\Delta_n^C(W_i)+\frac{1}{T_i+\mu_n^T(W_i)-1}[C_i-\mu_n^C(T_i,W_i)]\right]\\
&+\alpha\left[\mu_n^C(0,W_i)+\frac{1-T_i}{1-\mu_n^T(W_i)}[C_i-\mu_n^C(0,W_i)]\Bigg\}\right]-\kappa\Bigg\},
\end{aligned}$$

which is zero with probability tending to one as proved above. Therefore,

$$\psi_n - \psi_0 = (P_n - P_0) D_{\mathrm{TP}}(P_0) + \mathrm{o}_p(n^{-1/2}).$$

Conclusion: The asymptotic linearity result on ψ_n follows from the above results. Consequently, the asymptotic normality result on ψ_n holds by the central limit theorem and Slutsky's theorem. □

S4.5 Proof of Theorem S1

In this section, we prove Theorem S1. The arguments are almost identical to those in Supplement S9 Qiu et al. [34] with adaptations to the different treatment resource constraint.

Lemma S9 (Convergence rate of τ_n if $\eta_0 > -\infty$)**.** *Assume that the conditions for Theorem 4 hold. Suppose that $\eta_0 > -\infty$, that the Lebesgue density of the distribution of $\xi_0(V)$ under $V \sim P_0$ is well-defined, nonzero and finite in a neighborhood of and that $P_0 I(\xi_n = \eta_n) = \mathrm{O}_p(n^{-1/2})$. Under these conditions, the following implications hold with probability tending to one:*

- *If $\|\xi_n - \xi_0\|_{q,P_0} = \mathrm{o}_p(1)$ for some $0 < q < \infty$, then $|\tau_n - \tau_0| \lesssim \|\xi_n - \xi_0\|_{q,P_0}^{q/q+1} + \mathrm{O}_p(n^{-1/2})$.*
- *If $\|\xi_n - \xi_0\|_{\infty,P_0} = \mathrm{o}_p(1)$, then $|\tau_n - \tau_0| \lesssim \|\xi_n - \xi_0\|_{\infty,P_0} + \mathrm{O}_p(n^{-1/2})$.*

The condition that $P_0 I(\xi_n = \eta_n) = \mathrm{O}_p(n^{-1/2})$ is reasonable if $\xi_n(V)$ has a continuous distribution when $V \sim P_0$, in which case $P_0 I(\xi_n = \eta_n) = 0$.

Proof of Lemma S9. We study the three cases where $\eta_0 > 0$, $\eta_0 < 0$ and $\eta_0 = 0$ separately.

We first study the case where $\eta_0 > 0$. By Lemma S7, with probability tending to one, $\eta_n = \eta_n(k_n)$ where k_n is a solution to (5), and

$$P_0\{[I(\xi_n > \eta_n) - I(\xi_0 > \eta_0)]\Delta_0^C\} = P_0\{d_{n,k_n}\Delta_0^C\} - (\kappa - \alpha\phi_0) + \mathrm{O}_p(n^{-1/2}) = \mathrm{O}_p(n^{-1/2}).$$

We argue conditionally on the event that k_n is a solution to (5). Adding $\Gamma_0(\eta_n) - P_0\{I(\xi_n > \eta_n)\Delta_0^C\}$ to both sides shows that $\Gamma_0(\eta_n) - \Gamma_0(\eta_0) = -P_0\{[I(\xi_n > \eta_n) - I(\xi_0 > \eta_n)]\Delta_0^C\} + \mathrm{O}_p(n^{-1/2})$. By a Taylor expansion of Γ_0 under Conditions B2, B3 and A4, the left-hand side is equal to $-C(\eta_n - \eta_0) + \mathrm{o}_p(\eta_n - \eta_0)$ for some $C > 0$, yielding that

$$[C + \mathrm{o}_p(1)][\eta_n - \eta_0] = P_0\{[I(\xi_n > \eta_n) - I(\xi_0 > \eta_n)]\Delta_0^C\} + \mathrm{O}_p(n^{-1/2}),$$

which immediately implies that

$$\eta_n - \eta_0 = \mathrm{O}_p\Big(P_0\{[I(\xi_n > \eta_n) - I(\xi_0 > \eta_n)]\Delta_0^C\}\Big) + \mathrm{O}_p(n^{-1/2}). \tag{S17}$$

The rest of the proof for this case and the proof for the other two cases are identical to the proof of Lemma S14 in Qiu et al. [34]. We present the argument below for completeness. By Lemma S5 and Condition B4, for any $\epsilon > 0$ it holds that

$$\begin{aligned}
&|P_0\{[I(\xi_n > \eta_n) - I(\xi_0 > \eta_n)]\Delta_0^C\}| \\
&\lesssim |P_0\{[I(\xi_n > \eta_n) - I(\xi_0 > \eta_n)]\}| \\
&\leq P_0 I(|\xi_n - \xi_0| > \epsilon) + P_0 I(|\xi_0 - \eta_n| \leq \epsilon).
\end{aligned}$$

Fix a positive sequence $\{\epsilon_n\}_{n=1}^{\infty}$, where each ϵ_n may be random through observations $O_1, \ldots, O_n$, such that $\epsilon_n \xrightarrow{p} 0$ as $n \to \infty$. By a Taylor expansion of S_0, the survival function of the distribution of $\xi_0(V)$ when $V \sim P_0$, around η_0, which is valid under Condition B2 provided ϵ_n is sufficiently small, it follows that

$$|P_0\{[I(\xi_n > \eta_n) - I(\xi_0 > \eta_n)]\Delta_0^C\}| \lesssim P_0 I(|\xi_n - \xi_0| > \epsilon_n) - 2(S_0)'(\eta_0)\epsilon_n + \mathrm{o}_p(\epsilon_n).$$

Here we recall that $(S_0)'(\eta_0)$ is finite by Condition B2. Returning to (S17),

$$\eta_n - \eta_0 = \mathrm{O}_p\Big(P_0 I(|\xi_n - \xi_0| > \epsilon_n)\Big) - [2(S_0)'(\eta_0) + \mathrm{o}_p(1)]\epsilon_n + \mathrm{O}_p(n^{-1/2}).$$

If $\|\xi_n - \xi_0\|_{q,P_0} = \mathrm{o}_p(1)$ for some $0 < q < \infty$, by Markov's inequality, $P_0 I(|\xi_n - \xi_0| > \epsilon_n) \leq \|\xi_n - \xi_0\|_{q,P_0}^q / \epsilon_n^q$. In this case, taking $\epsilon_n = \|\xi_n - \xi_0\|_{q,P_0}^{q/(q+1)}$ yields that $|\eta_n - \eta_0| \lesssim \|\xi_n - \xi_0\|_{q,P_0}^{q/(q+1)} + \mathrm{O}_p(n^{-1/2})$ with probability tending to one. If $\|\xi_n - \xi_0\|_{\infty,P_0} = \mathrm{o}_p(1)$, then taking $\epsilon_n = \|\xi_n - \xi_0\|_{\infty,P_0}$ yields that $P_0 I(|\xi_n - \xi_0| > \epsilon_n) = 0$, and hence that $|\eta_n - \eta_0| \lesssim \|\xi_n - \xi_0\|_{\infty,P_0}^2 + \mathrm{O}_p(n^{-1/2})$ with probability tending to one. The desired result follows by noting that $\tau_0 = \eta_0$ and in both cases, $\tau_n = \eta_n(k_n)$ with probability tending to one.

We now study the case where $\eta < 0$. By Lemma S6, with probability tending to one, $\eta_n < 0$ and hence $\tau_n = 0 = \tau_0$, as desired.

We finally study the case where $\eta_0 = 0$. We argue conditional on the event that a solution k_n' to (5) exists, which happens with probability tending to one by Lemma S7. Recall that for convenience we let $k_n = k_n'$ when $\eta_n(\kappa) > 0$. Then, exactly one of the following two events happen: (i) $\eta_n(\kappa) \leq 0$ or $\eta_n(k_n') \leq 0$, in which case $\tau_n = 0 = \tau_0$; (2) $\eta_n(\kappa) > 0$ and $\eta_n(k_n') > 0$, in which case a similar argument as the above proof for the case where $\eta_0 > 0$ shows that the distance between $\tau_n = \eta_n(k_n')$ and τ_0 has the desired bound. The desired result holds conditional on either event, so it holds unconditional on either event. □

We finally prove Theorem S1.

Proof of Theorem S1. Observe that

$$\begin{aligned}
|P_0\{(\rho_n - \rho_0)(\delta_0^Y - \tau_0 \Delta_0^C)\}| &\leq P_0|\{I(\xi_n > \tau_n) - I(\xi_0 > \tau_0)\}(\xi_0 - \tau_0)\Delta_0^C| \\
&\lesssim P_0|\{I(\xi_n > \tau_n) - I(\xi_0 > \tau_0)\}(\xi_0 - \tau_0)| \\
&\leq P_0|\{I(\xi_n > \tau_n) - I(\xi_0 > \tau_n)\}(\xi_0 - \tau_n)| \\
&\quad + P_0|\{I(\xi_0 > \tau_n) - I(\xi_0 > \tau_0)\}(\xi_0 - \tau_0)| \\
&\quad + |\tau_n - \tau_0| P_0|I(\xi_n > \tau_n) - I(\xi_0 > \tau_n)|.
\end{aligned} \tag{S18}$$

Starting from this inequality, the rest of the proof is identical to that of Theorem 5 in Qiu et al. [34]. We present the argument below for completeness. Let $\{\epsilon_n\}_{n=1}^{\infty}$ be a positive sequence, where each ϵ_n is random through the observations $O_1, \ldots, O_n$, such that $\epsilon_n \xrightarrow{p} 0$ as $n \to \infty$.

We denote the three terms on the right-hand side by terms 1, 2, and 3, and study these terms separately. It is useful to note that $\tau_n - \tau_0 = \mathrm{o}_p(1)$, so the Lebesgue density of the distribution of $\xi_0(V)$, $V \sim P_0$, is finite in a neighborhood of τ_n with probability tending to one.

Study of term 1 in (S18)**:** Observe that

$$\begin{aligned}
&P_0|\{I(\xi_n > \tau_n) - I(\xi_0 > \tau_n)\}(\xi_0 - \tau_n)| \\
&\quad = P_0|\{I(\xi_n > \tau_n) - I(\xi_0 > \tau_n)\}(\xi_0 - \tau_n)| I(0 < |\xi_0 - \tau_n|).
\end{aligned}$$

First consider the bound with the $L^q(P_0)$-distance. Because $I(\xi_n(v) > \tau_n) \neq I(\xi_0(v) > \tau_n)$ if and only if (i) $\xi_n(v) - \tau_n$ and $\xi_0(v) - \tau_n$ take different signs or (ii) only one of them is zero, this event implies $|\xi_0(v) - \tau_n| \leq |\xi_n(v) - \xi_0(v)|$, and so this term is upper bounded by

$$P_0|\{I(\xi_n > \tau_n) - I(\xi_0 > \tau_n)\}(\xi_0 - \tau_n)| I(0 < |\xi_0 - \tau_n| \leq \epsilon_n)$$

$$
\begin{aligned}
&\quad + P_0|\{I(\xi_n > \tau_n) - I(\xi_0 > \tau_n)\}(\xi_0 - \tau_n)|I(|\xi_0 - \tau_n| > \epsilon_n) \\
&\le P_0|\xi_n - \xi_0|I(0 < |\xi_0 - \tau_n| \le \epsilon_n) + P_0|\xi_n - \xi_0|I(|\xi_n - \xi_0| > \epsilon_n) \\
&\le \|\xi_n - \xi_0\|_{q,P_0} \{P_0(0 < |\xi_0(V) - \tau_n| \le \epsilon_n)\}^{(q-1)/q} + \frac{P_0|\xi_n - \xi_0|^q}{\epsilon_n^{q-1}} \\
&\lesssim \|\xi_n - \xi_0\|_{q,P_0} \cdot \epsilon_n^{(q-1)/q} + \frac{\|\xi_n - \xi_0\|_{q,P_0}^q}{\epsilon_n^{q-1}},
\end{aligned}
$$

where second to last relation holds by Hölder's inequality and Markov's inequality, and the last relation holds with probability tending to one by the assumption that the distribution of $\xi_0(V)$, $V \sim P_0$, has a continuous finite Lebesgue density in a neighborhood of τ_0 and Lemma S7. Taking $\epsilon_n = \|\xi_n - \xi_0\|_{q,P_0}^{q/(q+1)}$ yields that $|P_0\{I(\xi_n > \tau_n) - I(\xi_0 > \tau_n)\}(\xi_0 - \tau_n)| \lesssim \|\xi_n - \xi_0\|_{q,P_0}^{2q/(q+1)}$.

Next consider the bound with the $L^\infty(P_0)$-distance. We have that

$$
\begin{aligned}
P_0|\{I(\xi_n > \tau_n) - I(\xi_0 > \tau_n)\}(\xi_0 - \tau_n)| &\le P_0 I(|\xi_0 - \tau_n| \le |\xi_n - \xi_0|)|\xi_0 - \tau_n| \\
&= P_0 I(0 < |\xi_0 - \tau_n| \le |\xi_n - \xi_0|)|\xi_0 - \tau_n| \\
&\le P_0 I(0 < |\xi_0 - \tau_n| \le \|\xi_n - \xi_0\|_{\infty,P_0})|\xi_0 - \tau_n| \\
&\le \|\xi_n - \xi_0\|_{\infty,P_0} P_0(0 < |\xi_0(V) - \tau_n| \le \|\xi_n - \xi_0\|_{\infty,P_0}) \\
&\lesssim \|\xi_n - \xi_0\|_{\infty,P_0}^2.
\end{aligned}
$$

Therefore, the first term is upper bounded by both $\|\xi_n - \xi_0\|_{q,P_0}^{2q/(q+1)}$ and $\|\xi_n - \xi_0\|_{\infty,P_0}^2$, up to an absolute constant.

Study of term 2 in (S18)**:** Because $I(\xi_0(v) > \tau_n) \neq I(\xi_0(v) > \tau_0)$ if and only if the two indicators take different signs or only one of them is zero, these indicators only take different values if $|\xi_0(v) - \tau_0| \le |\tau_n - \tau_0|$. Therefore, term 2 bounds as

$$
\begin{aligned}
P_0|\{I(\xi_0 > \tau_n) - I(\xi_0 > \tau_0)\}(\xi_0 - \tau_0)| &\le P_0 I(|\xi_0 - \tau_0| \le |\tau_n - \tau_0|)|\xi_0 - \tau_0| \\
&\le |\tau_n - \tau_0| P_0 I(|\xi_0 - \tau_0| \le |\tau_n - \tau_0|) \\
&\lesssim |\tau_n - \tau_0|^2,
\end{aligned}
$$

where the last step holds for with probability tending to one by the assumption that the distribution of $\xi_0(V)$, $V \sim P_0$, has a continuous finite Lebesgue density in a neighborhood of τ_0 and Lemma S7. If

$\eta_0 > -\infty$, by Lemma S9, with probability tending to one,

$$P_0|I(\xi_0 > \tau_n) - I(\xi_0 > \tau_0)||\xi_0 - \tau_0| \lesssim \begin{cases} \|\xi_n - \xi_0\|_{q,P_0}^{2q/(q+1)} + \mathrm{O}_p(n^{-1}), & \text{if } \|\xi_n - \xi_0\|_{q,P_0} = \mathrm{o}_p(1) \\ \|\xi_n - \xi_0\|_{\infty,P_0}^2 + \mathrm{O}_p(n^{-1}), & \text{if } \|\xi_n - \xi_0\|_{\infty,P_0} = \mathrm{o}_p(1) \end{cases}.$$

Otherwise, by Lemma S6, with probability tending to one, $\tau_n = 0 = \tau_0$ and the above result still holds.

Study of term 3 in (S18)**:** By Lemma S5,

$$P_0|I(\xi_n > \tau_n) - I(\xi_0 > \tau_n)| \leq P_0 I(|\xi_n - \xi_0| > \epsilon_n) + P_0 I(|\xi_0 - \tau_n| \leq \epsilon_n).$$

By a Taylor expansion of S_0 around τ_0, similarly to the proof of Lemma S9, with probability tending to one,

$$P_0 I(|\xi_0 - \tau_n| \leq \epsilon_n) = -2(S_0)'(\tau_0)\epsilon_n + \mathrm{o}_p(|\tau_n - \tau_0| + \epsilon_n),$$

where $|(S_0)'(\tau_0)| < \infty$. If $\|\xi_n - \xi_0\|_{q,P_0} = \mathrm{o}_p(1)$ for some $1 < q < \infty$, then $P_0 I(|\xi_n - \xi_0| > \epsilon_n) \leq \|\xi_n - \xi_0\|_{q,P_0}^q / \epsilon_n^q$. Taking $\epsilon_n = \|\xi_n - \xi_0\|_{q,P_0}^{q/(q+1)}$ yields that $|P_0\{I(\xi_n > \tau_n) - I(\xi_0 > \tau_n)\}| \lesssim \|\xi_n - \xi_0\|_{q,P_0}^{q/(q+1)}$. If $\|\xi_n - \xi_0\|_{\infty,P_0} = \mathrm{o}_p(1)$, then taking $\epsilon_n = \|\xi_n - \xi_0\|_{\infty,P_0}$ yields that $|P_0\{I(\xi_n > \tau_n) - I(\xi_0 > \tau_n)\}| \lesssim \|\xi_n - \xi_0\|_{\infty,P_0}$ with probability tending to one. Also note that, by Lemma S9, if $\eta_0 > -\infty$, then, with probability tending to one,

$$|\tau_n - \tau_0| \leq |\eta_n - \eta_0| \lesssim \begin{cases} \|\xi_n - \xi_0\|_{q,P_0}^{q/(q+1)} + \mathrm{O}_p(n^{-1/2}), & \text{if } \|\xi_n - \xi_0\|_{q,P_0} = \mathrm{o}_p(1), \\ \|\xi_n - \xi_0\|_{\infty,P_0} + \mathrm{O}_p(n^{-1/2}), & \text{if } \|\xi_n - \xi_0\|_{\infty,P_0} = \mathrm{o}_p(1). \end{cases}$$

The same holds when $\eta_0 = -\infty$ since then $|\tau_n - \tau_0| = 0$ with probability tending to one.

Therefore, with probability tending to one,

$$\begin{aligned} &|\tau_n - \tau_0| P_0 |I(\xi_n > \tau_n) - I(\xi_0 > \tau_n)| \\ &\lesssim \begin{cases} \|\xi_n - \xi_0\|_{q,P_0}^{2q/(q+1)} + \|\xi_n - \xi_0\|_{q,P_0}^{q/(q+1)} \mathrm{O}_p(n^{-1/2}) & \text{if } \|\xi_n - \xi_0\|_{q,P_0} = \mathrm{o}_p(1), \\ \|\xi_n - \xi_0\|_{\infty,P_0}^2 + \|\xi_n - \xi_0\|_{\infty,P_0} \mathrm{O}_p(n^{-1/2}) & \text{if } \|\xi_n - \xi_0\|_{\infty,P_0} = \mathrm{o}_p(1). \end{cases} \end{aligned}$$

Conclusion of the bound in (S18)**:** We finally combine the bounds for all three terms. Note that $a_n \mathrm{O}_p(b_n) \lesssim a_n^2 + \mathrm{O}_p(b_n^2)$ for any sequence of non-negative random variables a_n and sequence of constants

b_n. It follows that, with probability tending to one,

$$|P_0\{(\rho_n - \rho_0)(\delta_0^Y - \tau_0\nu_0)\}| \lesssim \begin{cases} \|\xi_n - \xi_0\|_{q,P_0}^{2q/(q+1)} + \mathrm{O}_p(n^{-1}), & \text{if } \|\xi_n - \xi_0\|_{q,P_0} = \mathrm{o}_p(1), \\ \|\xi_n - \xi_0\|_{\infty,P_0}^2 + \mathrm{O}_p(n^{-1}), & \text{if } \|\xi_n - \xi_0\|_{\infty,P_0} = \mathrm{o}_p(1). \end{cases}$$

□

S5 Additional simulations

S5.1 Results of simulation with nuisance functions being truth

In this section, we present the results of the simulation with an identical setting as that in Section 5 in the main text except that the nuisance functions are taken to be the truth rather than estimated via machine learning. The purpose of this simulation is to show that the performance of our proposed estimator may be significantly improved by using machine learning estimators of nuisance functions that outperform those used in the simulation study reported in the main text.

Table S1 presents the performance of our proposed estimator in this simulation. The Wald CI coverage is close to 95% for sample sizes of 1000 or more. The coverage of the confidence lower bounds is also close to the nominal coverage of 97.5%. Therefore, our proposed procedure appears to have the potential to be significantly improved when using improved estimators of nuisance functions. Figure S1 presents the width of our 95% Wald CI scaled by the square root of sample size n. For each estimand, the scaled width appears to stabilize as n grows and to be similar to the scaled width observed in the simulation reported in Section 5, where nuisance functions are estimated from data.

S5.2 Simulation under a low dimension and a parametric model

In this section, we describe the additional simulation in a setting with a low dimension and a parametric model as well as the simulation results.

The data is generated as follows. We first generate a univariate covariate $W \sim \mathrm{Unif}(-1, 1)$. We then generate T, C and Y as follows:

$$\begin{aligned} T \mid W &\sim \text{Bernoulli}\left(\text{expit}(W)\right), \\ C \mid T, W &\sim \text{Bernoulli}\left(\text{expit}(2T - 1 + W)\right), \end{aligned}$$

Table S1: Performance of estimators of average causal effects in the simulation with nuisance functions being the truth.

Performance measure	Sample size	FR	RD	TP
95% Wald CI coverage	500	93%	90%	90%
	1000	94%	94%	93%
	4000	96%	95%	95%
	16000	94%	96%	95%
97.5% confidence lower bound coverage	500	96%	96%	95%
	1000	97%	97%	96%
	4000	98%	97%	97%
	16000	97%	97%	97%
bias	500	0.0023	0.0004	0.0010
	1000	0.0013	0.0008	0.0007
	4000	0.0003	0.0003	0.0003
	16000	0.0002	0.003	0.0002
RMSE	500	0.048	0.023	0.029
	1000	0.033	0.015	0.020
	4000	0.016	0.008	0.010
	16000	0.009	0.004	0.005
Ratio of mean standard error to standard deviation	500	0.964	0.911	0.928
	1000	0.967	0.998	0.958
	4000	1.028	0.983	0.995
	16000	0.963	1.007	0.996

$$Y \mid T, W \sim \text{Bernoulli}\left(\text{expit}(1.4T - 0.7 - 0.3W)\right),$$

where C and Y are independent conditional on (W, T). We set $\rho^{\text{FR}} : v \mapsto 0$, $V = W$, and $\kappa = 0.35$, which is an active constraint with $\tau_0 > 0$ and $\rho_0^{\text{RD}} < 1$. We use logistic regression to estimate functions μ_0^T, μ_0^C and μ_0^C. All other simulation settings are identical to that in Section 5.

The simulation results are presented in Table S2 and Figure S2. The performance is generally between the nonparametric setting in Section 5 and the oracle setting in Section S5.1. The CI coverage is much better than the nonparametric case, thus suggesting that our method might perform better with improved estimators of nuisance functions μ_0^T, μ_0^C and μ_0^C.

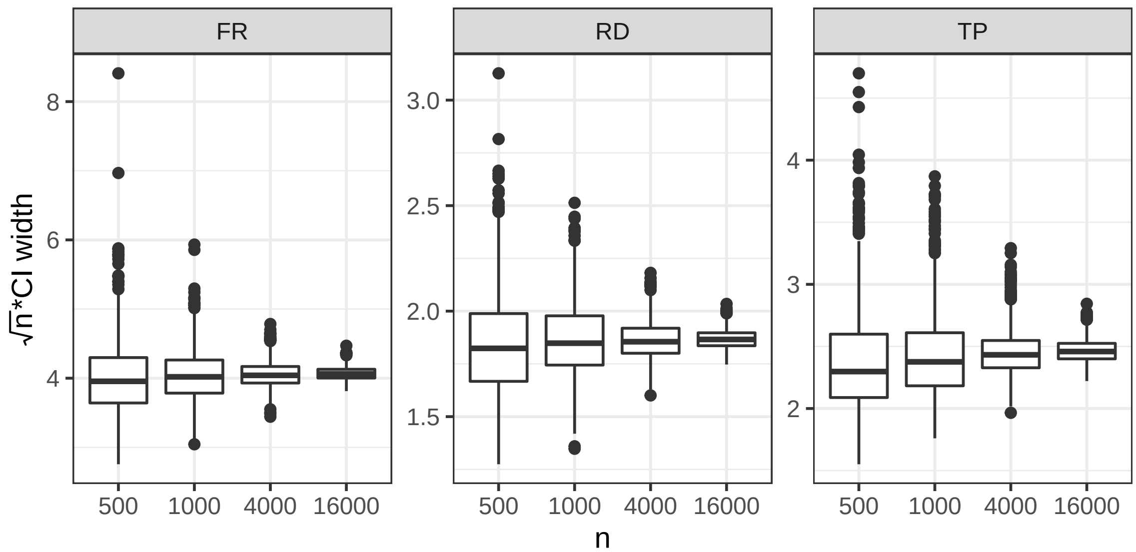

Figure S1: Boxplot of $\sqrt{n}\times$ CI width for ATE relative to each reference ITR in the simulation with nuisance functions being the truth.

Table S2: Performance of estimators of average causal effects in the simulation with nuisance functions in a parametric model.

Performance measure	Sample size	FR	RD	TP
95% Wald CI coverage	500	95%	83%	96%
	1000	91%	83%	93%
	4000	94%	88%	93%
	16000	94%	94%	95%
97.5% confidence lower bound coverage	500	99%	99%	99%
	1000	99%	99%	99%
	4000	99%	99%	98%
	16000	98%	99%	99%
bias	500	−0.0177	−0.0161	−0.0167
	1000	−0.0122	−0.0113	−0.0125
	4000	−0.0037	−0.0036	−0.0035
	16000	−0.0009	−0.0010	−0.0008
RMSE	500	0.035	0.029	0.040
	1000	0.026	0.021	0.029
	4000	0.012	0.009	0.013
	16000	0.006	0.004	0.006
Ratio of mean standard error to standard deviation	500	1.122	0.908	1.046
	1000	0.988	0.857	0.984
	4000	0.978	0.891	0.942
	16000	0.986	0.979	0.979

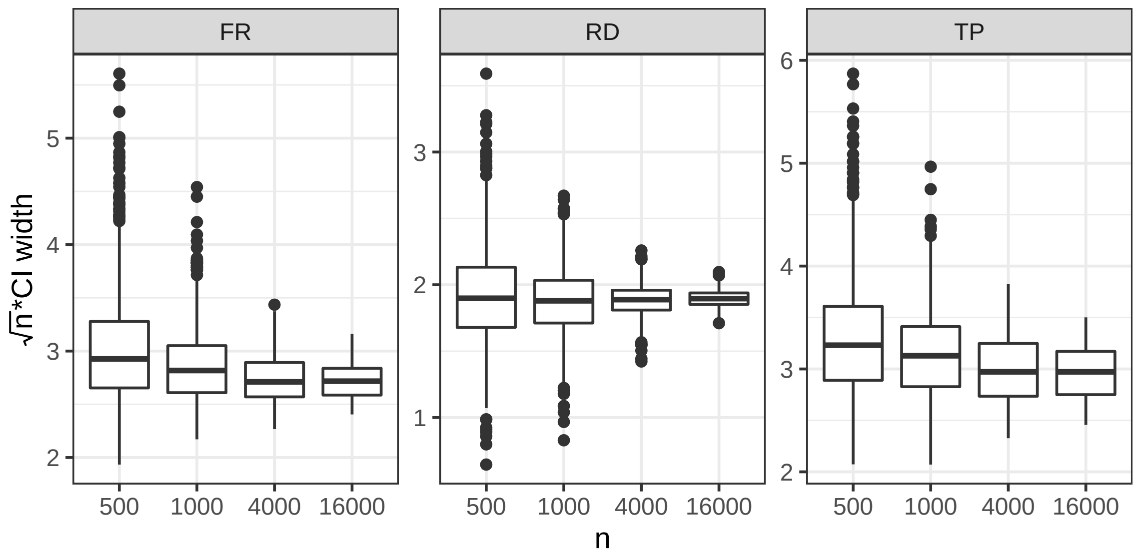

Figure S2: Boxplot of $\sqrt{n}\times$ CI width for ATE relative to each reference ITR in the simulation with nuisance functions in a parametric model.