Appendix

A Average Uplift in Terms of the Individual Uplift

$$\begin{aligned}
U(\pi) &= \iint \sum_{t=-1,1} yp(y \mid t, \boldsymbol{x})\pi(t \mid \boldsymbol{x})p(\boldsymbol{x})\mathrm{d}y\mathrm{d}\boldsymbol{x} - \iint \sum_{t=-1,1} yp(y \mid t, \boldsymbol{x})1[t=-1]p(\boldsymbol{x})\mathrm{d}y\mathrm{d}\boldsymbol{x} \\
&= \iint y[p(y \mid t=1, \boldsymbol{x})\pi(t=1 \mid \boldsymbol{x}) - p(y \mid t=-1, \boldsymbol{x})\pi(t=1 \mid \boldsymbol{x})]p(\boldsymbol{x})\mathrm{d}y\mathrm{d}\boldsymbol{x} \\
&= \iint y[p(y \mid t=1, \boldsymbol{x}) - p(y \mid t=-1, \boldsymbol{x})]\pi(t=1 \mid \boldsymbol{x})p(\boldsymbol{x})\mathrm{d}y\mathrm{d}\boldsymbol{x} \\
&= \int u(\boldsymbol{x})\pi(t=1 \mid \boldsymbol{x})p(\boldsymbol{x})\mathrm{d}\boldsymbol{x}.
\end{aligned} \tag{15}$$

B Area Under the Uplift Curve and Ranking

Define the following symbols:

- $C_\alpha := \Pr[f(\boldsymbol{x}) < \alpha]$,
- $U(\alpha; f) := \int u(\boldsymbol{x})1[\alpha \le f(\boldsymbol{x})]p(\boldsymbol{x})\mathrm{d}\boldsymbol{x}$,
- $\mathrm{Rank}(f) := \mathbf{E}[1[f(\boldsymbol{x}') \le f(\boldsymbol{x})][u(\boldsymbol{x}') - u(\boldsymbol{x})]]$,
- $\mathrm{AUUC}(f) := \int_0^1 U(\alpha; f)\mathrm{d}C_\alpha$.

Then, we have

$$\begin{aligned}
\mathrm{AUUC}(f) &= \int_{-\infty}^{\infty} U(\alpha)\frac{\mathrm{d}C_\alpha}{\mathrm{d}\alpha}\mathrm{d}\alpha \\
&= \int_{-\infty}^{\infty} U(\alpha)p_{f(\boldsymbol{x})}(\alpha)\mathrm{d}\alpha \\
&= \int_{\mathbb{R}^d} U(f(\boldsymbol{x}))p(\boldsymbol{x})\mathrm{d}\boldsymbol{x} \\
&= \iint 1[f(\boldsymbol{x}) \le f(\boldsymbol{x}')]u(\boldsymbol{x}')p(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}'p(\boldsymbol{x})\mathrm{d}\boldsymbol{x} \\
&= \mathbf{E}[1[f(\boldsymbol{x}) \le f(\boldsymbol{x}')]u(\boldsymbol{x}')] \\
&(= \mathbf{E}[1[f(\boldsymbol{x}) \le f(\boldsymbol{x}')][y^+ - y^-]]),
\end{aligned}$$

where $y^+ \sim p(y \mid \boldsymbol{x}', t=1)$ and $y^- \sim p(y \mid \boldsymbol{x}', t=-1)$.

Assuming $\Pr[f(\boldsymbol{x}') = f(\boldsymbol{x})] = 0$, we have

$$\begin{aligned}
\mathrm{Rank}(f) &:= \mathbf{E}[1[f(\boldsymbol{x}) \ge f(\boldsymbol{x}')][u(\boldsymbol{x}) - u(\boldsymbol{x}')]] \\
&= \mathbf{E}[1[f(\boldsymbol{x}) \ge f(\boldsymbol{x}')]u(\boldsymbol{x})] \\
&\quad - \mathbf{E}[1[f(\boldsymbol{x}) \ge f(\boldsymbol{x}')]u(\boldsymbol{x}')] \\
&= \mathrm{AUUC}(f) - \mathbf{E}[(1 - 1[f(\boldsymbol{x}) \le f(\boldsymbol{x}')])u(\boldsymbol{x}')] \\
&= \mathbf{E}[u(\boldsymbol{x})] - 2\,\mathrm{AUUC}(f).
\end{aligned}$$

Thus, $\mathrm{Rank}(f) = 2(\mathrm{AUUC}(f) - \mathrm{AUUC}(r))$, where $r : \mathbb{R}^d \to \mathbb{R}$ is the random ranking scoring function that outputs 1 or -1 with probability $1/2$ for any input $\boldsymbol{x}$. $\mathrm{Rank}(f)$ is maximized when $f(\boldsymbol{x}) \le f(\boldsymbol{x}') \iff u(\boldsymbol{x}) \le u(\boldsymbol{x}')$ for almost every pair of $\boldsymbol{x} \in \mathbb{R}^d$ and $\boldsymbol{x} \in \mathbb{R}^d$. In particular, $f = u$ is a maximizer of the objective.

C Proof of Lemma 1

Lemma 1. *For every $\boldsymbol{x}$ such that $p_1(\boldsymbol{x}) \neq p_2(\boldsymbol{x})$, $u(\boldsymbol{x})$ can be expressed as*

$$u(\boldsymbol{x}) = 2 \times \frac{\mathbf{E}_{y \sim p_1(y|\boldsymbol{x})}[y] - \mathbf{E}_{y \sim p_2(y|\boldsymbol{x})}[y]}{\mathbf{E}_{t \sim p_1(t|\boldsymbol{x})}[t] - \mathbf{E}_{t \sim p_2(t|\boldsymbol{x})}[t]}. \tag{16}$$

Proof.

$$\begin{aligned}
\mathbf{E}_{y\sim p_1(y|\boldsymbol{x})}[y] - \mathbf{E}_{y\sim p_2(y|\boldsymbol{x})}[y] &= \int \sum_{\tau=-1,1} yp(y \mid \boldsymbol{x}, t=\tau)p_1(t=\tau \mid \boldsymbol{x})\mathrm{d}y \\
&\quad - \int \sum_{\tau=-1,1} yp(y \mid \boldsymbol{x}, t=\tau)p_2(t=\tau \mid \boldsymbol{x})\mathrm{d}y \\
&= \int \sum_{\tau=-1,1} yp(y \mid \boldsymbol{x}, t=\tau)(p_1(t=\tau \mid \boldsymbol{x}) - p_2(t=\tau \mid \boldsymbol{x}))\mathrm{d}y \\
&= \sum_{\tau=-1,1} \mathbf{E}_{y\sim p(y|\boldsymbol{x},t=\tau)}[y](p_1(t=\tau \mid \boldsymbol{x}) - p_2(t=\tau \mid \boldsymbol{x})) \\
&= \mathbf{E}_{y\sim p(y|\boldsymbol{x},t=1)}[y](p_1(t=1 \mid \boldsymbol{x}) - p_2(t=1 \mid \boldsymbol{x})) \\
&\quad + \mathbf{E}_{y\sim p(y|\boldsymbol{x},t=-1)}[y](1 - p_1(t=1 \mid \boldsymbol{x}) - 1 + p_2(t=1 \mid \boldsymbol{x})) \\
&= u(\boldsymbol{x})(p_1(t=1 \mid \boldsymbol{x}) - p_2(t=1 \mid \boldsymbol{x})).
\end{aligned}$$

When $p_1(t=1 \mid \boldsymbol{x}) \neq p_2(t=1 \mid \boldsymbol{x})$, it holds that

$$\begin{aligned}
u(\boldsymbol{x}) &= \frac{\mathbf{E}_{y\sim p_1(y|\boldsymbol{x})}[y] - \mathbf{E}_{y\sim p_2(y|\boldsymbol{x})}[y]}{p_1(t=1 \mid \boldsymbol{x}) - p_2(t=1 \mid \boldsymbol{x})} \\
&= 2 \times \frac{\mathbf{E}_{y\sim p_1(y|\boldsymbol{x})}[y] - \mathbf{E}_{y\sim p_2(y|\boldsymbol{x})}[y]}{\mathbf{E}_{t\sim p_1(t|\boldsymbol{x})}[t] - \mathbf{E}_{t\sim p_2(t|\boldsymbol{x})}[t]}.
\end{aligned}$$

□

D Proof of Lemma 2

Lemma 2. *For every $\boldsymbol{x}$ such that $p_1(\boldsymbol{x}) \neq p_2(\boldsymbol{x})$, $u(\boldsymbol{x})$ can be expressed as*

$$u(\boldsymbol{x}) = 2 \times \frac{\mathbf{E}[z \mid \boldsymbol{x}]}{\mathbf{E}[w \mid \boldsymbol{x}]},$$

where $\mathbf{E}[z \mid \boldsymbol{x}]$ and $\mathbf{E}[w \mid \boldsymbol{x}]$ are the conditional expectations of z given $\boldsymbol{x}$ over $p(z \mid \boldsymbol{x})$ and w given $\boldsymbol{x}$ over $p(w \mid \boldsymbol{x})$, respectively.

Proof. We have

$$\begin{aligned}
\mathbf{E}[z \mid \boldsymbol{x}] &= \int \zeta \left[\frac{1}{2}p_1(y=\zeta \mid \boldsymbol{x}) + \frac{1}{2}p_2(y=-\zeta \mid \boldsymbol{x})\right]\mathrm{d}\zeta \\
&= \frac{1}{2}\int \zeta p_1(y=\zeta \mid \boldsymbol{x})\mathrm{d}\zeta + \frac{1}{2}\int \zeta p_2(y=-\zeta \mid \boldsymbol{x})\mathrm{d}\zeta \\
&= \frac{1}{2}\int yp_1(y \mid \boldsymbol{x})\mathrm{d}y - \frac{1}{2}\int yp_2(y \mid \boldsymbol{x})\mathrm{d}y \\
&= \frac{1}{2}\mathbf{E}_{y\sim p_1(y|\boldsymbol{x})}[y] - \frac{1}{2}\mathbf{E}_{y\sim p_2(y|\boldsymbol{x})}[y].
\end{aligned}$$

Similarly, we obtain

$$\mathbf{E}[w \mid \boldsymbol{x}] = \frac{1}{2}\mathbf{E}_{t\sim p_1(t|\boldsymbol{x})}[t] - \frac{1}{2}\mathbf{E}_{t\sim p_2(t|\boldsymbol{x})}[t].$$

Thus,

$$2 \times \frac{\mathbf{E}[z \mid \boldsymbol{x}]}{\mathbf{E}[w \mid \boldsymbol{x}]} = 2 \times \frac{\mathbf{E}_{y\sim p_1(y|\boldsymbol{x})}[y] - \mathbf{E}_{y\sim p_2(y|\boldsymbol{x})}[y]}{\mathbf{E}_{t\sim p_1(t|\boldsymbol{x})}[t] - \mathbf{E}_{t\sim p_2(t|\boldsymbol{x})}[t]} = u(\boldsymbol{x}).$$

□

E Proof of Theorem 2

We restate Theorem 2 below.

Theorem 2. *Assume that $n_1 = n_2$, $\widetilde{n}_1 = \widetilde{n}_2$, $p_1(\boldsymbol{x}) = p_2(\boldsymbol{x})$, $W := \inf_{x\in\mathcal{X}} |\mu_w(\boldsymbol{x})| > 0$, $M_{\mathcal{Z}} := \sup_{z\in\mathcal{Z}} |z| < \infty$, $M_F := \sup_{f\in F, x\in\mathcal{X}} |f(x)| < \infty$, and $M_G := \sup_{g\in G, x\in\mathcal{X}} |g(x)| < \infty$. Then, the following holds with probability at least $1-\delta$ that for every $f \in F$,*

$$\mathbf{E}_{\boldsymbol{x}\sim p(\boldsymbol{x})}[(f(\boldsymbol{x}) - u(\boldsymbol{x}))^2] \leq \frac{1}{W^2}\left[\sup_{g\in G} \widehat{J}(f,g) + \mathcal{R}_{F,G}^{n,\widetilde{n}} + \left(\frac{M_z}{\sqrt{2n}} + \frac{M_w}{\sqrt{2\widetilde{n}}}\right)\sqrt{\log\frac{2}{\delta}} + \varepsilon_G(f)\right],$$

where $M_z := 4M_{\mathcal{Y}}M_{\mathcal{G}} + M_{\mathcal{G}}^2/2$, $M_w = 2M_{\mathcal{F}}M_{\mathcal{G}} + M_{\mathcal{G}}^2/2$, $\mathcal{R}_{F,G}^{n,\widetilde{n}} := 2(M_F + 4M_Z)\mathfrak{R}_{p(\boldsymbol{x},z)}^n(G) + 2(2M_F + M_G)\mathfrak{R}_{p(\boldsymbol{x},w)}^{\widetilde{n}}(F) + 2(M_F + M_G)\mathfrak{R}_{p(\boldsymbol{x},w)}^{\widetilde{n}}(G)$.

Define $J(f,g)$ and $\widehat{J}(f,g)$ as in Section 3.2 and denote

$$\varepsilon_G(f) := \sup_{g\in L^2(p)} J(f,g) - \sup_{g\in G} J(f,g).$$

Definition 1 (Rademacher Complexity)**.** *We define the* Rademacher complexity *of H over N random variables following probability distribution q by*

$$\mathfrak{R}_p^N(H) = \mathbf{E}_{V_1,\dots,V_N,\sigma_1,\dots,\sigma_N}\left[\sup_{h\in H}\frac{1}{N}\sum_{i=1}^N \sigma_i h(V_i)\right],$$

where $\sigma_1,\dots,\sigma_N$ are independent, $\{-1,1\}$-valued uniform random variables.

Lemma 3. *Under the assumptions of Theorem 2, with probability at least $1-\delta$, it holds that for every $f\in F$,*

$$J(f,g) \le \widehat{J}(f,g) + \mathfrak{R}_{F,G} + \left(\frac{M_z}{\sqrt{n}} + \frac{M_w}{\sqrt{\widetilde{n}}}\right)\sqrt{\log\frac{2}{\delta}}.$$

To prove Lemma 3, we use the following lemma, which is a slightly modified version of Theorem 3.1 in Mohri et al. [22].

Lemma 4. *Let H be a set of real-valued functions on a measurable space $\mathcal{D}$. Assume that $M := \sup_{h\in H, v\in\mathcal{D}} h(v) < \infty$. Then, for any $h\in H$ and any $\mathcal{D}$-valued i.i.d. random variables $V, V_1,\dots,V_N$ following density q, we have*

$$\mathbf{E}[h(V)] \le \frac{1}{N}\sum_{i=1}^N h(V_i) + 2\mathfrak{R}_q^N(H) + \sqrt{\frac{M^2}{N}\log\frac{1}{\delta}}. \tag{17}$$

Proof of Lemma 4. We follow the proof of Theorem 3.1 in Mohri et al. [22] except that we set the constant B_ϕ in Eq. (28) to M/m when we apply McDiarmid's inequality (Section M). $\square$

Now, we prove Lemma 3.

Proof of Lemma 3. For any $f\in\mathcal{F}$, $g\in\mathcal{G}$, $\boldsymbol{x}',\widetilde{\boldsymbol{x}}'\in\mathcal{X}$, $z'\in\mathcal{Z} := \{y,-y \mid y\in\mathcal{Y}\}$, and $w'\in\{-1,1\}$, we define h_z and h_w as follows:

$$h_z(\boldsymbol{x}',z';g) := -4z'g(\boldsymbol{x}') - \frac{1}{2}g(\boldsymbol{x}')^2,$$
$$h_w(\widetilde{\boldsymbol{x}}',w';f,g) := w'f(\widetilde{\boldsymbol{x}}')g(\widetilde{\boldsymbol{x}}') - \frac{1}{2}g(\widetilde{\boldsymbol{x}}')^2.$$

Denoting $H_z := \{(\boldsymbol{x}',z')\mapsto h_z(\boldsymbol{x}',z';g) \mid g\in G\}$, we have

$$\sup_{h\in H_z,\boldsymbol{x}'\in\mathcal{X},z'\in\mathcal{Z}} \left|h(\boldsymbol{x}',z')\right| \le 4M_Z M_G + \frac{1}{2}M_G^2 =: M_z < \infty,$$

and thus, we can apply Lemma 4 to confirm that with probability at least $1-\delta/2$,

$$\mathbf{E}_{(\boldsymbol{x},z)\sim p(\boldsymbol{x},z)}[h_z(\boldsymbol{x},z;g)] \le \frac{1}{n}\sum_{(\boldsymbol{x}_i,z_i)\in S_z} h_z(\boldsymbol{x}_i,z_i;g) + 2\mathfrak{R}_p^n(H_z) + \sqrt{\frac{M_z^2}{n}\log\frac{2}{\delta}},$$

where $\{(\boldsymbol{x}_i,z_i)\}_{i=1}^n =: S_z$ are the samples defined in Section 4.1. Similarly, it holds that with probability at least $1-\delta/2$,

$$\mathbf{E}_{(\widetilde{\boldsymbol{x}},w)\sim p(\boldsymbol{x},w)}[h_w(\widetilde{\boldsymbol{x}},w;f,g)] \le \frac{1}{\widetilde{n}}\sum_{(\widetilde{\boldsymbol{x}},w_i)\in S_w} h_w(\widetilde{\boldsymbol{x}}_i,w_i;f,g) + 2\mathfrak{R}_p^{\widetilde{n}}(H_w) + \sqrt{\frac{M_w^2}{\widetilde{n}}\log\frac{2}{\delta}},$$

where $H_w := \{(\widetilde{\boldsymbol{x}}',w')\mapsto h_w(\widetilde{\boldsymbol{x}}',w';f,g) \mid f\in F, g\in G\}$, $M_w := M_F M_G + M_G^2/2$, and $\{(\widetilde{\boldsymbol{x}}_i,w_i)\}_{i=1}^n =: S_w$ are the samples defined in Section 4.1. By the union bound, we have the following with probability at least $1-\delta$:

$$\mathbf{E}_{(\boldsymbol{x},z)\sim p(\boldsymbol{x},z)}[h_z(\boldsymbol{x},z;g)] + \mathbf{E}_{(\widetilde{\boldsymbol{x}},w)\sim p(\boldsymbol{x},w)}[h_w(\widetilde{\boldsymbol{x}},w;f,g)] \tag{18}$$

$$\le \frac{1}{n}\sum_{(\boldsymbol{x}_i,z_i)\in S_z} h_z(\boldsymbol{x}_i,z_i,g) + \frac{1}{\widetilde{n}}\sum_{(\widetilde{\boldsymbol{x}},w_i)} h_w(\boldsymbol{x}_i,w_i,f,g) \tag{19}$$

$$+ 2(\mathfrak{R}_p^n(H_z) + \mathfrak{R}_p^{\widetilde{n}}(H_w)) + \left(\frac{M_z}{\sqrt{n}} + \frac{M_w}{\sqrt{\widetilde{n}}}\right)\sqrt{\log\frac{2}{\delta}}, \tag{20}$$

Using some properties of the Rademacher complexity including Talagrand's lemma, we can show that

$$\mathfrak{R}_p^n(H_z) \leq (M_F + 4M_Z)\mathfrak{R}_p^n(G), \tag{21}$$

$$\mathfrak{R}_p^{\widetilde{n}}(H_w) \leq (2M_F + M_G)\mathfrak{R}_p^{\widetilde{n}}(F) + (M_F + M_G)\mathfrak{R}_p^{\widetilde{n}}(G). \tag{22}$$

Clearly,

$$\widehat{J}(f,g) = \frac{1}{n}\sum_{(\boldsymbol{x}_i,z_i)\in S_z} h(\boldsymbol{x}_i, z_i; g) + \frac{1}{\widetilde{n}}\sum_{(\widetilde{\boldsymbol{x}}_i,w_i)\in S_w} h(\widetilde{\boldsymbol{x}}_i, w_i; f, g),$$

$$J(f,g) = \mathbf{E}_{(\boldsymbol{x},z)\sim p(\boldsymbol{x},z)}[h_z(\boldsymbol{x},z;g)] + \mathbf{E}_{(\widetilde{\boldsymbol{x}},w)\sim p(\boldsymbol{x},z)}[h_w(\widetilde{\boldsymbol{x}},w;f,g)].$$

From Eq. (20), Eq. (21), and Eq. (22), we obtain

$$J(f,g) \leq \widehat{J}(f,g) + \mathfrak{R}_{F,G} + \left(\frac{M_z}{\sqrt{n}} + \frac{M_w}{\sqrt{\widetilde{n}}}\right)\sqrt{\log\frac{2}{\delta}}, \tag{23}$$

where

$$\mathfrak{R}_{F,G} := 2(M_F + 4M_Z)\mathfrak{R}_p^n(G) + 2(2M_F + M_G)\mathfrak{R}_p^{\widetilde{n}}(F) + 2(M_F + M_G)\mathfrak{R}_p^{\widetilde{n}}(G).$$

□

Finally, we prove Theorem 2.

Proof of Theorem 2. From Lemma 3, with probability at least $1-\delta$, it holds that for all $f \in F$

$$\sup_{g\in G} J(f,g) \leq \sup_{g\in G}\widehat{J}(f,g) + \mathfrak{R}_{F,G} + \left(\frac{M_z}{\sqrt{n}} + \frac{M_w}{\sqrt{\widetilde{n}}}\right)\sqrt{\log\frac{2}{\delta}}. \tag{24}$$

Moreover, recalling $W := \inf_{\boldsymbol{x}\in\mathcal{X}}|\mu_w(\boldsymbol{x})|$ and $\sup_{g\in L^2(p)} J(f,g) = \mathbf{E}[(\mu_w(\boldsymbol{x})f(\boldsymbol{x}) - \mu_z(\boldsymbol{x}))^2]$, we have

$$\mathbf{E}\left[(f(\boldsymbol{x}) - u(\boldsymbol{x}))^2\right] = \mathbf{E}\left[\left(f(\boldsymbol{x}) - \frac{\mu_z(\boldsymbol{x})}{\mu_w(\boldsymbol{x})}\right)^2\right] \tag{25}$$

$$\leq \frac{1}{W^2}\mathbf{E}[(\mu_w(\boldsymbol{x})f(\boldsymbol{x}) - \mu_z(\boldsymbol{x}))^2] \tag{26}$$

$$= \frac{1}{W^2}\left[\varepsilon_G(f) + \sup_{g\in G} J(f,g)\right]. \tag{27}$$

Combining Eq. (24) and Eq. (27) yields the inequality of the theorem. □

F Proof of Corollary 1

Corollary 1. *Let $F = \{x \mapsto \boldsymbol{\alpha}^\top\boldsymbol{\phi}(\boldsymbol{x}) \mid \|\boldsymbol{\alpha}\|_2 \leq \Lambda_F\}$, $G = \{x \mapsto \boldsymbol{\beta}^\top\boldsymbol{\psi}(\boldsymbol{x}) \mid \|\boldsymbol{\beta}\|_2 \leq \Lambda_G\}$, and assume that $r_F := \sup_{\boldsymbol{x}\in\mathcal{X}}\|\boldsymbol{\phi}(\boldsymbol{x})\|_2 < \infty$ and $r_G := \sup_{\boldsymbol{x}\in\mathcal{X}}\|\boldsymbol{\psi}(\boldsymbol{x})\|_2 < \infty$, where $\|\cdot\|_2$ is the L_2-norm. Under the assumptions of Theorem 2, it holds with probability at least $1-\delta$ that for every $f \in F$,*

$$\mathbf{E}_{\boldsymbol{x}\sim p(\boldsymbol{x})}[(f(\boldsymbol{x}) - u(\boldsymbol{x}))^2] \leq \frac{1}{W^2}\left[\sup_{g\in G}\widehat{J}(f,g) + \frac{C_z\sqrt{\log\frac{2}{\delta}} + D_z}{\sqrt{2n}} + \frac{C_w\sqrt{\log\frac{2}{\delta}} + D_w}{\sqrt{2\widetilde{n}}} + \varepsilon_G(f)\right],$$

where $C_z := r_G^2\Lambda_G^2 + 4r_G\Lambda_G M_\mathcal{Y}$, $C_w := 2r_F^2\Lambda_F^2 + 2r_F r_G\Lambda_F\Lambda_G + r_G^2\Lambda_G^2$, $D_z := r_G^2\Lambda_G^2/2 + 4r_G\Lambda_G M_\mathcal{Y}$, and $D_w := r_G^2\Lambda_G^2/2 + 4r_F r_G\Lambda_F\Lambda_G$.

Proof. Under the assumptions, it is known that the Rademacher complexity of the linear-in-parameter model F can be upper bounded as follows [22]:

$$\mathfrak{R}_p^N(F) \leq \frac{r_F\Lambda_F}{\sqrt{N}}.$$

We can bound $\mathfrak{R}_p^N(G)$ similarly. Applying these bounds to Theorem 2, we obtain the statement of Corollary 1. □

G Proof of Theorem 3

We prove the following, formal version of Theorem 3.

Theorem 3. *Under the assumptions of Corollary 1, it holds with probability at least* $1-\delta$ *that* $\mathbf{E}[(\widehat{f}(\boldsymbol{x}) - u(\boldsymbol{x}))^2] \leq (4e_{n,\delta} + 2\varepsilon_G^F + \varepsilon_F)/W^2$*, where* $\varepsilon_G^F := \sup_{f\in F}\varepsilon_G(f)$*, and* $\varepsilon_F := \inf_{f\in F} J(f)$*,* $\widehat{f} \in F$ *is any approximate solution to* $\inf_{f\in F}\sup_{g\in G}\widehat{J}(f,g)$ *satisfying* $\sup_{g\in G}\widehat{J}(\widehat{f},g) \leq \inf_{f\in F}\sup_{g\in G}\widehat{J}(f,g) + e_{n,\delta}$*, and*

$$e_{n,\delta} := \frac{C_z\sqrt{\log\frac{2}{\delta}} + D_z}{\sqrt{2n}} + \frac{C_w\sqrt{\log\frac{2}{\delta}} + D_w}{\sqrt{2\widetilde{n}}}.$$

Proof. Let $J(f) := \sup_{g\in L^2} J(f,g) = \mathbf{E}[(\mu_w(\boldsymbol{x})f(\boldsymbol{x}) - \mu_z(\boldsymbol{x}))^2]$, $J_G(f) := \sup_{g\in G} J(f,g)$, $\widehat{J}_G(f) := \sup_{g\in G}\widehat{J}(f,g)$. Let $\widetilde{f}\in F$ be any approximate solution to $\inf_{f\in F} J(f)$ satisfying $J(\widetilde{f}) \leq \varepsilon_F + e_{n,\delta}$.

As a special case of Eq. 24, we can prove that with probability at least $1-\delta$, it holds for every $f\in F$ that $J_G(f) \leq \widehat{J}_G(f) + e_{n,\delta}$. From Corollary 1, it holds that with probability at least $1-\delta$,

$$\begin{aligned}
J(\widehat{f}) &\leq \left[J(\widehat{f}) - J_G(\widehat{f})\right] + \left[J_G(\widehat{f}) - \widehat{J}_G(\widehat{f})\right] + \left[\widehat{J}_G(\widehat{f}) - \widehat{J}_G(\widetilde{f})\right] \\
&\quad + \left[\widehat{J}_G(\widetilde{f}) - J_G(\widetilde{f})\right] + \left[J_G(\widetilde{f}) - J(\widetilde{f})\right] + J(\widetilde{f}) \\
&\leq \varepsilon_G^F + e_{n,\delta} + e_{n,\delta} \\
&\quad + e_{n,\delta} + \varepsilon_G^F + [\varepsilon_F + e_{n,\delta}] \\
&\leq 4e_{n,\delta} + 2\varepsilon_G^F + \varepsilon_F.
\end{aligned}$$

Since $\mathbf{E}[(\widehat{f}(\boldsymbol{x}) - u(\boldsymbol{x}))^2] \leq \frac{1}{W^2}J(\widehat{f})$, we obtain the bound in Theorem 3. □

H Binary Outcomes

When outcomes y take on binary values, e.g., success or failure, without loss of generality, we can assume that $y \in \{-1,1\}$. Then, by the definition of the individual uplift, $u(\boldsymbol{x}) \in [-2,2]$ for any $\boldsymbol{x}\in\mathbb{R}^d$. In order to incorporate this fact, we may add the following range constraints on f: $-2 \leq f(\boldsymbol{x}) \leq 2$ for every $\boldsymbol{x} \in \{\boldsymbol{x}_i\}_{i=1}^n \cup \{\widetilde{\boldsymbol{x}}_i\}_{i=1}^{\widetilde{n}}$.

I Cases Where $p_1(\boldsymbol{x}) \neq p_2(\boldsymbol{x})$ or $(n_1, \widetilde{n}_1) \neq (n_1, \widetilde{n}_1)$

So far, we have assumed that $p_1(\boldsymbol{x}) = p_2(\boldsymbol{x})$, $m_1 = m_2$, and $n_1 = n_2$. The proposed method can be adapted to the more general case where these assumptions may not hold.

Let $r_k(\boldsymbol{x}) = \frac{n}{2n_k}\cdot\frac{p(\boldsymbol{x})}{p_k(\boldsymbol{x})}$ and $\widetilde{r}_k(\boldsymbol{x}) = \frac{\widetilde{n}}{2\widetilde{n}_k}\cdot\frac{p(\boldsymbol{x})}{p_k(\boldsymbol{x})}$, $k=1,2$, for every $\boldsymbol{x}$ with $p_k(\boldsymbol{x}) > 0$. Let $k_i := 1$ if the sample $\boldsymbol{x}_i$ originally comes from $p_1(\boldsymbol{x})$, and $k_i := 2$ if it comes from $p_2(\boldsymbol{x})$. Similarly, define $\widetilde{k}_i \in \{1,2\}$ according to whether $\widetilde{\boldsymbol{x}}_i$ comes from $p_1(\boldsymbol{x})$ or $p_2(\boldsymbol{x})$. Then, unbiased estimators of the three terms in the proposed objective Eq. (10) are given as the following weighted sample averages using r_k and $\widetilde{r}_k$:

$$\begin{aligned}
\mathbf{E}_{\boldsymbol{x}\sim p(\boldsymbol{x})}[wf(\boldsymbol{x})g(\boldsymbol{x})] &\approx \frac{1}{\widetilde{n}}\sum_{i=1}^{\widetilde{n}}[w_i f(\widetilde{\boldsymbol{x}}_i)g(\widetilde{\boldsymbol{x}}_i)\widetilde{r}_{\widetilde{k}_i}(\widetilde{\boldsymbol{x}}_i)], \\
\mathbf{E}_{\boldsymbol{x}\sim p(\boldsymbol{x})}[zg(\boldsymbol{x})] &\approx \frac{1}{n}\sum_{i=1}^{n}[z_i g(\boldsymbol{x}_i) r_{k_i}(\boldsymbol{x}_i)] \\
\mathbf{E}_{\boldsymbol{x}\sim p(\boldsymbol{x})}[g(\boldsymbol{x})^2] &\approx \frac{1}{2n}\sum_{i=1}^{n}[g(\boldsymbol{x}_i)^2 r_{k_i}(\boldsymbol{x}_i)] + \frac{1}{2\widetilde{n}}\sum_{i=1}^{\widetilde{n}}[g(\widetilde{\boldsymbol{x}}_i)^2\widetilde{r}_{\widetilde{k}_i}(\widetilde{\boldsymbol{x}}_i)].
\end{aligned}$$

The density ratios $p_k(\boldsymbol{x})/p(\boldsymbol{x})$ can be accurately estimated using i.i.d. samples from $p_k(\boldsymbol{x})$ and $p(\boldsymbol{x})$ [21, 23, 35, 38].

J Unbiasedness of the Weighted Sample Average

Below, we show that the weighted sample averages are unbiased estimates. We only prove for $\mathbf{E}[wf(\boldsymbol{x})g(\boldsymbol{x})]$ since the other cases can be proven similarly. The expectation of the weighted sample average transforms as follows:

$$
\begin{aligned}
&\frac{1}{\widetilde{n}}\sum_{i=1}^{\widetilde{n}}\mathbf{E}_{\widetilde{\boldsymbol{x}}_i^{(k)}\sim p_k(\boldsymbol{x}),t_i^{(k)}\sim p_k(t|\widetilde{\boldsymbol{x}}_i^{(k)})}\left[w_i f(\widetilde{\boldsymbol{x}}_i)g(\widetilde{\boldsymbol{x}}_i)\widetilde{r}_{\widetilde{k}_i}(\widetilde{\boldsymbol{x}}_i)\right]\\
&=\frac{1}{\widetilde{n}}\sum_{k=1,2}\sum_{i=1}^{\widetilde{n}_k}\mathbf{E}_{\boldsymbol{x}\sim p_k(\boldsymbol{x}),t\sim p_k(t|\boldsymbol{x})}\left[(-1)^{k-1}tf(\boldsymbol{x})g(\boldsymbol{x})\frac{\widetilde{n}}{2\widetilde{n}_k}\cdot\frac{p(\boldsymbol{x})}{p_k(\boldsymbol{x})}\right]\\
&=\frac{1}{2}\sum_{k=1,2}\mathbf{E}_{\boldsymbol{x}\sim p(\boldsymbol{x}),t\sim p_k(t|\boldsymbol{x})}\left[(-1)^{k-1}tf(\boldsymbol{x})g(\boldsymbol{x})\right]\\
&=\iint(-1)^{k-1}t\sum_{k=1,2}\frac{1}{2}p_k(t\mid\boldsymbol{x})f(\boldsymbol{x})g(\boldsymbol{x})p(\boldsymbol{x})\mathrm{d}t\mathrm{d}\boldsymbol{x}\\
&=\iint wp(w\mid\boldsymbol{x})f(\boldsymbol{x})g(\boldsymbol{x})p(\boldsymbol{x})\mathrm{d}t\mathrm{d}\boldsymbol{x}\\
&=\mathbf{E}_{\boldsymbol{x}\sim p(\boldsymbol{x}),w\sim p(w|\boldsymbol{x})}[wf(\boldsymbol{x})g(\boldsymbol{x})].
\end{aligned}
$$

K Gaussian Basis Functions Used in Experiments

The l-th element of $\boldsymbol{\phi}(\boldsymbol{x})=(\phi_1(\boldsymbol{x}),\dots,\phi_{b_f}(\boldsymbol{x}))^\top$ is defined by

$$
\phi_l(\boldsymbol{x}):=\exp\left(\frac{-\left\|\boldsymbol{x}-\boldsymbol{x}^{(l)}\right\|^2}{\sigma^2}\right),
$$

where $\boldsymbol{x}^{(l)}$, $l=1,\dots,b_f$, are randomly chosen training data points. We used $b_f=100$ and $\sigma=25$ for all experiments. $\boldsymbol{\psi}$ is defined similarly.

L Justification of the Sub-Sampling Procedure

Suppose that we want a sample subset S_k following the treatment policy $p_k(t\mid\boldsymbol{x})$. For each sample $(\boldsymbol{x}_i,t_i,y_i)\sim p(\boldsymbol{x},t,y)$ in the original dataset, we randomly add it into S_k with probability proportional to $p_k(t_i\mid\boldsymbol{x}_i)/p(t_i\mid\boldsymbol{x}_i)$. Then,

$$
\begin{aligned}
p(\boldsymbol{x}_i,t_i,y_i\mid(\boldsymbol{x}_i,t_i,y_i)\in S_k)&=\frac{p((\boldsymbol{x}_i,t_i,y_i)\in S_k\mid\boldsymbol{x}_i,t_i,y_i)p(\boldsymbol{x}_i,t_i,y_i)}{\int\sum_{y_i,t_i}p((\boldsymbol{x}_i,t_i,y_i)\in S_k\mid\boldsymbol{x}_i,t_i,y_i)p(\boldsymbol{x}_i,t_i,y_i)\mathrm{d}\boldsymbol{x}_i}\\
&=\frac{p_k(t_i\mid\boldsymbol{x}_i)p(y_i\mid\boldsymbol{x}_i,t_i)p(\boldsymbol{x}_i)}{\int\sum_{y_i,t_i}p_k(t_i\mid\boldsymbol{x}_i)p(y_i\mid\boldsymbol{x}_i,t_i)p(\boldsymbol{x}_i)\mathrm{d}\boldsymbol{x}_i}\\
&=p_k(t_i\mid\boldsymbol{x}_i)p(y_i\mid\boldsymbol{x}_i,t_i)p(\boldsymbol{x}_i).
\end{aligned}
$$

This means that the subsamples S_k preserve the original $p(y\mid\boldsymbol{x},t)$ and $p(\boldsymbol{x})$ but follow the desired treatment policy $p_k(t\mid\boldsymbol{x})$.

M McDiarmid's Inequality

Although McDiarmid's inequality is a well known theorem, we present the statement to make the paper self-contained.

Theorem 4 (McDiarmid's inequality). *Let $\varphi:\mathcal{D}^N\to\mathbb{R}$ be a measurable function. Assume that there exists a real number $B_\varphi>0$ such that*

$$
\left|\varphi(v_1,\dots,v_N)-\varphi(v_1',\dots,v_N')\right|\le B_\varphi, \tag{28}
$$

for any $v_i,\dots,v_N,v_1,\dots,v_N'\in\mathcal{D}$ where $v_i=v_i'$ for all but one $i\in\{1,\dots,N\}$. Then, for any $\mathcal{D}$-valued independent random variables $V_1,\dots,V_N$ and any $\delta>0$ the following holds with probability at least $1-\delta$:

$$
\varphi(V_1,\dots,V_N)\le\mathbf{E}[\varphi(V_1,\dots,V_N)]+\sqrt{\frac{B_\varphi^2N}{2}\log\frac{1}{\delta}}.
$$