Supplementary Material

A Difinitions

We describe the formal notation of derivations of the propensity estimation and the potential outcome predictions.

DEFINITION A.1. *We represent the multiplicative deviations of the propensity score estimation as:*

$$\delta_i^{(1)} = 1 - \frac{e(\mathbf{X}_i)}{\hat{e}(\mathbf{X}_i)} \tag{A.1}$$

$$\delta_i^{(0)} = 1 - \frac{1 - e(\mathbf{X}_i)}{1 - \hat{e}(\mathbf{X}_i)} \tag{A.2}$$

If we have a perfect propensity score estimator (i.e., $\hat{e}(\mathbf{X}_i) = e(\mathbf{X}_i)$), $\delta_i^{(1)} = \delta_i^{(0)} = 0$. With regard to (A.1) and (A.2), the following equation holds.

$$\delta_i^{(0)} = -\frac{\hat{e}(\mathbf{X}_i)}{1 - \hat{e}(\mathbf{X}_i)} \delta_i^{(1)} \tag{A.3}$$

DEFINITION A.2. *The additive derivations of the potential outcome models are represented as:*

$$\Delta_i^{(1)} = \hat{\mu}_i^{(1)} - \mu_i^{(1)} \tag{A.4}$$

$$\Delta_i^{(0)} = \hat{\mu}_i^{(0)} - \mu_i^{(0)} \tag{A.5}$$

where $\hat{\mu}_i^{(1)}$ and $\hat{\mu}_i^{(0)}$ are predicted values for the expectations of i's potential outcomes.

DEFINITION A.3. *$\hat{Y}_i^{DR}$ is decomposed as:*

$$\hat{Y}_i^{DR} = \hat{Y}_i^{DR}(1) - \hat{Y}_i^{DR}(0) \tag{A.6}$$

where

$$\hat{Y}_i^{DR}(1) = \frac{W_i}{\hat{e}(\mathbf{X}_i)} \left(Y_i^{obs} - \hat{\mu}_i^{(1)}\right) + \hat{\mu}_i^{(1)}$$

$$\hat{Y}_i^{DR}(0) = \frac{1 - W_i}{1 - \hat{e}(\mathbf{X}_i)} \left(Y_i^{obs} - \hat{\mu}_i^{(0)}\right) + \hat{\mu}_i^{(0)}$$

B Proof of Theorem 3.3 and 3.4

First, we show the following Lemma B.1.

LEMMA B.1. *The covariance of $\hat{Y}_i^{DR}(1)$ and $\hat{Y}_i^{DR}(0)$ is*

$$\begin{aligned} Cov\left(\hat{Y}_i^{DR}(1), \hat{Y}_i^{DR}(0) \,\middle|\, \mathbf{X}_i\right) \\ = -\frac{e(\mathbf{X}_i)(1 - e(\mathbf{X}_i))}{\hat{e}(\mathbf{X}_i)(1 - \hat{e}(\mathbf{X}_i))} \Delta_i^{(1)} \Delta_i^{(0)} \end{aligned} \tag{B.7}$$

Proof. The covariance is decomposed as:

(B.8)

$$\begin{aligned} &Cov\left(\hat{Y}_i^{DR}(1), \hat{Y}_i^{DR}(0) \,\middle|\, \mathbf{X}_i\right) \\ &= \mathbb{E}\left[\hat{Y}_i^{DR}(1)\hat{Y}_i^{DR}(0) \,\middle|\, \mathbf{X}_i\right] - \mathbb{E}\left[\hat{Y}_i^{DR}(1) \,\middle|\, \mathbf{X}_i\right] \mathbb{E}\left[\hat{Y}_i^{DR}(0) \,\middle|\, \mathbf{X}_i\right] \end{aligned}$$

The first term of (B.8):

(B.9)

$$\begin{aligned} &\mathbb{E}\left[\hat{Y}_i^{DR}(1)\hat{Y}_i^{DR}(0) \,\middle|\, \mathbf{X}_i\right] \\ &= \mathbb{E}\Bigg[\left(\frac{W_i}{\hat{e}(\mathbf{X}_i)}\left(Y_i^{obs} - \hat{\mu}_i^{(1)}\right) + \hat{\mu}_i^{(1)}\right) \\ &\qquad \left(\frac{1 - W_i}{1 - \hat{e}(\mathbf{X}_i)}\left(Y_i^{obs} - \hat{\mu}_i^{(0)}\right) + \hat{\mu}_i^{(0)}\right) \,\Big|\, \mathbf{X}_i\Bigg] \\ &= \mathbb{E}\left[\frac{W_i}{\hat{e}(\mathbf{X}_i)} \,\middle|\, \mathbf{X}_i\right] \mathbb{E}\left[\left(Y_i^{(1)} - \hat{\mu}_i^{(1)}\right)\hat{\mu}_i^{(0)} \,\middle|\, \mathbf{X}_i\right] \\ &+ \mathbb{E}\left[\frac{1 - W_i}{1 - \hat{e}(\mathbf{X}_i)} \,\middle|\, \mathbf{X}_i\right] \mathbb{E}\left[\left(Y_i^{(0)} - \hat{\mu}_i^{(0)}\right)\hat{\mu}_i^{(1)} \,\middle|\, \mathbf{X}_i\right] + \hat{\mu}_i^{(1)}\hat{\mu}_i^{(0)} \\ &= \frac{e(\mathbf{X}_i)}{\hat{e}(\mathbf{X}_i)}\mu_i^{(1)}\hat{\mu}_i^{(0)} - \frac{e(\mathbf{X}_i)}{\hat{e}(\mathbf{X}_i)}\hat{\mu}_i^{(1)}\hat{\mu}_i^{(0)} \\ &+ \frac{1 - e(\mathbf{X}_i)}{1 - \hat{e}(\mathbf{X}_i)}\hat{\mu}_i^{(1)}\mu_i^{(0)} - \frac{1 - e(\mathbf{X}_i)}{1 - \hat{e}(\mathbf{X}_i)}\hat{\mu}_i^{(1)}\hat{\mu}_i^{(0)} + \hat{\mu}_i^{(1)}\hat{\mu}_i^{(0)} \\ &= \left(1 - \delta_i^{(1)}\right)\mu_i^{(1)}\hat{\mu}_i^{(0)} - \left(1 - \delta_i^{(1)} - \delta_i^{(0)}\right)\hat{\mu}_i^{(1)}\hat{\mu}_i^{(0)} \\ &+ \left(1 - \delta_i^{(0)}\right)\hat{\mu}_i^{(1)}\mu_i^{(0)} \end{aligned}$$

The second term of (B.8):

(B.10)

$$\begin{aligned} &\mathbb{E}\left[\hat{Y}_i^{DR}(1) \,\middle|\, \mathbf{X}_i\right] \mathbb{E}\left[\hat{Y}_i^{DR}(0) \,\middle|\, \mathbf{X}_i\right] \\ &= \left(\Delta_i^{(1)}\delta_i^{(1)} + \mu_i^{(1)}\right)\left(\Delta_i^{(0)}\delta_i^{(0)} + \mu_i^{(0)}\right) \quad \because Theorem\, 3.3 \\ &= \left(1 - \delta_i^{(1)}\right)\left(1 - \delta_i^{(0)}\right)\mu_i^{(1)}\mu_i^{(0)} + \delta_i^{(1)}\left(1 - \delta_i^{(0)}\right)\hat{\mu}_i^{(1)}\mu_i^{(0)} \\ &+ \left(1 - \delta_i^{(1)}\right)\delta_i^{(0)}\mu_i^{(1)}\hat{\mu}_i^{(0)} + \delta_i^{(1)}\delta_i^{(0)}\hat{\mu}_i^{(1)}\hat{\mu}_i^{(0)} \end{aligned}$$

Combining (B.8), (B.9), and (B.10), we have:

$$\begin{aligned} &Cov\left(\hat{Y}_i^{DR}(1), \hat{Y}_i^{DR}(0) \,\middle|\, \mathbf{X}_i\right) \\ &= \mathbb{E}\left[\hat{Y}_i^{DR}(1)\hat{Y}_i^{DR}(0) \,\middle|\, \mathbf{X}_i\right] - \mathbb{E}\left[\hat{Y}_i^{DR}(1) \,\middle|\, \mathbf{X}_i\right] \mathbb{E}\left[\hat{Y}_i^{DR}(0) \,\middle|\, \mathbf{X}_i\right] \\ &= \left(1 - \delta_i^{(1)}\right)\mu_i^{(1)}\hat{\mu}_i^{(0)} - \left(1 - \delta_i^{(1)} - \delta_i^{(0)}\right)\hat{\mu}_i^{(1)}\hat{\mu}_i^{(0)} \\ &+ \left(1 - \delta_i^{(0)}\right)\hat{\mu}_i^{(1)}\mu_i^{(0)} - \left(1 - \delta_i^{(1)}\right)\left(1 - \delta_i^{(0)}\right)\mu_i^{(1)}\mu_i^{(0)} \\ &- \delta_i^{(1)}\left(1 - \delta_i^{(0)}\right)\hat{\mu}_i^{(1)}\mu_i^{(0)} - \left(1 - \delta_i^{(1)}\right)\delta_i^{(0)}\mu_i^{(1)}\hat{\mu}_i^{(0)} - \delta_i^{(1)}\delta_i^{(0)}\hat{\mu}_i^{(1)}\hat{\mu}_i^{(0)} \\ &= -\left(1 - \delta_i^{(1)}\right)\left(1 - \delta_i^{(0)}\right)\left(\hat{\mu}_i^{(1)} - \mu_i^{(1)}\right)\left(\hat{\mu}_i^{(0)} - \mu_i^{(0)}\right) \\ &= -\left(1 - \delta_i^{(1)}\right)\left(1 - \delta_i^{(0)}\right)\Delta_i^{(1)}\Delta_i^{(0)} \\ &= -\frac{e(\mathbf{X}_i)(1 - e(\mathbf{X}_i))}{\hat{e}(\mathbf{X}_i)(1 - \hat{e}(\mathbf{X}_i))}\Delta_i^{(1)}\Delta_i^{(0)} \end{aligned}$$

□

THEOREM 3.3. *The bias of $\hat{Y}_i^{DR}$ is*

$$Bias\left(\hat{Y}_i^{DR} \mid \mathbf{X}_i\right) = \left|\mathbb{E}\left[\hat{Y}_i^{DR} \mid \mathbf{X}_i\right] - \tau_i\right|$$

$$= \left|\delta_i^{(1)}\left(\Delta_i^{(1)} + \frac{\hat{e}\left(\mathbf{X}_i\right)}{1-\hat{e}\left(\mathbf{X}_i\right)}\Delta_i^{(0)}\right)\right| \tag{B.11}$$

Proof. The expectation of the first term of (A.6) is:

(B.12)

$$\begin{aligned}
&\mathbb{E}\left[\hat{Y}_i^{DR}(1) \mid \mathbf{X}_i\right] \\
&= \mathbb{E}\left[\frac{W_i}{\hat{e}(\mathbf{X}_i)}\left(Y_i^{obs} - \hat{\mu}_i^{(1)}\right) + \hat{\mu}_i^{(1)} \mid \mathbf{X}_i\right] \\
&= \mathbb{E}\left[\left(\hat{\mu}_i^{(1)} - Y_i^{(1)}\right)\left(1 - \frac{W_i}{\hat{e}(\mathbf{X}_i)}\right) + Y_i^{(1)} \mid \mathbf{X}_i\right] \\
&= \mathbb{E}\left[\hat{\mu}_i^{(1)} - Y_i^{(1)} \mid \mathbf{X}_i\right]\mathbb{E}\left[1 - \frac{W_i}{\hat{e}(\mathbf{X}_i)} \mid \mathbf{X}_i\right] + \mathbb{E}\left[Y_i^{(1)} \mid \mathbf{X}_i\right] \\
&= \left(\hat{\mu}_i^{(1)} - \mu_i^{(1)}\right)\left(1 - \frac{e(\mathbf{X}_i)}{\hat{e}(\mathbf{X}_i)}\right) + \mu_i^{(1)} \\
&= \Delta_i^{(1)}\delta_i^{(1)} + \mu_i^{(1)}
\end{aligned}$$

Similarly, we obtain

$$\mathbb{E}\left[\hat{Y}_i^{DR}(0) \mid \mathbf{X}_i\right] = \Delta_i^{(0)}\delta_i^{(0)} + \mu_i^{(0)} \tag{B.13}$$

We have (B.11) by (A.3), (B.12), and (B.13).

□

THEOREM 3.4. *The variance of $\hat{Y}_i^{DR}$ is*

(B.14)

$$\begin{aligned}
Var\left(\hat{Y}_i^{DR} \mid \mathbf{X}_i\right) = {} & \mathbb{E}\left[\left(\epsilon_i^{(1)}\right)^2 \mid \mathbf{X}_i\right] + \mathbb{E}\left[\left(\epsilon_i^{(0)}\right)^2 \mid \mathbf{X}_i\right] \\
& + \frac{1-e\left(\mathbf{X}_i\right)}{e\left(\mathbf{X}_i\right)}\left(\Delta_i^{(1)}\right)^2\left(1-\delta_i^{(1)}\right)^2 \\
& + \frac{e\left(\mathbf{X}_i\right)}{1-e\left(\mathbf{X}_i\right)}\left(\Delta_i^{(0)}\right)^2\left(1-\delta_i^{(0)}\right)^2 \\
& + \frac{2e\left(\mathbf{X}_i\right)\left(1-e\left(\mathbf{X}_i\right)\right)}{\hat{e}\left(\mathbf{X}_i\right)\left(1-\hat{e}\left(\mathbf{X}_i\right)\right)}\Delta_i^{(1)}\Delta_i^{(0)}
\end{aligned}$$

Proof. The second moment of the first term of (A.6) is

$$\begin{aligned}
&\mathbb{E}\left[\left(\hat{Y}_i^{DR}(1)\right)^2 \mid \mathbf{X}_i\right] \\
&= \mathbb{E}\left[\left(\left(\hat{\mu}_i^{(1)} - Y_i^{(1)}\right)\left(1 - \frac{W_i}{\hat{e}(\mathbf{X}_i)}\right) + Y_i^{(1)}\right)^2 \mid \mathbf{X}_i\right] \\
&= \mathbb{E}\left[\left(\Delta_i^{(1)}\left(1 - \frac{W_i}{\hat{e}(\mathbf{X}_i)}\right) + \mu_i^{(1)} + \epsilon_i^{(1)}\right)^2 \mid \mathbf{X}_i\right] \\
&= \mathbb{E}\left[\left(\epsilon_i^{(1)}\right)^2 \mid \mathbf{X}_i\right] + 2\mathbb{E}\left[\mu_i^{(1)}\Delta_i^{(1)}\left(1 - \frac{W_i}{\hat{e}(\mathbf{X}_i)}\right) \mid \mathbf{X}_i\right] \\
&+ \mathbb{E}\left[\left(\Delta_i^{(1)}\right)^2\left(1 - \frac{2W_i}{\hat{e}(\mathbf{X}_i)} + \frac{W_i}{\left(\hat{e}(\mathbf{X}_i)\right)^2}\right) \mid \mathbf{X}_i\right] + \left(\mu_i^{(1)}\right)^2 \\
&= \mathbb{E}\left[\left(\epsilon_i^{(1)}\right)^2 \mid \mathbf{X}_i\right] + 2\mu_i^{(1)}\Delta_i^{(1)}\delta_i^{(1)} \\
&+ \left(\Delta_i^{(1)}\right)^2\left(\left(\delta_i^{(1)}\right)^2 + \frac{e(\mathbf{X}_i)(1-e(\mathbf{X}_i))}{\left(\hat{e}(\mathbf{X}_i)\right)^2}\right) + \left(\mu_i^{(1)}\right)^2 \\
&= \mathbb{E}\left[\left(\epsilon_i^{(1)}\right)^2 \mid \mathbf{X}_i\right] + \left(\mu_i^{(1)} + \Delta_i^{(1)}\delta_i^{(1)}\right)^2 \\
&+ \frac{1-e(\mathbf{X}_i)}{e(\mathbf{X}_i)}\left(\Delta_i^{(1)}\right)^2\left(1-\delta_i^{(1)}\right)^2
\end{aligned}$$

Therefore the variance is

(B.15)

$$\begin{aligned}
&Var\left(\hat{Y}_i^{DR}(1) \mid \mathbf{X}_i\right) \\
&= \mathbb{E}\left[\left(\hat{Y}_i^{DR}(1)\right)^2 \mid \mathbf{X}_i\right] - \left(\mathbb{E}\left[\hat{Y}_i^{DR}(1) \mid \mathbf{X}_i\right]\right)^2 \\
&= \mathbb{E}\left[\left(\epsilon_i^{(1)}\right)^2 \mid \mathbf{X}_i\right] + \frac{1-e(\mathbf{X}_i)}{e(\mathbf{X}_i)}\left(\Delta_i^{(1)}\right)^2\left(1-\delta_i^{(1)}\right)^2
\end{aligned}$$

Similarly, we obtain

(B.16)

$$\begin{aligned}
&Var\left(\hat{Y}_i^{DR}(0) \mid \mathbf{X}_i\right) \\
&= \mathbb{E}\left[\left(\hat{Y}_i^{DR}(0)\right)^2 \mid \mathbf{X}_i\right] - \left(\mathbb{E}\left[\hat{Y}_i^{DR}(0) \mid \mathbf{X}_i\right]\right)^2 \\
&= \mathbb{E}\left[\left(\epsilon_i^{(0)}\right)^2 \mid \mathbf{X}_i\right] + \frac{e(\mathbf{X}_i)}{1-e(\mathbf{X}_i)}\left(\Delta_i^{(0)}\right)^2\left(1-\delta_i^{(0)}\right)^2
\end{aligned}$$

Finally, we have by (B.15) and (B.16), and Lemma B.1 that:

$$\begin{aligned}
&Var(\hat{Y}_i^{DR} \mid \mathbf{X}_i) \\
&= Var\left(\hat{Y}_i^{DR}(1) \mid \mathbf{X}_i\right) + Var\left(\hat{Y}_i^{DR}(0) \mid \mathbf{X}_i\right) \\
&- 2Cov\left(\hat{Y}_i^{DR}(1), \hat{Y}_i^{DR}(0) \mid \mathbf{X}_i\right) \\
&= \mathbb{E}\left[\left(\epsilon_i^{(1)}\right)^2 \mid \mathbf{X}_i\right] + \mathbb{E}\left[\left(\epsilon_i^{(0)}\right)^2 \mid \mathbf{X}_i\right] \\
&+ \frac{1-e(\mathbf{X}_i)}{e(\mathbf{X}_i)}\left(\Delta_i^{(1)}\right)^2\left(1-\delta_i^{(1)}\right)^2 \\
&+ \frac{e(\mathbf{X}_i)}{1-e(\mathbf{X}_i)}\left(\Delta_i^{(0)}\right)^2\left(1-\delta_i^{(0)}\right)^2 \\
&+ \frac{2e(\mathbf{X}_i)(1-e(\mathbf{X}_i))}{\hat{e}(\mathbf{X}_i)(1-\hat{e}(\mathbf{X}_i))}\Delta_i^{(1)}\Delta_i^{(0)}
\end{aligned}$$

□

C Proof of Theorem 3.1 and 3.2

THEOREM 3.1. *The bias of the transformed outcome with a biased propensity score is*

$$Bias\left(\hat{Y}_i^{TO}\,|\,\mathbf{X}_i\right) = \left|\mathbb{E}\left[\hat{Y}_i^{TO}\,|\,\mathbf{X}_i\right] - \tau_i\right|$$
$$= \left|\delta_i^{(1)}\left(\mu_i^{(1)} + \frac{\hat{e}\left(\mathbf{X}_i\right)}{1-\hat{e}\left(\mathbf{X}_i\right)}\mu_i^{(0)}\right)\right| \tag{C.17}$$

Proof. We have (C.17) by replacing $\Delta_i^{(1)}$ and $\Delta_i^{(0)}$ in (B.11) with $\mu_i^{(1)}$ and $\mu_i^{(0)}$ respectively.

□

THEOREM 3.2. *The variance of the transformed outcome with a biased propensity score is*

(C.18)

$$Var\left(\hat{Y}_i^{TO}\,|\,\mathbf{X}_i\right) = \mathbb{E}\left[\left(\epsilon_i^{(1)}\right)^2\,|\,\mathbf{X}_i\right] + \mathbb{E}\left[\left(\epsilon_i^{(0)}\right)^2\,|\,\mathbf{X}_i\right]$$
$$+ \frac{1-e\left(\mathbf{X}_i\right)}{e\left(\mathbf{X}_i\right)}\left(\mu_i^{(1)}\right)^2\left(1-\delta_i^{(1)}\right)^2$$
$$+ \frac{e\left(\mathbf{X}_i\right)}{1-e\left(\mathbf{X}_i\right)}\left(\mu_i^{(0)}\right)^2\left(1-\delta_i^{(0)}\right)^2$$
$$+ \frac{2e\left(\mathbf{X}_i\right)\left(1-e\left(\mathbf{X}_i\right)\right)}{\hat{e}\left(\mathbf{X}_i\right)\left(1-\hat{e}\left(\mathbf{X}_i\right)\right)}\mu_i^{(1)}\mu_i^{(0)}$$

Proof. We have (C.18) by replacing $\Delta_i^{(1)}$ and $\Delta_i^{(0)}$ in (B.14) with $\mu_i^{(1)}$ and $\mu_i^{(0)}$ respectively.

□

D Proof of Theorem 3.5

THEOREM 3.5. *Given a set of realized training dataset* $\{\mathbf{x}_i, w_i, y_i^{obs}\}$, *and suppose* $\zeta_i = 0$, *the bias and variance of* $\hat{Y}_i^{SDR}(\gamma)$ *are*

$$Bias\left(\hat{Y}_i^{SDR}(\gamma)\,|\,\zeta_i = 0\right) = \left|\Delta_i^{(1)} - \Delta_i^{(0)}\right| \tag{D.19}$$

$$Var\left(\hat{Y}_i^{SDR}(\gamma)\,|\,\zeta_i = 0\right) = 0 \tag{D.20}$$

Proof. Suppose $\zeta_i = 0$, then,

$$\hat{Y}_i^{SDR}(\gamma) = \hat{\mu}_i^{(1)} - \hat{\mu}_i^{(0)}$$

Therefore, by simply subtracting i's true ITE from both sides, we have:

$$Bias\left(\hat{Y}_i^{SDR}(\gamma)\,|\,\zeta_i = 0\right)$$
$$= \left|\mathbb{E}\left[\hat{Y}_i^{SDR}(\gamma)\,|\,\zeta_i = 0\right] - \tau_i\right|$$
$$= \left|\left(\hat{\mu}_i^{(1)} - \hat{\mu}_i^{(0)}\right) - \left(\mu_i^{(1)} - \mu_i^{(0)}\right)\right|$$
$$= \left|\Delta_i^{(1)} - \Delta_i^{(0)}\right|$$

As for the variance, when i's feature vector is given, $\hat{Y}_i^{SDR}(\gamma) = \hat{\mu}_i^{(1)} - \hat{\mu}_i^{(0)}$ is a constant value. Therefore, (D.20) holds. □

E Proof of Theorem 4.1 and 4.2

First, we prove Theorem 4.2 and use it to prove Theorem 4.1.

THEOREM 4.2. *The bias of SDR-MSE with* $\gamma = 0$ *from the true MSE is*

(E.21)

$$\left|\mathbb{E}\left[\left(\hat{Y}_i^{SDR}(0) - \hat{\tau}_i\right)^2\right] - \mathbb{E}\left[\left(\tau_i - \hat{\tau}_i\right)^2\right]\right|$$
$$= \mathbb{E}\left[\left(\hat{Y}_i^{SDR}(0) - \tau_i\right)^2\right]$$
$$+ 2\left|\mathbb{E}\left[\delta_i^{(1)}\left(\hat{\tau}_i - \tau_i\right)\left(\Delta_i^{(1)} + \frac{\hat{e}\left(\mathbf{X}_i\right)}{1-\hat{e}\left(\mathbf{X}_i\right)}\Delta_i^{(0)}\right)\right]\right|$$

Proof. We have:

$$\mathbb{E}\left[\left(\hat{Y}_i^{SDR}(0) - \hat{\tau}_i\right)^2\right]$$
$$= \mathbb{E}\left[\left(\hat{Y}_i^{SDR}(0) - \tau_i + \tau_i - \hat{\tau}_i\right)^2\right]$$
$$= \mathbb{E}\left[\left(\hat{Y}_i^{SDR}(0) - \tau_i\right)^2\right] + \mathbb{E}\left[\left(\tau_i - \hat{\tau}_i\right)^2\right]$$
$$+ 2\mathbb{E}\left[\left(\hat{\tau}_i - \tau_i\right)\ \mathbb{E}\left[\left(\hat{Y}_i^{SDR}(\gamma = 0) - \tau_i\right)\,|\,\mathbf{X}_i\right]\right]$$
$$= \mathbb{E}\left[\left(\hat{Y}_i^{SDR}(0) - \tau_i\right)^2\right] + \mathbb{E}\left[\left(\tau_i - \hat{\tau}_i\right)^2\right]$$
$$+ 2\mathbb{E}\left[\delta_i^{(1)}\left(\hat{\tau}_i - \tau_i\right)\left(\Delta_i^{(1)} + \frac{\hat{e}(\mathbf{X}_i)}{1-\hat{e}(\mathbf{X}_i)}\Delta_i^{(0)}\right)\right]$$

Therefore, by subtracting $\mathbb{E}\left[\left(\tau_i - \hat{\tau}_i\right)^2\right]$ from both sides, we have (E.21).

□

THEOREM 4.1. *The bias of TO-MSE from the true MSE is*

(E.22)

$$\left|\mathbb{E}\left[\left(\hat{Y}_i^{TO} - \hat{\tau}_i\right)^2\right] - \mathbb{E}\left[\left(\check{\tau}_i - \hat{\tau}_i\right)^2\right]\right|$$
$$= \mathbb{E}\left[\left(\hat{Y}_i^{TO} - \tau_i\right)^2\right]$$
$$+ 2\left|\mathbb{E}\left[\delta_i^{(1)}\left(\hat{\tau}_i - \tau_i\right)\left(\mu_i^{(1)} + \frac{\hat{e}\left(\mathbf{X}_i\right)}{1-\hat{e}\left(\mathbf{X}_i\right)}\mu_i^{(0)}\right)\right]\right|$$

Proof. We have (E.22) by replacing $\Delta_i^{(1)}$ and $\Delta_i^{(0)}$ in (E.21) with $\mu_i^{(1)}$ and $\mu_i^{(0)}$ respectively.

□

F Details of the Experiments

F.1 Synthetic Data Here we present the details of parameter tuning in Section 5.1.

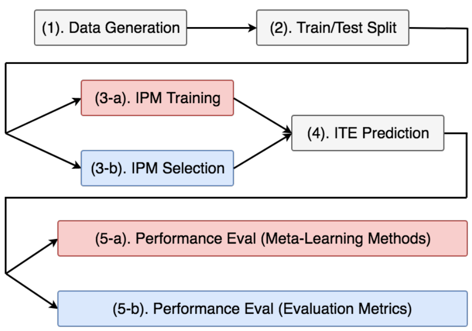

Figure 8: Overall flow of the experiments. Red box:meta-learning methods experiment. Blue box: evaluation metrics experiment.

F.1.1 Details of the Base Models: We used the same 50 base models in Section 5.1.1 and 5.1.2.

Elastic Net: 20 base models were based on Elastic Net. The regularization parameter α was between 0.01 and 1, and the ratio of the L1 regularization term λ_1 was between 0.01 and 0.9.

GBR[6]: 30 base models were based on GBR. The number of boosting stages n_{trees} was between 50 and 400. The maximum depth of the individual regression estimators Δ_{depth} was 2 or 4. The rate that shrinks the contribution of each tree η was 0.1 or 0.2.

F.1.2 Parameter Tuning Procedures for Outcome Models: Here, we describe the model selection and the hyper-parameter tuning procedures for the Potential Outcome Models (POMs) used in our proposed methods and the Observed Outcome Models (OOMs) used in τ-risk$_R$. Note that we only used the observed outcome, feature vectors, and treatment assignments, i.e., $(\mathbf{X}_i, W_i, Y_i^{obs})$, because these are available in real-world settings.

For the POM selection, we used μ-risk [19]. We selected the model and the corresponding hyper-parameters that minimized μ-risk as POM for each scenario. For the OOM selection, we selected the model and the corresponding hyper-parameters that had the minimum MSE for the observed outcomes. We relied on 3-fold cross-validation for the model selections, and used 3,000 samples from the first iteration of the experiments. Table F.1 lists the resulting POMs and OOMs for each scenario [7].

Table F.1: Selected models and hyper-parameters.

	POM	OOM
1	Elastic Net $\alpha = 0.1,\ \lambda_1 = 0.9$	Elastic Net $\alpha = 0.1,\ \lambda_1 = 0.8$
2	GBR $n_{trees} = 250,\ \Delta_{depth} = 2,\ \eta = 0.2$	Elastic Net $\alpha = 0.1,\ \lambda_1 = 0.1$
3	Elastic Net $\alpha = 0.01,\ \lambda_1 = 0.9$	Elastic Net $\alpha = 0.1,\ \lambda_1 = 0.9$
4	GBR $n_{trees} = 325,\ \Delta_{depth} = 2,\ \eta = 0.2$	Elastic Net $\alpha = 0.1,\ \lambda_1 = 0.1$
5	Elastic Net $\alpha = 0.01,\ \lambda_1 = 0.9$	Elastic Net $\alpha = 0.1,\ \lambda_1 = 0.9$
6	GBR $n_{trees} = 50,\ \Delta_{depth} = 2,\ \eta = 0.2$	Elastic Net $\alpha = 0.1,\ \lambda_1 = 0.1$
7	GBR $n_{trees} = 50,\ \Delta_{depth} = 2,\ \eta = 0.2$	Elastic Net $\alpha = 0.1,\ \lambda_1 = 0.9$
8	GBR $n_{trees} = 50,\ \Delta_{depth} = 2,\ \eta = 0.2$	Elastic Net $\alpha = 0.1,\ \lambda_1 = 0.2$

F.1.3 Full Results Table F.2 and Table F.3 show the complete results of the experiments in Section 5.1 including six values for γ.

G Right Heart Catheterization Data

Here we present the details of parameter tuning in Section 5.2.

G.1 Details of the Base Models: We used 20 base models for each meta-learning method.

For TMA:

Logistic Regression: 10 base models were Logistic Regression. The Regularization parameter α was between 0.01 and 500.

RFC[8]: 10 base models were RFC. The number of trees was fixed ($n_{trees} = 300$), the maximum depth of the tree Δ_{depth} was between 1 and 5, the minimum number of samples required to be at a leaf node $n_{min-leaf}$ was 1 or 3.

For TOM & SDRM:

Elastic Net: 10 base models were Elastic Net. The regularization parameter α was between 0.01 and

[6] Gradient Boosting Regressor.

[7] Undescribed parameters of each algorithm are the default values defined by scikit-learn (http://scikit-learn.org/stable/).

[8] Random Forest Classifier.

Table F.2: Experimental results of meta-learning methods. Each value is the average RMSE over 50 iterations.

Scenario	1	2	3	4
TMA	1.004	0.941	1.167	1.358
TOM	7.644	4.268	19.754	4.742
SDRM(0.0)	1.785	0.684	3.501	0.771
SDRM(0.1)	0.643	0.604	0.748	0.771
SDRM(0.2)	0.461	0.588	0.607	0.763
SDRM(0.3)	0.401	0.583	0.540	0.756
SDRM(0.4)	0.368	0.580	0.502	0.749
SDRM(0.5)	**0.342**	**0.576**	**0.473**	**0.743**
Scenario	5	6	7	8
TMA	2.448	**1.000**	2.128	1.948
TOM	27.247	1.139	3.113	3.329
SDRM(0.0)	3.439	1.104	2.326	2.016
SDRM(0.1)	0.762	1.104	2.296	2.017
SDRM(0.2)	0.658	1.094	2.221	1.982
SDRM(0.3)	0.616	1.076	2.150	1.933
SDRM(0.4)	0.597	1.045	2.062	1.886
SDRM(0.5)	**0.580**	1.003	**1.988**	**1.836**

10, and the ratio of the L1 regularization term λ_1 was between 0.01 and 0.9.

RFR[9]: 10 base models were RFRs. The number of trees was fixed ($n_{trees} = 300$), the maximum depth of the tree Δ_{depth} was between 1 and 5, the minimum number of samples required to be at a leaf node $n_{min-leaf}$ was 1 or 3.

G.2 Details of the POM and OOM: We followed the same procedures as in F.1.2. Table G.4 lists the selected POM and OOM.

G.3 Full Results Table G.5 lists the complete result of the experiment on the RHC dataset in Section 5.2.

Table F.3: Experimental results of evaluation metrics. Each value is the average MSE of models selected by each metric. Oracle is the best performing model's performance.

Scenario	1	2	3	4
Oracle	0.004	0.207	0.022	0.235
TO-MSE	0.265	0.546	1.001	22.446
μ-risk	0.041	0.462	0.037	0.777
τ-risk	0.028	**0.272**	0.078	7.075
SDR-MSE(0.0)	0.031	0.295	0.335	0.613
SDR-MSE(0.1)	**0.028**	0.298	0.034	**0.610**
SDR-MSE(0.2)	0.029	0.294	**0.033**	0.614
SDR-MSE(0.3)	0.030	0.294	0.033	0.619
SDR-MSE(0.4)	0.031	0.294	0.034	0.622
SDR-MSE(0.5)	0.031	0.294	0.035	0.624
Scenario	5	6	7	8
Oracle	0.032	0.710	2.937	1.432
TO-MSE	5.754	**0.873**	6.960	9.531
μ-risk	0.037	0.882	3.477	3.054
τ-risk	0.046	0.891	6.792	3.092
SDR-MSE(0.0)	0.129	0.887	3.309	2.870
SDR-MSE(0.1)	**0.037**	0.887	3.310	2.872
SDR-MSE(0.2)	0.037	0.891	3.305	2.860
SDR-MSE(0.3)	0.037	0.884	**3.299**	2.860
SDR-MSE(0.4)	0.037	0.895	3.306	2.841
SDR-MSE(0.5)	0.037	0.913	3.309	**2.818**

Table G.4: Selected models and hypter-parameters.

	POM	OOM
model	RFC	RFC
params	$\Delta_{depth} = 5$, $n_{min-leaf} = 1$	$\Delta_{depth} = 5$, $n_{min-leaf} = 1$

Table G.5: Average AUUCs with their standard errors.

Procedure	AUUC
TMA & μ-risk	7.247 ± 1.092
TMA & TO-MSE	10.806 ± 0.997
TMA & τ-risk$_R$	10.957 ± 1.028
TOM & TO-MSE	3.849 ± 1.389
TOM & τ-risk$_R$	3.114 ± 1.381
SDRM & SDR-MSE	**17.269 ± 1.023**

[9]Random Forest Regressor.