Counterfactual Cross-Validation: 
Effective Causal Model Selection from Observational Data

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Abstract

What is the most effective way to select the best causal model among potential candidates? In this paper, we propose a method to effectively select the best individual-level treatment effect (ITE) predictors from a set of candidates using only an observational validation set. In model selection or hyperparameter tuning, we are interested in choosing the best model or the value of hyperparameter from potential candidates. Thus, we focus on accurately preserving the rank order of the ITE prediction performance of candidate causal models. The proposed evaluation metric is theoretically proved to preserve the true ranking of the model performance in expectation and to minimize the upper bound of the finite sample uncertainty in model selection. Consistent with the theoretical result, empirical experiments demonstrate that our proposed method is more likely to select the best model and set of hyperparameter in both model selection and hyperparameter tuning.

1 Introduction

Predicting the Individual-level Treatment Effects (ITE) for certain actions is essential for optimizing metrics of interest in various domains. In digital marketing, for instance, incrementality is becoming increasingly important for performance metrics [7]. For this purpose, users to be shown ads for a given product should be chosen based on the ITE to avoid showing ads to a user who will already buy that product. Healthcare is also an important application of ITE prediction [3]. For precision medicine, we need to know which treatments will be more beneficial or harmful for a given patient. The fundamental problem of causal inference is that we never observe both treated and untreated outcomes from the same unit at the same time, and it is the central problem in ITE prediction [14]. Because of this situation, we are unable to observe a causal effect itself and to use causal effects as labels in the prediction model. Most of the previous papers related to the topic of ITE focus on prediction methods using observational data [2, 8, 18, 26, 29, 30]. In model evaluation and selection, the fundamental problem of causal inference poses an additional critical challenge. Because labels are not observed directly, we are unable to calculate loss metrics such as Mean Squared Error (MSE). Therefore, data-driven validation procedures such as cross-validation are not applicable in model selection and hyperparameter tuning. In other words, we are unsure which model and which hyperparameter values should be used when applying ITE prediction to real world problems.

There are only a few studies that tackle this problem. [12] proposed using the inverse probability weighting (IPW) outcome as the pseudo label for the true ITE in the calculation of a loss metric such as MSE. [24] used the loss function of R-learner [20], which outperforms T- and S-learner in both theoretical and empirical results [20], as the loss metrics. [4] used influence functions to obtain a more efficient estimator for the loss. These literatures are mainly interested in estimating the loss more accurately and efficiently.
In this paper, we focus on the problem of choosing the best ITE predictors among a set of candidates using only an observational validation set. Typically, we are interested in choosing the best model or hyperparameters from potential candidates in model selection and hyperparameter tuning. In such a situation, we only need to know the rank order of the value of the loss for those candidates. Thus, we construct a plug-in oracle that accurately ranks the performance using a given validation dataset. Then we propose Counterfactual Cross-Validation, which uses the above plug-in oracle. Our proposed metric is theoretically proven to preserve the ranking of candidate predictors and minimize the upper bound of the finite sample uncertainty in model selection. To show the practical significance of our evaluation metric, we conducted two experiments. In those experiments, our proposed method accurately finds the best performance model among candidates compared with other benchmark methods.

The rest of our paper is organized as follows. In Section 2, we review related works. Section 3 describes the problem setting and notation. Section 4 presents our approach for model evaluation in ITE prediction. We explain the procedure of our experiments and show the results in Section 5. We conclude in Section 6 with a summary of our contributions and future research directions.

2 Related Work

ITE prediction has been extensively studied by combining causal inference and machine learning techniques aiming for the best possible personalization of interventions. State-of-the-art approaches are constructed by utilizing the adversarial generative model, Gaussian process, and latent variable models [2, 3, 18, 30]. Among the diverse methods that predict ITE from observational data, the approach that is most related to this work is the method based on representation learning [6]. All the methods based on representation learning attempt to map the original feature vectors into the desirable latent representation space such that it eliminates selection biases. Balancing Neural Network [17] is the most basic method and uses discrepancy distance [19], a domain discrepancy measure in unsupervised domain adaptation, for the regularization term. CounterFactual Regression [26] minimizes the upper bound of the true loss by utilizing an Integral Probability Metric (IPM)[27]. In addition to these, methods that obtain a latent representation by preserving a local similarity [29] or by applying adversarial learning [8] have been proposed.

The prediction methods stated above have provided promising results on standard benchmark datasets; however, the evaluation of such ITE predictors have been conducted by using synthetic datasets or simple heuristic metrics such as policy risk, in previous studies [26, 29, 30]. These evaluations do not guarantee which models would actually be best on a given real-world dataset [4, 25]. Therefore, to bridge the gap between causal inference and applications, developing a reliable evaluation metric is critical.

There are only a few studies directly tackling the evaluation problem of ITE prediction models. [24] conducted an extensive survey of several heuristic metrics and provided experimental comparisons. In particular, they introduced inverse probability weighting (IPW) validation, which utilizes an unbiased estimator for the true ITE as the oracle, and $\tau$-risk, which is based on a loss function of R-learner as proposed in [20]. In addition, they showed that these metrics empirically outperformed another naive metric, $\mu$-risk, where predictive risk is estimated separately for treated and control outcomes using factual samples only. On the other hand, [4] improved those heuristic plug-in metrics by introducing a meta-estimation technique using the influence functions (IF) in a theoretically principal way. Our proposed metric can be further improved by the IF-based estimation method.

All the existing metrics so far aim to estimate the true metric of interest (e.g., MSE for the true ITE) accurately. However, to conduct accurate model selection and hyperparameter tuning, accurate ranking of model performance is critical, although these above metrics do not guarantee the preservation of such ranking.
Therefore, in contrast to previous works, we investigate a way to construct a metric that accurately preserves the ranking of candidate ITE predictors.

3 Problem Setting and Notation

In this section, we introduce some notation and formulate the evaluation of ITE prediction models.

3.1 Notation

We denote $X \in \mathcal{X} \subset \mathbb{R}^d$ as the $d$-dimensional feature vector and $T \in \mathcal{T} = \{0, 1\}$ as a binary treatment assignment indicator. When an individual $i$ receives treatment, then $T_i = 1$, otherwise, $T_i = 0$. Here, we follow the potential outcome framework \cite{15, 21, 23} and assume that there exist two potential outcomes denoted as $(Y^{(0)}, Y^{(1)}) \in \mathcal{Y} \times \mathcal{Y}$ for each individual. $Y^{(0)}$ is a potential outcome associated with $T = 0$, and $Y^{(1)}$ is associated with $T = 1$. Note that each individual receives only one treatment and reveals the outcome value for the received treatment. We use $p(X, T, Y^{(0)}, Y^{(1)})$, or simply $p$, to denote the joint probability distribution of these random variables. In addition, the treated and control feature distributions conditioned on treatment assignment are defined as $p^{t=1}(x) := p(x|t = 1)$ and $p^{t=0}(x) := p(x|t = 0)$, respectively.

We formally define the Individual-level Treatment Effect for an individual with a feature vector $x \in \mathcal{X}$ as:

$$\tau(x) = E \left[ Y^{(1)} - Y^{(0)} \mid X = x \right]$$

In addition, we use some notation to represent parameters of $p$. First, the conditional expectations of potential outcomes are:

$$m^{(k)}(x) = E \left[ Y^{(k)} \mid X = x \right], \forall k \in \{0, 1\}.$$  \hspace{1cm} (2)

Next, we define the conditional probability of treatment assignment as:

$$e(x) = P \left( T = 1 \mid X = x \right)$$

This parameter is called propensity score in causal inference and is widely used to estimate treatment effects from observational data \cite{15, 21, 22}.

Throughout this paper, we make the following standard assumptions in causal inference:

**Assumption 1.** (Unconfoundedness) Potential outcomes $(Y^{(0)}, Y^{(1)})$ are independent of the treatment assignment indicator $T$ conditioned on feature vector $X$, i.e.,

$$(Y^{(0)}, Y^{(1)}) \perp T \mid X$$ \hspace{1cm} (4)

**Assumption 2.** (Overlap) For any point in feature space $X \in \mathcal{X}$, the true propensity score is strictly between 0 and 1, i.e.,

$$P \left( e(X) \in (0, 1) \right) = 1$$ \hspace{1cm} (5)

**Assumption 3.** (Consistency) Observed outcome $Y^{\text{obs}}$ is represented using potential outcomes and the treatment assignment indicator as follows:

$$Y^{\text{obs}} = T Y^{(1)} + (1 - T) Y^{(0)}$$ \hspace{1cm} (6)
Under these assumptions, the ITE is identifiable from observational data (i.e., $\tau(X) = \mathbb{E}[Y_{\text{obs}} \mid X, T = 1] - \mathbb{E}[Y_{\text{obs}} \mid X, T = 0]$) [26].

Furthermore, we define some critical notation following [26].

**Definition 1.** (Representation Function) $\Phi : \mathcal{X} \rightarrow \mathcal{R}$ is a representation function and $\mathcal{R}$ is called the representation space. We assume that $\Phi$ is a twice differentiable, one-to-one function. Moreover, $p^l_\Phi(r) = p_\Phi(r \mid t = 1)$ and $p^u_\Phi(r) = p_\Phi(r \mid t = 0)$ are feature distributions for the treated and controlled induced over the representation space.

**Definition 2.** (Factual and Counterfactual Loss Functions) Let $h : \mathcal{R} \times \mathcal{T} \rightarrow \mathcal{Y}$ be a hypothesis, $w : \mathcal{X} \rightarrow \mathbb{R}_{\geq 0}$ be a weighting function, and $L : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathcal{R}$ be a loss function. In addition, The expected loss for the unit and treatment pair $(x, t) \in \mathcal{X} \times \mathcal{T}$ is denoted as:

$$\ell_{h, \Phi}(x, t) = \int_{\mathcal{Y}} L(\phi(t), h(\Phi(x), t)) p(\phi(t) \mid x) \, d\phi(t)$$

$$\ell_{h, \Phi, w}(x, t) = \int_{\mathcal{Y}} w(x)L(\phi(t), h(\Phi(x), t)) p(\phi(t) \mid x) \, d\phi(t)$$

Then, the expected factual and counterfactual losses of a combination of a hypothesis $h$ and a representation function $\Phi$ are defined as:

$$\epsilon_{F}(h, \Phi, w) = \int_{\mathcal{X} \times \mathcal{T}} \ell_{h, \Phi, w}(x, t)p(x, t)dxdt$$

$$\epsilon_{CF}(h, \Phi, w) = \int_{\mathcal{X} \times \mathcal{T}} \ell_{h, \Phi, w}(x, t)p(x, 1 - t)dxdt$$

Further, the expected factual and counterfactual losses on the treated $(t = 1)$ and on the controlled $(t = 0)$ are represented as:

$$\epsilon_{F}^{t=1}(h, \Phi, w) = \int_{\mathcal{X}} \ell_{h, \Phi, w}(x, t = 1)p^{t=1}(x)dx$$

$$\epsilon_{F}^{t=0}(h, \Phi, w) = \int_{\mathcal{X}} \ell_{h, \Phi, w}(x, t = 0)p^{t=0}(x)dx$$

$$\epsilon_{CF}^{t=1}(h, \Phi, w) = \int_{\mathcal{X}} \ell_{h, \Phi, w}(x, t = 1)p^{t=0}(x)dx$$

$$\epsilon_{CF}^{t=0}(h, \Phi, w) = \int_{\mathcal{X}} \ell_{h, \Phi, w}(x, t = 0)p^{t=1}(x)dx$$

By the definition of the conditional probability, the following equations hold for factual and counterfactual losses:

$$\epsilon_{F}(h, \Phi, w) = u \cdot \epsilon_{F}^{t=1}(h, \Phi, w) + (1 - u) \cdot \epsilon_{F}^{t=0}(h, \Phi, w)$$

$$\epsilon_{CF}(h, \Phi, w) = (1 - u) \cdot \epsilon_{CF}^{t=1}(h, \Phi, w) + u \cdot \epsilon_{CF}^{t=0}(h, \Phi, w)$$

where $u = P(t = 1)$.

We also define a class of metrics between probability distributions [27].

**Definition 3.** (Integral Probability Metric) For two probability density functions defined over a space $\mathcal{S} \subset \mathbb{R}^d$ and for a family of functions $G = \{g : \mathcal{S} \rightarrow \mathbb{R}\}$. The IPM between the two density functions $p$ and $q$ is defined as:

$$\text{IPM}_G(p, q) = \sup_{g \in G} \left| \int_{\mathcal{S}} g(s) (p(s) - q(s)) \, ds \right|$$
Function families $G$ can be the family of bounded continuous functions, the family of 1-Lipschitz functions, and the unit-ball of functions in a universal reproducing Hilbert kernel space.

**Definition 4.** (Weighted Variance of Potential Outcomes) The weighted expected variance of a potential outcome $Y(t)$ with respect to a conditional feature distribution $p^t(x)$ is defined as:

$$\sigma^2_{t,w}(p^t(x)) = \int_{X \times Y} w(x) \left( m^t(x) - Y^t(x) \right)^2 p^t(Y^t, x) dY^t dx$$

### 3.2 Evaluating ITE prediction models

In previous studies [4, 12, 24], the evaluation of an ITE predictor $\hat{\tau}(\cdot)$ has been formulated as accurately estimating the following metric from observational validation dataset $V = \{X_i, T_i, Y_{obs}^i\}$ as:

$$R_{true}(\hat{\tau}) = \mathbb{E}_X \left[ (\tau(X) - \hat{\tau}(X))^2 \right]$$

(7)

Here, $R_{true}$ is the true performance metric of an ITE predictor $\hat{\tau}(\cdot)$.

This approach is intuitive and ideal. However, the realizations of the true ITE are never observable, and thus, accurate performance estimation is difficult. Moreover, estimating the true metric values is not always necessary to conduct valid model selection or hyperparameter tuning of causal models. It may be possible to construct a better metric under an objective specific to selection and tuning. Thus, we take a different approach from previous works and aim to construct a performance estimator $\hat{R}$ satisfying the following condition:

$$R_{true}(\hat{\tau}) \leq R_{true}(\hat{\tau}') \Rightarrow \hat{R}(\hat{\tau}) \leq \hat{R}(\hat{\tau}') \quad \forall \hat{\tau}, \hat{\tau}' \in M.$$  

(8)

where $M = \{\hat{\tau}_1, \ldots, \hat{\tau}_{|M|}\}$ is a set of candidate ITE predictors.

An estimator satisfying Eq. (8) gives accurate ranking of candidate predictors by the true metric values, and we can select the best model among $M$ using the estimator. The main focus of this paper is to propose a theoretically sophisticated way to construct a performance estimator $\hat{R}$ that achieves the condition described in Eq. (8) as much as possible.

### 4 Method

To achieve our goal of interest, we consider the following feasible estimator of the performance metric:

$$\hat{R}(\hat{\tau}) = \frac{1}{n} \sum_{i=1}^n \left( \hat{\tau} \left( X_i, T_i, Y_{obs}^i \right) - \hat{\tau}(X_i) \right)^2$$

(9)

where $\hat{\tau}(\cdot)$ is called the oracle and is constructed from validation set $V$. We consider the estimator for the true risk as represented in Eq. (9) because it can be applied to estimating the performance of a predictor, directly predicting an ITE such as R-learner [20], Domain Adaptation Learner, or Doubly Robust Learner [11].

Under our formulation, we aim to answer the following question: What is the best plug-in oracle to rank the performance of given candidate ITE predictors from an observational validation dataset?

In the following subsections, we theoretically analyze the performance estimator as represented in the form of Eq. (9) and propose an oracle that gives accurate ranking of candidate ITE prediction models by the true performance metric.

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1Several papers have called $R_{true}$ the expected Precision in Estimation of Heterogeneous Effect (PEHE).
4.1 Theoretical Analysis of the Performance Estimator

First, the following proposition states that an oracle that is unbiased against the ITE provides a desirable property of the performance estimator.

**Proposition 1.** If an oracle is an unbiased estimator for the true ITE:

\[ \mathbb{E} \left[ \hat{\tau} \left( X, T, Y^{\text{obs}} \right) \mid X \right] = \tau(X) \]

then, the expectation of performance estimator \( \hat{R} \) is decomposed into the true performance metric and the MSE of the given oracle:

\[
\mathbb{E} \left[ \hat{R} \left( \hat{\tau} \right) \right] = R_{\text{true}} \left( \hat{\tau} \right) + \mathbb{E} \left[ \left( \tau(X) - \hat{\tau}(X, T, Y^{\text{obs}}) \right)^2 \right] \tag{10}
\]

The first term of RHS of Eq. (10) is the true performance metric, and the second term is independent of the given predictor. Therefore, the expectations of the performance estimators preserve the difference between the true metric values as follows:

\[
\mathbb{E} \left[ \hat{R} \left( \hat{\tau}_1 \right) \right] - \mathbb{E} \left[ \hat{R} \left( \hat{\tau}_2 \right) \right] = R_{\text{true}} \left( \hat{\tau}_1 \right) - R_{\text{true}} \left( \hat{\tau}_2 \right)
\]

where \( \hat{\tau}_1, \hat{\tau}_2 \in \mathcal{M} \) are arbitrary candidate predictors. This property is desirable because the predictor that has the smallest expected value of \( \hat{R} \) among candidate predictors also has the smallest value of \( R_{\text{true}} \) among them; one can expect to select the best predictor among a set of candidates.

However, the expectation of the performance estimator is incalculable because we can only use a finite sample validation dataset. This motivates us to consider the finite sample uncertainty of the performance estimator. Here, the empirical version of the performance estimator can be decomposed as:

\[
\hat{R} \left( \hat{\tau} \right) = \frac{1}{n} \sum_{i=1}^{n} \left( \tau(X_i) - \hat{\tau}(X_i) \right)^2 \\
- \frac{2}{n} \sum_{i=1}^{n} \left( \hat{\tau}(X_i) - \tau(X_i) \right) \left( \hat{\tau} \left( X_i, T_i, Y^{\text{obs}}_i \right) - \tau(X_i) \right) \\
+ \frac{1}{n} \sum_{i=1}^{n} \left( \tau(X_i) - \hat{\tau}(X_i, T_i, Y^{\text{obs}}_i) \right)^2 \tag{11}
\]

In Eq. (11), the second term of RHS (\( \mathcal{W} \)) is critical to the uncertainty and is controllable by the oracle. Thus, we consider the oracle minimizing the variance of \( \mathcal{W} \) to construct the performance estimator. The following theorem states the upper bound of the variance of \( \mathcal{W} \).

**Theorem 1.** Assume that \( \left( \tau(X) - \hat{\tau}(X) \right)^2 \) is upper bounded by a positive constant \( C \) for a given predictor. Additionally, the oracle is unbiased for the ITE and the output of the oracle for an instance is independent of that of other instances. Then, we have the upper bound of the variance of \( \mathcal{W} \) as follows:

\[
\mathbb{V} \left( \mathcal{W} \right) \leq \frac{4C}{n} \left( \mathbb{E} \left[ \mathbb{V} \left( \hat{\tau} \left( X, T, Y^{\text{obs}} \right) \mid X \right) \right] + \mathbb{V} \left( \tau(X) \right) \right) \tag{12}
\]
In Eq. (12), the expectation of the conditional variance of oracle is the only controllable term by the construction of the oracle. Thus, an oracle satisfying the following condition is desirable to construct the performance estimator $\hat{R}$:

$$\min \mathbb{E} \left[ \mathcal{V} \left( \hat{\tau}(X, T, Y^{\text{obs}}) \mid X \right) \right] \quad (13)$$

s.t. $\mathbb{E}[\hat{\tau}(X, T, Y^{\text{obs}})] = \tau(X). \quad (14)$

A performance estimator using an oracle that satisfies the conditions above is expected to preserve the difference of the true performance metric and minimizes the upper bound of the finite sample uncertainty term $\mathcal{W}$ in Eq. (11). In the next subsection, we investigate and propose a method to derive an oracle achieving our goal.

### 4.2 Proposed Oracle

In this subsection, we present our class of counterfactual cross-validation (CF-CV) performance estimators. In particular, we propose a method to construct an oracle that leads to an effective estimator based on the theoretical analysis in the previous subsection. The main idea of CF-CV is to gain an unbiased oracle minimizing its own variance to better satisfy the conditions in Eq. (13) and Eq. (14).

Here we define the proposed oracle inspired by the doubly robust (DR) estimator used to estimate average causal effects of treatments or performance of bandit policies [5, 9, 10, 16].

**Definition 5.** Let $f(\cdot, \cdot) : X \times T \rightarrow Y$ be a hypothesis predicting potential outcomes and is defined as $f(x, t) = h(\Phi(x), t)$. Then, the oracle for a given data $(X, T, Y^{\text{obs}})$ is defined as follows:

$$\tilde{\tau}_{DR}(X, T, Y^{\text{obs}}) = \frac{T}{e(X)} \left( Y^{\text{obs}} - f(X, 1) \right) - \frac{1 - T}{1 - e(X)} \left( Y^{\text{obs}} - f(X, 0) \right) + (f(X, 1) - f(X, 0)) \quad (15)$$

We rely on the class of DR estimators for constructing the oracle because it theoretically and empirically achieves better bias-variance trade-off in a variety of fields than other unbiased estimators including IPW estimators. [9, 10, 16, 28].

First, the oracle in the form of Eq. (15) is proved to be unbiased against the true ITE, thus satisfying Eq. (14).

**Proposition 2.** Given true propensity scores, the doubly robust oracle is unbiased against the true ITE:

$$\mathbb{E}[\tilde{\tau}_{DR} \mid X] = \tau(X) \quad (16)$$

Next, to consider the condition in Eq. (13), we state the expectation of the conditional variance of the DR oracle.

**Proposition 3.** Given true propensity scores, the expectation of the conditional variance of the doubly robust oracle is represented as:

$$\mathbb{E}[\mathcal{V}(\tilde{\tau}_{DR} \mid X)] = \mathbb{E}\left[ (\xi^{(1)})^2 \right] + \mathbb{E}\left[ (\xi^{(0)})^2 \right] + Z \quad (17)$$

where

$$\xi^{(1)} = \frac{T}{e(x)} \left( Y^{(1)} - m^{(1)}(x) \right), \quad \xi^{(0)} = \frac{1 - T}{1 - e(x)} \left( Y^{(0)} - m^{(0)}(x) \right), \quad w(t)(x) = \frac{t(1 - 2e(x)) + e(x)^2}{e(x)(1 - e(x))}$$

$$Z = \int_X \left( \sqrt{w^{(1)}(x)(f(x, 1) - m^{(1)}(x))} + \sqrt{w^{(0)}(x)(f(x, 0) - m^{(0)}(x))} \right)^2 p(x) dx$$
We used the Infant Health Development Program (IHDP) dataset provided by [13]. IHDP is an interventional program aimed to improve the health of premature infants [2, 13]. This is a standard semi-synthetic dataset.

Algorithm 1 Counterfactual Cross-Validation (CF-CV)

**Input:** A set of candidate ITE predictors $\mathcal{M} = \{\tau_1, \ldots, \tau_{|\mathcal{M}|}\}$; observational validation dataset $\mathcal{V} = \{X_i, T_i, Y_{\text{obs}}\}_{i=1}^n$; A trade-off hyperparameter $\alpha$.

**Output:** An ITE predictor $\hat{\tau}^* \in \mathcal{M}$.

1. Train a function $f(X, T)$ by minimizing Eq. (19) using validation set $\mathcal{V}$.
2. Drive the oracle values $\hat{\tau}_{DR}$ for $\mathcal{V}$.
3. Estimate performance of candidate predictors in $\mathcal{M}$ based on the performance estimator $\hat{\mathcal{R}}$ in Eq. (9).
4. Select a predictor minimizing the performance estimator among $\mathcal{M}$.
5. return $\hat{\tau}^* = \arg \min_{\tau \in \mathcal{M}} \hat{\mathcal{R}}(\tau)$.

To find an oracle satisfying the variance condition in Eq. (13), we aim to train a hypothesis $f$ minimizing the variance derived in Eq. (17). In the variance, $\xi(1)$ and $\xi(0)$ are independent of $f$, and are thus uncontrollable. On the other hand, the third term of RHS of Eq. (17) ($\mathcal{Z}$) is dependent on both $m(0)(x)$ and $m(1)(x)$. However, either $m(0)(x)$ or $m(1)(x)$ is always counterfactual, and thus, the direct minimization of $\mathcal{Z}$ is infeasible.

Therefore, to find the appropriate hypothesis $f$ that minimizes $\mathcal{Z}$ from an observational validation set, we derive the upper bound of $\mathcal{Z}$ depending only on observable variables.

**Theorem 2.** Let $G$ be a family of functions $g : \mathcal{R} \to \mathcal{Y}$ and assume that, for any given $t \in \mathcal{T}$, there exists a positive constant $B_\Phi$ such that the per-unit expected loss functions obey $\frac{1}{B_\Phi} \cdot \ell_h(\Psi(r), t) \in G$ where $\Psi$ is the inverse image of $\Phi$. Then, the following inequality holds:

$$
\mathcal{Z} \leq 2 \left( \epsilon_F^{t=1} \left( h, \Phi, w(1) \right) + \epsilon_F^{t=0} \left( h, \Phi, w(0) \right) - 2\sigma^2 \right) + 2B_\Phi \left( (1 - u) \cdot \text{IPM}_G \left( p_{\Phi, w(1)}^{t=1}(r), p_{\Phi, w(1)}^{t=0}(r) \right) + u \cdot \text{IPM}_G \left( p_{\Phi, w(0)}^{t=1}(r), p_{\Phi, w(0)}^{t=0}(r) \right) \right)
$$

(18)

where $\sigma^2 = \min_{(t', t) \in \mathcal{T}^2} \sigma^2_{t', w(t)}(p(x | \tau'))$, $p_{\Phi, w}(r) = w(\Psi(r)) \cdot p^t(r)$.

Eq. (18) in Theorem 2 consists of factual losses and an IPM on the representation space and thus can be estimated from finite samples. From the theoretical implications above, the loss function to derive a hypothesis $h$ and a representation function $\Phi$ is:

$$
h, \Phi = \min_{h, \Phi} \frac{1}{n} \sum_{i=1}^n w(t_i)(x_i) \cdot L(h(\Phi(x_i), t_i), y_i) + \alpha \cdot \text{IPM}_G \left( \{\Phi(x_i)\}_{i:t_i=0}, \{\Phi(x_i)\}_{i:t_i=1} \right)
$$

(19)

where $\alpha$ is a trade-off hyperparameter.

The derived oracle for our CF-CV is unbiased for the true metric and minimizes the upper bound of the variance in Eq. (18). A summary of the resulting CF-CV is given in Algorithm 1.

5 Experiments

In this section, we compare our proposed performance estimator and the other baselines using a standard semi-synthetic dataset.

5.1 Basic Experimental Setups

5.1.1 Dataset

We used the Infant Health Development Program (IHDP) dataset provided by [13]. IHDP is an interventional program aimed to improve the health of premature infants [2, 13]. This is a standard semi-synthetic dataset.
containing 747 children with 25 features and has been widely used to evaluate ITE prediction models [2, 26, 30]. The detailed description of this dataset can be found in Section 5.1 of [26]. We used the simulated outcome implemented in EconML package\(^2\).

5.1.2 Baselines

We compared our CF-CV with the following baseline metrics.

- **IPW validation [12, 24]**: This metric utilizes the following form of performance estimator:
  \[
  \frac{1}{n} \sum_{i=1}^{n} \left( \hat{\tau}_{IPW}(X_i, T_i, Y_{i}^{obs}) - \hat{\tau}(X_i) \right)^2
  \]
  where \(\hat{\tau}_{IPW}(X_i, T_i, Y_{i}^{obs}) = \frac{T_i}{e(X_i)} Y_{i}^{obs} - \frac{1-T_i}{1-e(X_i)} Y_{i}^{obs}\) is an estimator for the ITE. This IPW oracle satisfies the unbiasedness for the true ITE.

- **Plug-in validation**: This uses predicted values of potential outcomes by an arbitrary machine learning algorithm as the oracle of the performance estimator in Eq. (9).
  \[
  \frac{1}{n} \sum_{i=1}^{n} \left( \hat{\tau}_i^{(1)} - \hat{\tau}_i^{(0)} - \hat{\tau}(X_i) \right)^2
  \]
  where \(\hat{\tau}_i^{(1)}\) and \(\hat{\tau}_i^{(0)}\) are predictions for potential outcomes. We used Counterfactual Regression [26] to construct the oracle \(\hat{\tau}(1)(\cdot)\) and \(\hat{\tau}(0)(\cdot)\) to ensure a fair comparison.

- **\(\tau\)-risk [24]**: This metric is derived from the loss function of R-learner in [20] and is defined as follows:
  \[
  \frac{1}{n} \sum_{i=1}^{n} \left( (Y_i^{obs} - m(X_i)) - (T_i - e(X_i))\hat{\tau}(X_i) \right)^2
  \]
  where \(m(\cdot)\) is the expectation of observed outcome \(E[Y^{obs}|X]\). We used Gradient Boosting Regressor to estimate this parameter.

5.2 Comparison on Model Selection Performance

We first compared the model selection performance of our CF-CV with the other baselines.

5.2.1 Experimental Procedure

We follow the experimental procedure in [24]; We first trained candidate predictors on the training set, and then made predictions on both validation and test sets by pre-trained predictors. Then, we ranked those predictors by using each metric on the observational validation set. Finally, we compare these estimated performances on the validation set and the true performance on the testing set. We conducted the experimental procedure over 30 realizations with 35/35/30 train/validation/test splits.

\(^2\)https://github.com/microsoft/EconML/blob/master/econml/data/dgps.py
5.2.2 Candidate Models

We constructed a set of candidate predictors $\mathcal{M}$ by combining five machine learning algorithms (Decision Tree, Random Forest, Gradient Boosting Tree, Ridge Regressor, and Support Vector Regressor with RBF kernel) and five meta-learners (S-Learner, X-Learner, T-Learner, Domain Adaptation Learner, and Doubly Robust Learner) as implemented in EconML package\(^3\). Thus, we had a set of 25 ITE predictors to select among (i.e., $|\mathcal{M}| = 25$).

5.2.3 Results

Table 1 reports the averaged and the worst-case performance over 30 realizations. We evaluated the worst-case model selection performance of each metric because, in real-world causal inference problems, we never know the ground truth performance of any predictor, and stable model selection performance is essential. Rank Correlation is the Spearman rank correlation between the ranking by the true performance and the estimated metric values. Relative RMSE is the true performance of the selected model in each metric relative to the best one in $\mathcal{M}$. We used Relative RMSE defined as below because potential outcomes of the IHDP dataset have different scales among realizations.

$$\text{Relative RMSE} = \frac{R_{\text{true}}(\hat{\tau}^*)}{\min_{\hat{\tau} \in \mathcal{M}} R_{\text{true}}(\hat{\tau})}, \quad \hat{\tau}^* = \arg \min_{\hat{\tau} \in \mathcal{M}} \hat{R}(\hat{\tau})$$

Table 1 shows the effective model selection performance of the proposed CF-CV on average. Moreover, ours significantly outperformed with respect to worst-case performance, and this empirically suggests the stability of the proposed metric.

|                | Rank Correlation | Relative RMSE |
|----------------|------------------|---------------|
|                | Avg ($\pm$ SE)   | Worst-Case    | Avg ($\pm$ SE) | Worst-Case |
| IPW            | 0.224 ($\pm$ 0.073) | $-0.659$   | 2.027 ($\pm$ 0.242) | 7.779 |
| $\tau$-risk    | $-0.399$ ($\pm$ 0.051) | $-0.797$   | 3.408 ($\pm$ 0.250) | 8.884 |
| Plug-in        | 0.887 ($\pm$ 0.021) | 0.385       | 1.123 ($\pm$ 0.039) | 1.841 |
| CF-CV          | 0.929 ($\pm$ 0.008) | 0.830       | 1.040 ($\pm$ 0.019) | 1.515 |

Table 1: The results of model selection experiments on IHDP dataset over 30 realizations. For both Spearman rank correlation and relative RMSE, the averaged results with their standard errors (SE) and the worst-case performance are reported. The results show that our metric outperformed the other baselines with respect to both rank correlation and the relative RMSE.

5.3 Comparison on Hyperparameter Tuning Performance

Next, we compared the hyperparameter tuning performance of our CF-CV with the other baseline metrics.

5.3.1 Tuned Model

We tuned the hyperparameters of the combinations of Gradient Boosting Regressor and Domain Adaptation Learner as implemented in scikit-learn and EconML, respectively. Domain Adaptation Learner consists of three base learners including treated_model, controls_model, and overall_model. Thus, we aimed to

\(^3\)https://econml.azurewebsites.net/spec/estimation/metalearners.html
find the best three sets of hyperparameters of Gradient Boosting Regressor to construct Domain Adaptation Learner.

5.3.2 Experimental Procedure

We used Optuna software [1] with a TPE sampler to tune the ITE predictor and set each metric as the objective function of Optuna. For each metric, we sought 100 points in the hyperparameter searching space. The hyperparameter tuning performance of each metric was evaluated by the true performance of the tuned model on the testing set. We conducted the experimental procedure over the same 30 realizations, using 35/35/30 train/validation/test splits as the model selection experiment.

![Figure 1: Results of the hyperparameter tuning experiment. Averaged RMSE of ITE predictors tuned by each metric relative to the results of IPW and their standard errors are reported. The result shows that our CF-CV outperformed the other metrics and led to a better set of hyperparameters for an ITE predictor.](image)

5.3.3 Results

Figure 1 provides the results of the hyperparameter tuning experiment. We report the averaged performance of each metric relative to the performance of the IPW metric because potential outcomes of the IHDP dataset have different scales among realizations.

The results suggest that our metric improved by over 17.9% in comparison to IPW and by 6.2% comparison to Plug-in. Thus, our metric allows one to conduct valid hyperparameter tuning of the causal inference model.

6 Conclusion

In this paper, we explored the evaluation problem of ITE prediction models. In contrast to previous studies, we proposed a new approach called counterfactual cross-validation that preserves the ranking of the true performance with high confidence using only an observational validation set. The proposed evaluation metric was theoretically proved to preserve the true ranking of the model performance in expectation and to minimize the upper bound of the finite sample uncertainty in model evaluation. Empirical evaluation using the IHDP dataset demonstrated the effective and stable model selection and hyperparameter tuning performance of the proposed metric.
Important future research directions are theoretical analysis on choosing the hyper parameters of potential outcome models used in the proposed metric, and how to consider situations with hidden confounders.

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Supplementary Materials

For all the proofs below, we denote $\tau(X_i)$, $\hat{\tau}(X_i)$, and $\tilde{\tau}(X_i, T_i, Y_i^{\text{obs}})$ as $\tau_i$, $\hat{\tau}_i$, and $\tilde{\tau}_i$ for simplicity.

A Proof of Proposition 1

**Proof.** First, the following equality holds:

$$
\mathbb{E} \left[ \hat{R}(\hat{\tau}) \right] = \frac{1}{n} \sum_{i=1}^{n} (\tilde{\tau}_i - \hat{\tau}_i)^2
$$

$$
= \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[ (\tilde{\tau}_i - \tau_i + \tau_i - \hat{\tau}_i)^2 \right]
$$

$$
= \mathbb{E} \left[ (\tilde{\tau}_i - \tau(X))^2 \right] - \frac{2}{n} \sum_{i=1}^{n} \mathbb{E} \left[ \underbrace{(\tilde{\tau}_i - \tau_i)(\tilde{\tau}_i - \tau_i)}_{(a)} \right] + \mathbb{E} \left[ (\hat{\tau}(X) - \tau(X))^2 \right] - R_{\text{true}}
$$

Then, we have,

$$(a) = \mathbb{E} \left[ (\tilde{\tau}_i - \tau_i)(\tilde{\tau}_i - \tau_i) \right]
$$

$$
= \mathbb{E} \left[ \mathbb{E} \left[ (\tilde{\tau}_i - \tau_i)(\tilde{\tau}_i - \tau_i) \mid X \right] \right]
$$

$$
= \mathbb{E} \left[ \mathbb{E} \left[ (\tilde{\tau}_i - \tau_i) \mid X \right] \mathbb{E} \left[ (\tilde{\tau}_i - \tau_i) \mid X \right] \right] = 0 \quad \vdots \quad \text{unbiasedness of } \tilde{\tau}_i.
$$

Thus, we obtain,

$$
\mathbb{E} \left[ \hat{R}(\hat{\tau}) \right] = R_{\text{true}}(\hat{\tau}) + R_{\text{true}}(\tilde{\tau}) + \mathbb{E} \left[ (\tilde{\tau}(X) - \tau(X))^2 \right]
$$

\[ \square \]

B Derivation of Eq. (11)

**Proof.** Following the same procedure as in the proof of Proposition 1,

$$
\hat{R}(\hat{\tau}) = \frac{1}{n} \sum_{i=1}^{n} (\tilde{\tau}_i - \hat{\tau}_i)^2
$$

$$
= \frac{1}{n} \sum_{i=1}^{n} (\tilde{\tau}_i - \tau_i + \tau_i - \hat{\tau}_i)^2
$$

$$
= \frac{1}{n} \sum_{i=1}^{n} (\tilde{\tau}_i - \tau_i)^2 - \frac{2}{n} \sum_{i=1}^{n} (\tilde{\tau}_i - \tau_i)(\tilde{\tau}_i - \tau_i) + \frac{1}{n} \sum_{i=1}^{n} (\tilde{\tau}_i - \tau_i)^2
$$

\[ \square \]
C Proof of Proposition 2

Proof. We define the DR oracle as:

\[
\tilde{\tau}_{DR}(X, T, Y) = \frac{T}{e(X)} \left( Y^{obs} - f(X, 1) \right) - \frac{1-T}{1-e(X)} \left( Y^{obs} - f(X, 0) \right) + (f(X, 1) - f(X, 0))
\]

\[
= \tilde{\tau}^{(1)}_{DR}(X, T, Y) - \tilde{\tau}^{(0)}_{DR}(X, T, Y)
\]

where

\[
\tilde{\tau}^{(1)}_{DR}(X, T, Y) = \frac{T}{e(X)} \left( Y^{obs} - f(X, 1) \right) + f(X, 1)
\]

\[
\tilde{\tau}^{(0)}_{DR}(X, T, Y) = \frac{1-T}{1-e(X)} \left( Y^{obs} - f(X, 0) \right) + f(X, 0)
\]

Then, the expectation of \(\tilde{\tau}^{(1)}_{DR}\) is:

\[
E \left[ \tilde{\tau}^{(1)}_{DR} \mid X \right] = E \left[ \left( Y^{(1)} - f(X, 1) \right) + f(X, 1) \mid X \right]
\]

\[
= \frac{T}{e(X)} E \left[ Y^{(1)} \mid X \right] + f(X, 1) \quad \because \text{Unconfoundedness}
\]

\[
= E \left[ Y^{(1)} \mid X \right]
\]

We also have \(E \left[ \tilde{\tau}^{(0)}_{DR} \mid X \right] = E \left[ Y^{(0)} \mid X \right]\) is the same way. Thus,

\[
E \left[ \tilde{\tau}_{DR} \mid X \right] = E \left[ \tilde{\tau}^{(1)}_{DR} - \tilde{\tau}^{(0)}_{DR} \mid X \right] = E \left[ Y^{(1)} - Y^{(0)} \mid X \right] = \tau(X)
\]

D Proof of Proposition 3

Proof. The second moment of \(\tilde{\tau}^{(1)}_{DR}\) is

\[
E \left[ \left( \tilde{\tau}^{(1)}_{DR} \right)^2 \mid X \right] = E \left[ \left( \frac{T}{e(X)} \left( Y^{(1)} - f(X, 1) \right) + f(X, 1) \right)^2 \mid X \right]
\]

\[
= E \left[ \left( \left( 1 - \frac{T}{e(X)} \right) \left( f(X, 1) - Y^{(1)} \right) + Y^{(1)} \right)^2 \mid X \right]
\]

\[
= E \left[ \left( \xi^{(1)} \right)^2 \mid X \right] + \left( m^{(1)}(X) \right)^2 + \frac{1-e(X)}{e(X)} \left( f(X, 1) - m^{(1)}(X) \right)^2
\]

We also have the second moment of \(\tilde{\tau}^{(0)}_{DR}\) in the same manner as follows:

\[
E \left[ \left( \tilde{\tau}^{(0)}_{DR} \right)^2 \mid X \right] = E \left[ \left( \xi^{(0)} \right)^2 \mid X \right] + \left( m^{(0)}(X) \right)^2 + \frac{e(X)}{1-e(X)} \left( f(X, 0) - m^{(0)}(X) \right)^2
\]
Thus, by using the result of Proposition 2, we obtain

\[
\text{Var} \left( \tilde{\tau}_{DR}^{(1)} | X \right) = \mathbb{E} \left[ \left( \tilde{\tau}_{DR}^{(1)} \right)^2 | X \right] - \left( \mathbb{E} \left[ \tilde{\tau}_{DR}^{(1)} | X \right] \right)^2 \\
= \mathbb{E} \left[ \left( \xi^{(1)} \right)^2 | X \right] + \frac{1 - e(X)}{e(X)} \left( f(X, 1) - m^{(1)}(X) \right)^2
\]

\[
\text{Var} \left( \tilde{\tau}_{DR}^{(0)} | X \right) = \mathbb{E} \left[ \left( \tilde{\tau}_{DR}^{(0)} \right)^2 | X \right] - \left( \mathbb{E} \left[ \tilde{\tau}_{DR}^{(0)} | X \right] \right)^2 = \mathbb{E} \left[ \left( \xi^{(0)} \right)^2 | X \right] + \frac{e(X)}{1 - e(X)} \left( f(X, 0) - m^{(0)}(X) \right)^2
\]

In addition, from Lemma 3.

\[
\text{Cov} \left( \tilde{\tau}_{DR}^{(1)}, \tilde{\tau}_{DR}^{(0)} | X \right) = - \left( f(X, 1) - m^{(1)}(X) \right) \left( f(X, 0) - m^{(0)}(X) \right)
\]

Therefore,

\[
\text{Var} \left( \tilde{\tau}_{DR} | X \right) = \text{Var} \left( \tilde{\tau}_{DR}^{(1)} - \tilde{\tau}_{DR}^{(0)} | X \right) \\
= \text{Var} \left( \tilde{\tau}_{DR}^{(1)} | X \right) - 2 \text{Cov} \left( \tilde{\tau}_{DR}^{(1)}, \tilde{\tau}_{DR}^{(0)} | X \right) + \text{Var} \left( \tilde{\tau}_{DR}^{(0)} | X \right) \\
= \mathbb{E} \left[ \left( \xi^{(1)} \right)^2 | X \right] + \mathbb{E} \left[ \left( \xi^{(0)} \right)^2 | X \right] + \frac{1 - e(X)}{e(X)} \left( f(X, 1) - m^{(1)}(X) \right)^2 \\
+ \frac{e(X)}{1 - e(X)} \left( f(X, 0) - m^{(0)}(X) \right)^2 + 2 \left( f(X, 1) - m^{(1)}(X) \right) \left( f(X, 0) - m^{(0)}(X) \right)
\]

\[
= \mathbb{E} \left[ \left( \xi^{(1)} \right)^2 | X \right] + \mathbb{E} \left[ \left( \xi^{(0)} \right)^2 | X \right] \\
+ \left( \sqrt{\frac{1 - e(X)}{e(X)}} \left( f(X, 1) - m^{(1)}(X) \right) + \sqrt{\frac{e(X)}{1 - e(X)}} \left( f(X, 0) - m^{(0)}(X) \right) \right)^2
\]

\[
= \mathbb{E} \left[ \left( \xi^{(1)} \right)^2 | X \right] + \mathbb{E} \left[ \left( \xi^{(0)} \right)^2 | X \right] + Z
\]
E Proof of Theorem 1

Proof.

\[
\mathbb{V}(\frac{1}{n} \sum_{i=1}^{n} (\tilde{\tau}_i - \tau_i)(\tilde{\tau}_i - \tau_i)) = \frac{4}{n^2} \mathbb{V}(\sum_{i=1}^{n} (\tilde{\tau}_i - \tau_i)(\tilde{\tau}_i - \tau_i)) \\
= \frac{4}{n^2} \mathbb{E}\left[\left(\sum_{i=1}^{n} (\tilde{\tau}_i - \tau_i)(\tilde{\tau}_i - \tau_i)\right)^2\right] \quad \because (a) = 0 \\
= \frac{4}{n^2} \sum_{i=1}^{n} \mathbb{E}\left[(\tilde{\tau}_i - \tau_i)^2(\tilde{\tau}_i - \tau_i)^2\right] \\
\because \mathbb{E}[(\tilde{\tau}_i - \tau_i)(\tilde{\tau}_i - \tau_i)(\tilde{\tau}_j - \tau_j)(\tilde{\tau}_j - \tau_j)] = 0, \forall i, j(i \neq j) \\
\leq \frac{4C}{n} \mathbb{E}\left[(\tilde{\tau}_i - \tau_i)^2\right] \\
= \frac{4C}{n} \mathbb{V}(\tilde{\tau}_i) \quad \because \mathbb{E}[\tilde{\tau}_i | X] = \tau_i \\
= \frac{4C}{n} \left(\mathbb{E}[\mathbb{V}(\tilde{\tau}_i | X)] + \mathbb{V}[\mathbb{E}(\tilde{\tau}_i | X)]\right) \quad \because \text{law of total variance} \\
= \frac{4C}{n} \left(\mathbb{E}[\mathbb{V}(\tilde{\tau}_i | X)] + \mathbb{V}(\tau_i)\right) \quad \because \mathbb{E}[\tilde{\tau}_i | X] = \tau_i
\]

F Proofs of Technical Lemmas

First, we prove some lemmas.

Lemma 1. (Similar to Lemma A.4 of [26]) Let \( \Phi : \mathcal{X} \rightarrow \mathcal{R} \) be an invertible representation with \( \Psi \) its inverse. Let \( G \) be a family of functions \( g : \mathcal{R} \rightarrow \mathbb{R} \) and \( h : \mathcal{R} \times \mathcal{T} \rightarrow \mathcal{Y} \) be a hypothesis. Assume that, for any given \( t \in \mathcal{T} \), there exists a constant \( B_\Phi > 0 \), such that \( \frac{1}{B_\Phi} \cdot \ell_{h, \Phi}(\Psi(r), t) \in G \). Then we have:

\[
\epsilon_{CF}^l(h, \Phi, w) \leq \epsilon_{F}^l(h, \Phi, w) + B_\Phi \cdot IPM_G \left( p_{\Phi, w}^{t=1}(r), p_{\Phi, w}^{t=0}(r) \right)
\]

Proof.

\[
\epsilon_{CF}^l(h, \Phi, w) - \epsilon_{F}^l(h, \Phi, w) = \int_{\mathcal{X}} w(x) \ell_{h, \Phi}(x, t) \left( p_{1-t}^l(x) - p_t^l(x) \right) dx \\
= \int_{\mathcal{R}} w(\Psi(r)) \ell_{h, \Phi}(\Psi(r), t) \left( p_{1-t}^\Phi(r) - p_t^\Phi(r) \right) dr \\
= B_\Phi \cdot \int_{\mathcal{R}} \frac{\ell_{h, \Phi}(\Psi(r), t)}{B_\Phi} \left( w(\Psi(r))p_{1-t}^\Phi(r) - w(\Psi(r))p_t^\Phi(r) \right) dr \\
\leq B_\Phi \cdot \sup_{g \in G} \left| \int_{\mathcal{R}} g(r) \left( w(\Psi(r))p_{1-t}^\Phi(r) - w(\Psi(r))p_t^\Phi(r) \right) dr \right| \\
= B_\Phi \cdot IPM_G \left( w(\Psi(r))p_{1-t}^\Phi(r), w(\Psi(r))p_t^\Phi(r) \right)
\]

\[\square\]
Lemma 2. (Similar to Lemma A.5 of [26]) For any function \(f: \mathcal{X} \times \mathcal{T} \to \mathcal{Y}\) and conditional probability distribution \(p^t(x)\) over the space \(\mathcal{X} \times \mathcal{T}\), the following equalities hold:

\[
\int_{\mathcal{X}} w(x) \left( f(x, t) - m^t(x) \right)^2 p^t(x) dx = \epsilon_F^t(f, w) - \sigma^2_{t,w} (p^t(x))
\]

\[
\int_{\mathcal{X}} w(x) \left( f(x, t) - m^t(x) \right)^2 p(x | 1-t) dx = \epsilon_{CF}(f, w) - \sigma^2_{t,w} (p^{1-t}(x))
\]

Proof.

\[
\epsilon_F^t(f, w) = \int_{\mathcal{X} \times \mathcal{Y}} w(x) \left( f(x, t) - Y^t \right)^2 p \left( Y^t | x \right) p(x | t) dY^t dx
\]

\[
= \int_{\mathcal{X}} w(x) \left( f(x, t) - m^t(x) \right)^2 p(x | t) dx
\]

\[
- 2 \int_{\mathcal{X} \times \mathcal{Y}} w(x) \left( f(x, t) - m^t(x) \right) \left( Y^t - m^t(x) \right) p \left( Y^t, x | t \right) dY^t dx
\]

\[
+ \int_{\mathcal{X} \times \mathcal{Y}} w(x) \left( Y^t - m^t(x) \right)^2 p \left( Y^t, x | t \right) dY^t dx
\]

\[
= \int_{\mathcal{X}} w(x) \left( f(x, t) - m^t(x) \right)^2 p(x | t) dx + \sigma^2_{t,w} (p(x | t))
\]

Thus, we have,

\[
\int_{\mathcal{X}} w(x) \left( f(x, t) - m^t(x) \right)^2 p^t(x) dx = \epsilon_F^t(f, w) - \sigma^2_{t,w} (p^t(x))
\]

We can derive the analogous equality for counterfactual losses in the same manner. \(\square\)

Lemma 3. The covariance of \(\hat{\tau}^{(1)}_{DR}\) and \(\hat{\tau}^{(0)}_{DR}\) is:

\[
\text{Cov} \left( \hat{\tau}^{(1)}_{DR}, \hat{\tau}^{(0)}_{DR} \mid X \right) = - \left( f(X, 1) - m^{(1)}(X) \right) \left( f(X, 0) - m^{(0)}(X) \right)
\]

Proof.

\[
\text{Cov} \left( \hat{\tau}^{(1)}_{DR}, \hat{\tau}^{(0)}_{DR} \mid X \right) = \mathbb{E} \left[ \hat{\tau}^{(1)}_{DR} \cdot \hat{\tau}^{(0)}_{DR} \mid X \right] - \mathbb{E} \left[ \hat{\tau}^{(1)}_{DR} \mid X \right] \cdot \mathbb{E} \left[ \hat{\tau}^{(0)}_{DR} \mid X \right]
\]

Then,

\[
\mathbb{E} \left[ \hat{\tau}^{(1)}_{DR} \cdot \hat{\tau}^{(0)}_{DR} \mid X \right] = f(X, 1)f(X, 0) + f(X, 1)\mathbb{E} \left[ \frac{1 - T}{1 - e(X)} \left( Y^{(0)} - f(X, 0) \right) \mid X \right]
\]

\[
+ f(X, 0)\mathbb{E} \left[ \frac{T}{e(X)} \left( Y^{(1)} - f(X, 1) \right) \mid X \right]
\]

\[
= f(X, 1)f(X, 0) + f(X, 1)(m^{(0)}(X) - f(X, 0)) + f(X, 0)(m^{(1)}(X) - f(X, 1))
\]

Therefore,

\[
\mathbb{E} \left[ \hat{\tau}^{(1)}_{DR} \cdot \hat{\tau}^{(0)}_{DR} \mid X \right] - m^{(1)}(X)m^{(0)}(X)
\]

\[
= f(X, 1)f(X, 0) + f(X, 1)(m^{(0)}(X) - f(X, 0)) + f(X, 0)(m^{(1)}(X) - f(X, 1)) - m^{(1)}(X)m^{(0)}(X)
\]

\[
= - \left( f(X, 1) - m^{(1)}(X) \right) \left( f(X, 0) - m^{(0)}(X) \right)
\]

\(\square\)
G Proof of Theorem 2

Proof.

\[ Z \leq 2 \int_{X} \left( w^{(1)}(x) \left( f(x, 1) - m^{(1)}(x) \right)^2 + w^{(0)}(x) \left( f(x, 0) - m^{(0)}(x) \right)^2 \right) p(x) \, dx \quad \because (x + y)^2 \leq 2(x^2 + y^2) \]

\[ = 2u \int_{X} w^{(1)}(x) \left( f(x, 1) - m^{(1)}(x) \right)^2 p^{t=1}(x) \, dx + 2u \int_{X} w^{(0)}(x) \left( f(x, 0) - m^{(0)}(x) \right)^2 p^{t=0}(x) \, dx \]

\[ \leq 2u \left( \epsilon_{F}^{t=1}(f, w^{(1)}) - \sigma_{t=1,w^{(1)}}^{2} \left( p^{t=1}(x) \right) \right) + 2\left( 1 - u \right) \left( \epsilon_{C_{F}}^{t=1}(f, w^{(1)}) - \sigma_{t=1,w^{(1)}}^{2} \left( p^{t=0}(x) \right) \right) \]

\[ \quad + 2\left( 1 - u \right) \left( \epsilon_{F}^{t=0}(f, w^{(0)}) - \sigma_{t=0,w^{(0)}}^{2} \left( p^{t=0}(x) \right) \right) + 2u \left( \epsilon_{C_{F}}^{t=0}(f, w^{(0)}) - \sigma_{t=0,w^{(0)}}^{2} \left( p^{t=1}(x) \right) \right) \quad \because \text{Lemma 2} \]

\[ \leq 2\epsilon_{F}^{t=1}(f, w^{(1)}) + 2\epsilon_{F}^{t=0}(f, w^{(0)}) \]

\[ + 2B_{\Phi} \left( 1 - u \right) \cdot \text{IPM}_{G} \left( p^{t=1}_{\Phi,w^{(1)}}(r), p^{t=0}_{\Phi,w^{(1)}}(r) \right) + u \cdot \text{IPM}_{G} \left( p^{t=1}_{\Phi,w^{(0)}}(r), p^{t=0}_{\Phi,w^{(0)}}(r) \right) \] - 4\sigma^2 \quad \because \text{Lemma 1} \]

where \( \sigma^2 = \min_{(t,t') \in T^2} \{ \sigma_{t,w(t)}^2(p(x \mid t')) \} \), \( p^{t}_{\Phi,w}(r) = w(\Psi(r)) \cdot p^{t}(r) \).

\hfill \Box

H Hyperparameter Searching Space

Table 2 provides the hyperparameter searching space of the Gradient Boosting Regressor used in the hyperparameter tuning experiment in Section 5.3.

| Hyperparameters | Range |
|-----------------|-------|
| n_estimators    | 100 (fixed) |
| max_depth      | [1, 20] |
| min_samples_leaf | [1, 20] |
| learning_rate  | [1e^{-5}, 1e^{-1}] |
| subsample      | {0.1, 0.2, \ldots 1.0} |