Learning Counterfactual Outcomes Under Rank Preservation

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Abstract

Counterfactual inference aims to estimate the counterfactual outcome at the individual level given knowledge of an observed treatment and the factual outcome, with broad applications in fields such as epidemiology, econometrics, and management science. Previous methods rely on a known structural causal model (SCM) or assume the homogeneity of the exogenous variable and strict monotonicity between the outcome and exogenous variable. In this paper, we propose a principled approach for identifying and estimating the counterfactual outcome. We first introduce a simple and intuitive rank preservation assumption to identify the counterfactual outcome without relying on a known structural causal model. Building on this, we propose a novel ideal loss for theoretically unbiased learning of the counterfactual outcome and further develop a kernel-based estimator for its empirical estimation. Our theoretical analysis shows that the rank preservation assumption is not stronger than the homogeneity and strict monotonicity assumptions, and shows that the proposed ideal loss is convex, and the proposed estimator is unbiased. Extensive semi-synthetic and real-world experiments are conducted to demonstrate the effectiveness of the proposed method.

1 Introduction

Understanding causal relationships is a fundamental goal across various domains, such as epidemiology [1], econometrics [2], and management science [3]. Pearl and Mackenzie [4] define the three-layer causal hierarchy—association, intervention, and counterfactuals—to distinguish three types of queries with increasing complexity and difficulty [5]. Counterfactual inference, the most challenging level, aims to explore the impact of a treatment on an outcome given knowledge about a different observed treatment and the factual outcome. For example, given a patient who has not taken medication before and now suffers from a headache, we want to know whether the headache would have occurred if the patient had taken the medication initially. Answering such counterfactual queries can provide valuable instructions in scenarios such as credit assignment [6], root-causal analysis [7], attribution [8, 9, 10, 11], as well as fair and safe decision-making [12, 13, 14, 15, 16].

Different from interventional queries, which are prospective and estimate the counterfactual outcome in a hypothetical world via only the observations obtained before treatment (as pre-treatment variables), counterfactual inference is retrospective and further incorporates the factual outcome (as a post-treatment variable) in the observed world. This inherent conflict between the hypothetical

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and the observed world poses a unique challenge and makes the counterfactual outcome generally unidentifiable, even in randomized controlled experiments (RCTs) [5, 8, 13, 17].

For counterfactual inference, Pearl et al. [8] proposed a three-step procedure (abduction, action, and prediction) to estimate counterfactual outcomes. However, it relies on the availability of structural causal models (SCMs) that fully describe the data-generating process [18, 19]. In real-world applications, the ground-truth SCM is likely to be unknown, and estimating it requires additional assumptions to ensure identifiability, such as linearity [20] and additive noise [21, 22, 23]. Unfortunately, these assumptions are hard to satisfy in practice and restrict the applicability.

To tackle the above problems, several counterfactual learning approaches have been proposed with respect to different identifiability assumptions. For example, Lu et al. [24], Nasr-Esfahany et al. [25], and Xie et al. [19] established the identifiability of counterfactual outcomes based on homogeneity and strict monotonicity assumptions [23, 26]. The homogeneity assumption posits that the exogenous variable for each individual remains constant across different interventional environments, and the strict monotonicity assumption asserts that the outcome is a strictly monotone function of the exogenous variable given the features. In terms of counterfactual learning, [24] and [25] adopted Pearl's three-step procedure that needs to estimate the SCM initially. In addition, [19] proposed using quantile regression to estimate counterfactual outcomes that effectively avoid the estimation of SCM. Nevertheless, it relies on a stringent assumption that the conditional quantile functions for different counterfactual outcomes come from the same model and it requires estimating a different quantile value for each individual, leading to a challenging bi-level optimization problem [27].

In this work, we propose a principled counterfactual learning approach with *intuitive identifiability assumptions and theoretically guaranteed estimation methods*. **On one hand**, we introduce the simple and intuitive rank preservation assumption, positing that an individual's factual and counterfactual outcomes have the same rank in the corresponding distributions of factual and counterfactual outcomes for all individuals. We establish the identifiability of counterfactual outcomes under the rank preservation assumption and show that it is slightly less restrictive than the homogeneity and monotonicity assumptions used in previous studies.

On the other hand, we further propose a theoretically guaranteed method for unbiased estimation of counterfactual outcomes. The proposed estimation method has several desirable merits. First, unlike Pearl's three-step procedure, it does not necessitate a prior estimation of SCMs and thus relies on fewer assumptions than that in [24] and [25]. Second, in contrast to the quantile regression method proposed by [19], our approach neither restricts conditional quantile functions for different counterfactual outcomes to originate from the same model, nor does it require estimating a different quantile value for each unit. Third, we improve the previous learning approaches by adopting a convex loss for estimating counterfactual outcomes, which leads to a unique solution.

In summary, the main contributions are as follows: (1) We introduce the intuitive rank preservation assumption to identify the counterfactual outcomes with unknown SCM; (2) We propose a novel ideal loss for unbiased learning of the counterfactual outcome and further develop a kernel-based estimator for the ideal loss. In addition, we provide a comprehensive theoretical analysis for the proposed learning approach; (3) We conduct extensive experiments on both semi-synthetic and real-world datasets to demonstrate the effectiveness of the proposed method.

2 Problem Formulation

Throughout, capital letters represent random variables and lowercase letters denote their realizations.

Structural Causal Model (SCM, [28]). An SCM $\mathcal{M}$ consists of a causal graph $\mathcal{G}$ and a set of structure equation models $\mathcal{F} = \{f_1, ..., f_p\}$. The nodes in $\mathcal{G}$ are divided into two categories: (a) exogenous variables $\mathbf{U} = (U_1, ..., U_p)$, which represent the environment during data generation, assumed to be mutually independent; (b) endogenous variables $\mathbf{V} = \{V_1, ..., V_p\}$, which denote the relevant features that we need to model in a question of interest. For variable V_j, its value is determined by a structure equation $V_j = f_j(PA_j, U_j),\ j = 1, ..., p$, where PA_j stands for the set of parents of V_j. SCM provides a formal language for describing how the variables interact and how the resulting distribution would change in response to certain interventions. Based on SCM, we introduce the counterfactual inference problem in the following.

Counterfactual Inference. Suppose that we have three sets of variables denoted by $X, Y, \mathbf{E} \subseteq \mathbf{V}$, counterfactual inference revolves around the question, "given evidence $\mathbf{E} = \mathbf{e}$, what would have happened if we had set X to a different value x'?". Pearl et al. [8] propose using the three-step procedure to answer the problem: (a) **Abduction**: determine the value of $\mathbf{U}$ according to the evidence $\mathbf{E} = \mathbf{e}$; (b) **Action**: modify the model $\mathcal{M}$ by removing the structural equations for X and replacing them with $X = x'$, yielding the modified model $\mathcal{M}_{x'}$; (c) **Prediction**: Use $\mathcal{M}_{x'}$ and the value of $\mathbf{U}$ to calculate the counterfactual outcome of Y. In this paper, we focus on estimating the counterfactual outcome for each individual. To illustrate the main ideas, we formulate the common counterfactual inference problem within the context of the backdoor criterion.

Problem Formulation. Let $\mathbf{V} = (Z, X, Y)$, where X causes Y, Z affects both X and Y, and the structure equation of Y is given as

$$Y = f_Y(X, Z, U_X). \tag{1}$$

Let $Y_{x'}$ denotes the potential outcome if we had set $X = x'$. The counterfactual question, "given evidence $(X = x, Z = z, Y = y)$ of an individual, what would have happened had we set $X = x'$ for this individual", is formally expressed as estimating $y_{x'}$, the realization of $Y_{x'}$ for the individual. Here, we adhere to the deterministic viewpoint of [28] and [8], treating the value of $Y_{x'}$ for each individual as a fixed constant. According to Pearl's three-step procedure, given the evidence $(X = x, Z = z, Y = y)$ for an individual, the identifiability of its counterfactual value $y_{x'}$ can be achieved by determining the structural equation f_Y and the value of U_X for this individual. This is the key idea underlying most of the existing methods.

For clarity, we use $y_{x'}$ to denote the realization of the counterfactual outcome $Y_{x'}$ *for a specific individual* with observed evidence $(X = x, Z = z, Y = y)$.

3 Analysis of Existing Methods

In this section, we elucidate the challenges of counterfactual inference. Subsequently, we summarize the existing methods and shed light on their limitations.

3.1 Challenges in Counterfactual Inference

The main challenge lies in that the counterfactual value $y_{x'}$ is generally not identifiable, even in randomized controlled experiments (RCTs). By definition, $y_{x'}$ is a quantity involving two "different worlds" at the same time: the observed world with $(X = x, Z = z, Y = y)$ and the hypothetical world where $X = x'$. We only observe the factual outcome $Y_x = y$ but never observe the counterfactual outcome $Y_{x'}$, which is the fundamental problem in causal inference [29, 30]. This inherent conflict prevents us from simplifying the expression of $y_{x'}$ to a do-calculus expression, making it generally unidentifiable, even in RCTs [8]. Therefore, in addition to the widely used assumptions such as conditional exchangeability, overlapping, and consistency [1], counterfactual inference requires extra assumptions to ensure identifiability. Essentially, estimating $y_{x'}$ is equivalent to estimating the individual treatment effect $y_{x'} - y_x$, while the conditional average treatment effect (CATE) $\mathbb{E}[Y_{x'} - Y_x | Z = z]$ represents the ATE for a subpopulation with $Z = z$, overlooking the inherent heterogeneity in this subpopulation caused by the noise terms such as U_X [13, 31, 32, 33, 34, 35, 36].

3.2 Summary of Existing Methods

We summarize the existing methods in terms of identifiability assumptions and estimation strategies.

We first present an equivalent expression of Eq. (1) using $(Y_x, Y_{x'})$. Eq. (1) be reformulated as the following system

$$Y_x = f_Y(x, Z, U_x), \; Y_{x'} = f_Y(x', Z, U_{x'}),$$

where U_x and $U_{x'}$ denote the values of U_X given $X = x$ and $X = x'$, respectively. The exogenous variable U_X denotes the background and environment information induced by many unmeasured factors [8], and thus U_x and $U_{x'}$ account for the heterogeneity of Y_x and $Y_{x'}$ in the observed and hypothetical worlds, respectively. These two worlds may exhibit different levels of noise due to unmeasured factors [32, 34, 37]. For identification, previous work [19, 24, 25] relies on the key homogeneity and strict monotonicity assumptions.

Assumption 3.1 (Homogeneity)**.** $U_x = U_{x'}$.

Assumption 3.2 (Strict Monotonicity)**.** For any given (x, z), $Y_x = f_Y(x, z, U_x)$ is a smooth and strictly monotonic function of U_x; or it is a bijective mapping from U_x to Y_x.

Assumption 3.1 implies that the value of U_X for each individual remains unchanged across x. Assumption 3.2 implies that Y_x is a strict monotonic function of U_x in the subpopulation of $(X = x, Z = z)$. In Assumption 3.2, the smoothness and strict monotonicity of $f_Y(x, z, U_x)$ are akin to a bijective mapping of Y_x and U_x and serve the same purpose, so we don't distinguish them in detail.

Lemma 3.3. *Under Assumptions 3.1-3.2, $y_{x'}$ is identifiable.*

For estimation of $y_{x'}$, following Pearl's three-step procedure, [24] and [25] initially estimate f_Y and U_X for each individual. However, estimating f_Y and U_X needs to impose extra assumptions, such as linearity [20] and additive noise [22]. In addition, [19] demonstrate that $y_{x'}$ corresponds to the τ^*-th quantile of the distribution $\mathbb{P}(Y|X = x', Z = z)$, where τ^* is the quantile of y in $\mathbb{P}(Y|X = x, Z = z)$ (See the proof of Lemma 3.3 or Section 4.1 for more details). Based on it, the authors uses quantile regression to estimate $y_{x'}$, which avoids the problem of estimating f_Y and U_X. Nevertheless, this method fits a single model to obtain the conditional quantile functions for both the counterfactual and factual outcomes. Thus, its validity relies on the underlying assumption that the conditional quantile functions of outcomes for different treatment groups stem from the same model. In addition, it involves estimating a distinct quantile value for each individual before deriving the counterfactual outcomes, posing a challenging bi-level optimization problem.

4 Identification through Rank Preservation

We introduce the rank preservation assumption for identifying $y_{x'}$. *From a high-level perspective, identifying $y_{x'}$ essentially involves establishing the relationship between Y_x and $Y_{x'}$ for each individual.* Pearl's three-step procedure achieves this by estimating f_Y and U_X.

4.1 Rank Preservation Assumption

Our identifiability assumption is based on Kendall's rank correlation coefficient defined below.

Definition 4.1 (Kendall [38])**.** Let $(x_1, y_1), ..., (x_n, y_n)$ be a set of observations of two random variables (X, Y), such that all the values of x_i and y_i are unique (ties are neglected for simplicity). Any pair of (x_i, y_i) and (x_j, y_j), if $(x_j - x_i)(y_j - y_i) > 0$, they are said to be concordant; otherwise they are discordant. The *sample* Kendall rank correlation coefficient is defined as

$$\rho_n(X, Y) = \frac{2}{n(n-1)} \sum_{1 \le i < j \le n} \text{sign}((x_i - x_j)(y_i - y_j)),$$

where $\text{sign}(t) = -1, 0, 1$ for $t < 0$, $t = 0$, $t > 0$, respectively. For any two random variables (X, Y), we define $\rho(X, Y) = 1$, if $\rho_n(X, Y) = 1$ for all integers $n \ge 2$.

The $\rho_n(X, Y)$ also can be written as $2(N_c - N_d)/n(n-1)$, where N_c is the number of concordant pairs, N_d is the number of discordant pairs. It is easy to see that $-1 \le \rho_n(X, Y) \le 1$ and if the agreement between the two rankings is perfect (i.e., perfect concordance), $\rho_n(X, Y) = 1$.

Assumption 4.2 (Rank Preservation)**.** $\rho(Y_x, Y_{x'}|Z) = 1$.

Assumption 4.2 is a high-level condition that establishes a connection between Y_x and $Y_{x'}$. This assumption is satisfied in many common scenarios, as illustrated below.

- Causal models with additive noise: $Y = g(X, Z) + U$ for an arbitrary function g.
- Heteroscedastic noise models: $Y = g(X, Z) + h(X, Z)U$ for arbitrary functions g and h, with $h(X, Z) > 0$ denoting the conditional standard deviation of Y given (X, Z).

For the individual with observation $(X = x, Z = z, Y = y)$, we denote $(y_x = y, y_{x'})$ as its true values of $(Y_x, Y_{x'})$. Assumption 4.2 implies that for this individual, its rankings of y_x and $y_{x'}$ are the same in the distributions of $\mathbb{P}(Y_x|Z = z)$ and $\mathbb{P}(Y_{x'}|Z = z)$, respectively. Therefore, we have

$$\mathbb{P}(Y_x \le y_x|Z = z) = \mathbb{P}(Y_{x'} \le y_{x'}|Z = z). \quad (2)$$

Since $y_x = y$ is observed and the distributions $\mathbb{P}(Y_x|Z=z)$ and $\mathbb{P}(Y_{x'}|Z=z)$ can be identified as $\mathbb{P}(Y|X=x, Z=z)$ and $\mathbb{P}(Y|X=x', Z=z)$, respectively, by the backdoor criterion (i.e., $(Y_x, Y_{x'}) \perp\!\!\!\perp X|Z$). Therefore, we have the following Proposition 4.3 (see Appendix A for proofs).

Proposition 4.3. *Under Assumption 4.2, $y_{x'}$ is identified as the τ^*-th quantile of $\mathbb{P}(Y|X=x', Z=z)$, where τ^* is the quantile of y in the distribution of $\mathbb{P}(Y|X=x, Z=z)$.*

Proposition 4.3 shows that Assumption 4.2 can serve as a substitute for Assumptions 3.1-3.2 in identifying $y_{x'}$. Unlike Assumptions 3.1-3.2, Assumption 4.2 is simple and intuitive, as it directly links Y_x and $Y_{x'}$ for each individual. To clarify the relationship between Assumption 4.2 introduced by this work and Assumptions 3.1-3.2 from previous work, we present Proposition 4.4 below.

Proposition 4.4. *The proposed Assumption 4.2 is strictly weaker than Assumptions 3.1-3.2.*

Proposition 4.4 is intuitive, as correlation (Assumption 4.2) does not necessarily imply identity (Assumption 3.1). To illustrate, consider a SCM with $X \in \{0, 1\}$, $Y_1 = Z + U_1$, $Y_0 = Z/2 + U_0$, $U_1 = U_0^3$. In this case, $\rho(Y_0, Y_1|Z) = 1$, but $U_1 \neq U_0$. Nevertheless, Assumption 4.2 is only slightly weaker than Assumptions 3.1-3.2 by allowing $U_{x'} \neq U_x$. Specifically, we can show that if U_x is a strictly monotone increasing function of $U_{x'}$, Assumption 4.2 is equivalent to Assumption 3.2, see Appendix A for proofs.

4.2 Further Relaxation of Strict Monotonicity

In Definition 4.1, we ignore ties for simplicity. However, when the outcome Y is discrete or continuous variables with tied observations, $\rho(Y_x, Y_{x'})$ will always be less than 1. To accommodate such cases, we introduce a modified version of the Kendall rank correlation coefficient given below.

Definition 4.5 (Kendall [39]). Let $(x_1, y_1), ..., (x_n, y_n)$ be the observations of two random variables (X, Y), the modified Kendall rank correlation coefficient is define as

$$\tilde{\rho}_n(X, Y) = \sum_{1 \le i < j \le n} \frac{\text{sign}((x_i - x_j)(y_i - y_j))}{\sqrt{n(n-1)/2 - T_x} \cdot \sqrt{n(n-1)/2 - T_y}},$$

where T_x is the number of tied pairs in $\{x_1, ..., x_n\}$ and T_y is the number of tied pairs in $\{y_1, ..., y_n\}$. We define $\tilde{\rho}(X, Y) = 1$, if $\tilde{\rho}_n(X, Y) = 1$ for all integers $n \ge 2$.

Compared with Definition 4.1, one can see that $\tilde{\rho}(X, Y)$ adjusts $\rho(X, Y)$ by eliminating the ties in the denominator, and $\tilde{\rho}(X, Y)$ reduces to $\rho(X, Y)$ if there are no ties.

Assumption 4.6 (Rank Preservation). $\tilde{\rho}(Y_x, Y_{x'}|Z) = 1$.

Assumption 4.6 is less restrictive than Assumption 4.2 as it accommodates broader data types of Y. To illustrate, consider a dataset with four individuals where the true values of $(Y_x, Y_{x'})$ are $(1, 1), (2, 1.5), (2, 1.5), (3, 2.5)$. In this scenario, $\sum_{1 \le i < j \le n} \text{sign}((y_{i,x} - y_{j,x})(y_{i,x'} - y_{j,x'}) = 5$, $T_{Y_x} = 1$, $T_{Y_{x'}} = 1$, resulting in $\rho(Y_x, Y_{x'}) = 5/6$ and $\tilde{\rho}(Y_x, Y_{x'}) = 5/(\sqrt{6-1} \cdot \sqrt{6-1}) = 1$.

Assumption 4.6 also guarantees the identifiability of $y_{x'}$.

Proposition 4.7. *Under Assumption 4.6, the conclusion in Proposition 4.3 also holds.*

5 Counterfactual Learning

We propose a novel estimation method for counterfactual inference. Suppose that $\{(x_k, z_k, y_k) : k = 1, ..., N\}$ is a sample consisting of N realizations of random variables (X, Z, Y). For an individual, given its evidence $(X = x, Z = z, Y = y)$, we aim to estimate its counterfactual outcome $y_{x'}$, i.e., the realization of $Y_{x'}$ for this individual.

5.1 Rationale and Limitations of Quantile Regression

For estimating $y_{x'}$, Xie et al. [19] formulate it as the following bi-level optimization problem

$$\tau^* = \arg\min_{\tau} |f_\tau(x, z) - y|, \quad f_\tau^* = \arg\min_{f} \frac{1}{N} \sum_{k=1}^{N} l_\tau(y_k - f(x_k, z_k)),$$

where $l_\tau(\xi) = \tau\xi \cdot \mathbb{I}(\xi \geq 0) + (\tau - 1)\xi \cdot \mathbb{I}(\xi < 0)$ is the check function [40], the upper level optimization is to estimate τ^*, the quantile of y in the distribution $\mathbb{P}(Y|X = x, Z = z)$, and the lower level optimization is to estimate the conditional quantile function $q(x, z; \tau) \triangleq \inf_y\{y : \mathbb{P}(Y \leq y|X = x, Z = z) \geq \tau\}$ for a given τ. Then $y_{x'}$ can be estimated using $q(x', z; \tau^*)$.

We define two conditional quantile regression functions,

$$q_x(z;\tau) \triangleq \inf_y\{y : \mathbb{P}(Y_x \leq y|Z = z) \geq \tau\}, \quad q_{x'}(z;\tau) \triangleq \inf_y\{y : \mathbb{P}(Y_{x'} \leq y|Z = z) \geq \tau\}.$$

By Eq. (2), $y_{x'}$ can be expressed as $q_{x'}(z; \tau^*)$ with τ^* being the quantile of y in the distribution of $\mathbb{P}(Y_x|Z = z)$, i.e., $\mathbb{P}(Y_x \leq y|Z = z) = \tau^*$. Lemma 5.1 (see Appendix B for proofs) shows the rationale behind employing the check function as the loss to estimate conditional quantiles.

Lemma 5.1. *We have that*
(i) $q_x(Z; \tau) = \arg\min_f \mathbb{E}[l_\tau(Y_x - f(Z))]$ *for any given* x*;*
(ii) $q(X, Z; \tau) = \arg\min_f \mathbb{E}[l_\tau(Y - f(X, Z))]$.

There are two major concerns with the estimation method of [19]. First, it only fits a single quantile regression model for $q(X, Z; \tau)$ to obtain estimates of $q_x(Z; \tau)$ and $q_{x'}(Z; \tau)$. When the two conditional quantile functions $q_x(Z; \tau)$ and $q_{x'}(Z; \tau)$ originate from different models, this method may yield inaccurate estimates. Second, it explicitly requires estimating the quantile τ^* for each individual before estimating the counterfactual outcome $y_{x'}$.

Inspired by [41], a simple improvement is to estimate $q_x(z; \tau)$ and $q_{x'}(z; \tau)$ separately. For example, for estimating $q_x(z; \tau)$, the associated loss function is given as

$$R_x(f, \tau) = \frac{1}{N}\sum_{k=1}^{N} \frac{\mathbb{I}(x_k = x) \cdot l_\tau(y_k - f(z_k))}{\hat{p}_x(z_k)},$$

where $p_x(z) = \mathbb{P}(X = x|Z = z)$ is the propensity score, $\hat{p}_x(z)$ is its estimate. Likewise, we could define $R_{x'}(f, \tau)$ by replacing x with x'. Then the estimation procedure for $y_{x'}$ involves four steps: (1) estimating $p_x(z)$; (2) estimating $q_x(z; \tau)$ by minimizing $R_x(f, \tau)$ for a range of candidate values of τ; (3) identifying the τ^* in the candidate set of τ, that corresponds to the quantile of y in the distribution $\mathbb{P}(Y|X = x, Z = z)$; (4) estimating $y_{x'}$ using $q_{x'}(z; \tau^*)$, where $q_{x'}(z; \tau^*)$ is obtained by minimizing $R_{x'}(f, \tau^*)$. Despite this four-step estimation method that allows $q_x(Z; \tau)$ and $q_{x'}(Z; \tau)$ to come from different models, it still needs to estimate a different τ^* for each individual.

5.2 Enhanced Counterfactual Learning Method

To address the limitations mentioned above in directly applying quantile regression and improve estimation accuracy, we propose a novel loss that produces an unbiased estimator of $y_{x'}$ for the individual with evidence $(X = x, Z = z, Y = y)$. The proposed ideal loss is constructed as

$$R_{x'}(t|x, z,y) = \mathbb{E}\left[|Y_{x'} - t| \;\middle|\; Z = z\right] + \mathbb{E}\left[\text{sign}(Y_x - y) \;\middle|\; Z = z\right] \cdot t,$$

which is a function of t and the expectation operator is taken on the random variable of $(Y_x, Y_{x'})$ given $Z = z$. The proposed estimation method is based on Theorem 5.2.

Theorem 5.2 (Validity of the Proposed Ideal Loss)**.** *The loss* $R_{x'}(t|x, z, y)$ *is convex with respect to* t *and is minimized uniquely at* t^**, where* t^* *is the solution satisfying*

$$\mathbb{P}(Y_{x'} \leq t^*|Z = z) = \mathbb{P}(Y_x \leq y|Z = z).$$

Theorem 5.2 (see Appendix B for proofs) implies that given the evidence $(X = x, Z = z, Y = y)$ for an individual, the counterfactual outcome $y_{x'}$ satisfies $y_{x'} = \arg\min_t R_{x'}(t|x, z, y)$ under Assumption 4.6. **Importantly**, *the loss* $R_{x'}(t|x, z, y)$ *neither estimates the SCM a priori, nor restricts* $q_x(z; \tau)$ *and* $q_{x'}(z; \tau)$ *stem from the same model, and it does not need to estimate a different quantile value for each individual explicitly.*

To optimize the ideal loss $R_{x'}(t; x, z, y)$, we first need to estimate it, which presents two significant challenges: (1) $R_{x'}(t|x, z, y)$ involves both Y_x and $Y_{x'}$, but for each unit, we only observe one of them; (2) The terms $\mathbb{E}\left[|Y_{x'} - t| \;\middle|\; Z = z\right]$ and $\mathbb{E}\left[\text{sign}(Y_x - y) \;\middle|\; Z = z\right]$ in $R_{x'}(t|x, z, y)$ is conditioned on $Z = z$, and when Z is a continuous variable with infinite possible values, it cannot be estimated

Table 1: $\sqrt{\epsilon_{\text{PEHE}}}$ of individual treatment effect estimation on the simulated Sim-m dataset, where m is the dimension of Z.

	Sim-5		Sim-10		Sim-20		Sim-40	
Methods	In-sample	Out-sample	In-sample	Out-sample	In-sample	Out-sample	In-sample	Out-sample
T-learner	2.95 ± 0.02	2.66 ± 0.01	2.99 ± 0.01	3.17 ± 0.01	3.36 ± 0.02	3.19 ± 0.03	5.12 ± 0.02	4.74 ± 0.04
X-learner	2.94 ± 0.01	2.66 ± 0.01	2.98 ± 0.02	3.19 ± 0.02	3.31 ± 0.02	3.21 ± 0.02	5.08 ± 0.04	4.77 ± 0.03
BNN	2.91 ± 0.08	2.64 ± 0.07	2.90 ± 0.11	3.08 ± 0.12	3.21 ± 0.13	3.13 ± 0.16	4.81 ± 0.10	4.54 ± 0.09
TARNet	2.89 ± 0.07	2.64 ± 0.06	2.94 ± 0.07	3.16 ± 0.08	3.18 ± 0.07	3.11 ± 0.07	4.82 ± 0.07	4.56 ± 0.07
CFRNet	2.88 ± 0.07	2.62 ± 0.06	2.94 ± 0.07	3.15 ± 0.08	3.15 ± 0.07	3.08 ± 0.07	4.71 ± 0.12	4.45 ± 0.11
CEVAE	2.92 ± 0.27	2.65 ± 0.21	3.04 ± 0.27	3.11 ± 0.18	3.16 ± 0.17	3.11 ± 0.17	4.88 ± 0.23	4.53 ± 0.20
DragonNet	2.90 ± 0.08	2.63 ± 0.08	3.02 ± 0.07	3.25 ± 0.08	3.16 ± 0.11	3.09 ± 0.10	4.78 ± 0.11	4.50 ± 0.12
DeRCFR	2.88 ± 0.06	2.61 ± 0.06	2.87 ± 0.05	3.07 ± 0.06	3.11 ± 0.07	3.04 ± 0.06	4.77 ± 0.11	4.50 ± 0.10
DESCN	2.93 ± 0.11	2.66 ± 0.09	3.27 ± 0.81	3.46 ± 0.79	3.12 ± 0.20	3.06 ± 0.20	4.91 ± 0.37	4.59 ± 0.35
ESCFR	2.87 ± 0.08	2.62 ± 0.07	2.94 ± 0.08	3.15 ± 0.09	3.03 ± 0.09	3.06 ± 0.09	4.71 ± 0.15	4.43 ± 0.15
CFQP	2.91 ± 0.09	2.67 ± 0.11	3.14 ± 0.30	3.40 ± 0.37	3.21 ± 0.12	3.18 ± 0.11	4.93 ± 0.14	4.55 ± 0.13
Quantile-Reg	2.80 ± 0.06	2.54 ± 0.05	2.78 ± 0.08	3.05 ± 0.09	2.92 ± 0.07	3.01 ± 0.08	4.39 ± 0.13	4.12 ± 0.10
Ours	$\mathbf{2.45 \pm 0.17}$	$\mathbf{2.28 \pm 0.23}$	$\mathbf{2.25 \pm 0.07}$	$\mathbf{2.33 \pm 0.07}$	$\mathbf{2.51 \pm 0.07}$	$\mathbf{2.46 \pm 0.06}$	$\mathbf{3.74 \pm 0.26}$	$\mathbf{3.66 \pm 0.21}$

Table 2: $\sqrt{\epsilon_{\text{PEHE}}}$ of individual treatment effect estimation on the simulated Sim-m dataset, where m is the dimension of Z.

	Sim-80 ($\rho = 0.3$)		Sim-80 ($\rho = 0.5$)		Sim-40 ($\rho = 0.3$)		Sim-40 ($\rho = 0.5$)	
Methods	In-sample	Out-sample	In-sample	Out-sample	In-sample	Out-sample	In-sample	Out-sample
TARNet	12.63 ± 0.93	12.51 ± 0.90	12.35 ± 1.24	12.68 ± 1.51	8.91 ± 0.97	8.78 ± 0.74	8.76 ± 0.76	8.51 ± 0.68
DragonNet	12.50 ± 0.75	12.36 ± 0.80	12.71 ± 1.29	13.02 ± 1.54	8.83 ± 0.90	8.73 ± 0.72	8.62 ± 0.70	8.39 ± 0.53
ESCFR	12.61 ± 1.09	12.53 ± 1.09	12.56 ± 1.36	12.87 ± 1.64	8.76 ± 1.03	8.65 ± 0.79	8.76 ± 0.78	8.50 ± 0.48
X_learner	12.82 ± 0.91	12.68 ± 0.95	12.74 ± 1.22	12.99 ± 1.43	8.97 ± 0.87	8.81 ± 0.64	8.91 ± 0.75	8.61 ± 0.58
Quantile-Reg	11.59 ± 0.94	11.57 ± 0.97	11.59 ± 1.26	11.91 ± 1.47	8.05 ± 0.73	8.08 ± 0.75	7.74 ± 0.73	7.58 ± 0.73
Ours	$\mathbf{9.28 \pm 0.72}$	$\mathbf{9.28 \pm 0.72}$	$\mathbf{9.03 \pm 1.09}$	$\mathbf{9.27 \pm 0.97}$	$\mathbf{7.07 \pm 0.39}$	$\mathbf{7.05 \pm 0.41}$	$\mathbf{7.07 \pm 1.23}$	$\mathbf{6.98 \pm 1.08}$

by simply splitting the data based on Z. We employ inverse propensity score and kernel smoothing techniques to overcome these two challenges. Specifically, we propose a kernel-smoothing-based estimator for the ideal loss, which is given as

$$\hat{R}_{x'}(t|x,z,y) = \frac{\sum_{k=1}^{N} K_h(z_k - z)\frac{\mathbb{I}(x_k=x')}{\hat{p}_{x'}(z_k)}|y_k - t|}{\sum_{k=1}^{N} K_h(z_k - z)} + \frac{\sum_{k=1}^{N} K_h(z_k - z)\frac{\mathbb{I}(x_k=x)}{\hat{p}_{x}(z_k)} \cdot \text{sign}(y_k - y)}{\sum_{k=1}^{N} K_h(z_k - z)} \cdot t,$$

where h is a bandwidth/smoothing parameter, $K_h(u) = K(u/h)/h$, and $K(\cdot)$ is a symmetric kernel function [42, 43, 44] that satisfies $\int K(u)du = 1$ and $\int uK(u)du = 1$, such as Epanechnikov kernel $K(u) = 3(1 - u^2) \cdot \mathbb{I}(|u| \leq 1)/4$ and Gaussian kernel $K(u) = \exp(-u^2/2)/\sqrt{2\pi}$ for $u \in \mathbb{R}$. Then we can estimate $y_{x'}$ by minimizing $\hat{R}_{x'}(t; x, z, y)$ directly.

Proposition 5.3 (Consistency). *If $h \to 0$ as $N \to \infty$, $\hat{p}_x(z)$ and $\hat{p}_{x'}(z)$ are consistent estimates of $p_x(z)$ and $p_{x'}(z)$, and the density function of Z is differentiable, then $\hat{R}_{x'}(t|x, z, y)$ converges to $R_{x'}(t|x, z, y)$ in probability.*

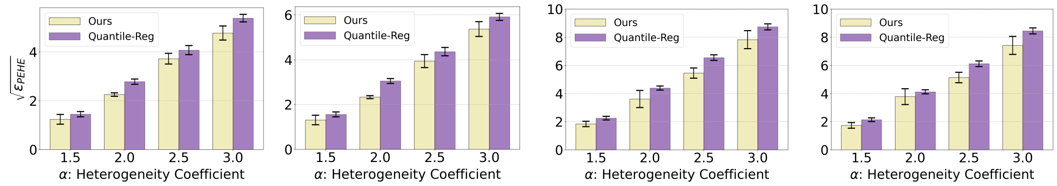
Proposition 5.3 (see Appendix B for proofs) indicates that $\hat{R}_{x'}(t|x, z, y)$ is a consistent estimator of $R_{x'}(t|x, z, y)$, demonstrating the validity of the estimated ideal loss. The loss $\hat{R}_{x'}(t|x, z, y)$ is applicable only for discrete treatments due to the terms $\mathbb{I}(x_k = x')$ and $\mathbb{I}(x_k = x)$. However, it can be easily extended to continuous treatments, as detailed in Appendix C.

It is well known that kernel-smoothing-based estimators suffer from scalability issues in high-dimensional settings (i.e., the high-dimensional covariates) [42]. Therefore, for implementation, we avoid applying kernel functions directly to the original covariates. Instead, we first learn a low-dimensional representation of the covariates, and then apply the kernel-smoothing-based estimator to this representation to learn the counterfactual outcomes.

6 Experiments

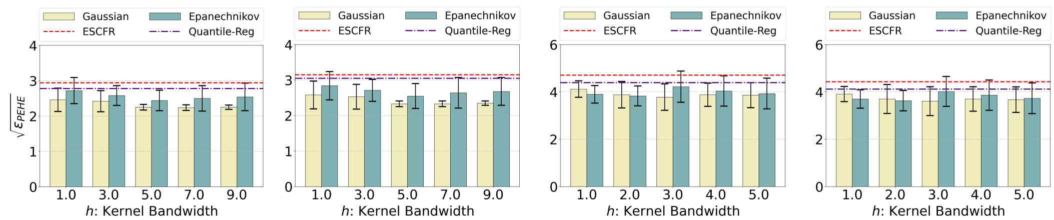
6.1 Synthetic Experiment

Simulation Process. We generate the synthetic dataset by the following process. First, we sample the covariate $Z \sim \mathcal{N}(0, I_m)$ and the treatment $X \sim \text{Bern}(\pi(Z))$, where $\text{Bern}(\cdot)$ is the Bernoulli



(a) Sim-10 (In-sample) (b) Sim-10 (Out-sample) (c) Sim-40 (In-sample) (d) Sim-40 (Out-sample)

Figure 1: Estimation performance of individual treatment effects under varying heterogeneity degrees.



(a) Sim-10 (In-sample) (b) Sim-10 (Out-sample) (c) Sim-40 (In-sample) (d) Sim-40 (Out-sample)

Figure 2: The estimation performance with different kernels and bandwidths.

distribution with probability $\pi(Z) = \mathbb{P}(X = 1 \mid Z) = \sigma(W_x \cdot Z)$, $\sigma(\cdot)$ is the sigmoid function, and $W_x \sim \text{Unif}(-1, 1)^m$, $\text{Unif}(\cdot)$ is the uniform distribution. Then, we sample the noise $U_0 \sim \mathcal{N}(0, 1)$ and $U_1 = \alpha \cdot U_0$ to consider the heterogeneity of the exogenous variables, where α is the hyper-parameter to control the heterogeneity degree. Finally, we simulate $Y_1 = W_y \cdot Z + U_1$ and $Y_0 = W_y \cdot Z/\alpha + U_0$ with $W_y \sim \mathcal{N}(0, I_m)$. We generate 10,000 samples with 63/27/10 train/validation/test split and vary $m \in \{5, 10, 20, 40\}$ in our synthetic experiment.

Baselines and Evaluation Metrics. The competing baselines includes: T-learner [45], X-learner [45], BNN [46], TARNet [47], CFRNet [47], CEVAE [48], DragonNet [49], DeRCFR [50], DESCN [51], ESCFR [52], CFQP [18], and Quantile-Reg [19]. We evaluate the individual treatment effect estimation using the *individual level Precision in Estimation of Heterogeneous Effects* (PEHE):

$$\epsilon_{\text{PEHE}} = \frac{1}{N}\sum_{i=1}^{N}[(\hat{Y}_i(1) - \hat{Y}_i(0)) - (Y_i(1) - Y_i(0))]^2,$$

where $\hat{Y}_i(1)$ and $\hat{Y}_i(0)$ are the predicted values for the corresponding true potential outcomes of unit i. It is noteworthy that ϵ_{PEHE} is tailored for individual-level evaluation and counterfactual estimation, which is different from the common metric [47] given by $\frac{1}{N}\sum_{i=1}^{N}[(\hat{\mu}_1(X_i) - \hat{\mu}_0(X_i)) - (\mu_1(X_i) - \mu_0(X_i))]^2$, where $\mu_1(X_i) - \mu_0(X_i) := \mathbb{E}[Y(1)|X] - \mathbb{E}[Y(0)|X]$ are the true CATE, and $\hat{\mu}_1(X_i) - \hat{\mu}_0(X_i)$ is its estimate. Both in-sample and out-of-sample performances are reported in our experiments. In addition, we run all experiments on the Google Colab platform. For the representation model, we use the MLP for the base model and tune the layers in $\{1, 2, 3\}$. In addition, we adopt the logistic regression model as the propensity model. We tune the learning rate in $\{0.001, 0.005, 0.01, 0.05, 0.1\}$. For the kernel choice, we select the kernel function between the Gaussian kernel function and the Epanechnikov kernel function, and tune the bandwidth in $\{1, 3, 5, 7, 9\}$.

Performance Analysis. The results of estimation performance are shown in Table 1. Our method stably outperforms all baselines with varying covariate dimensions m, demonstrating the effectiveness of the proposed method. In addition, we investigate our method performance with violated assumptions on rank and uncorrelated covariates. Specifically, we modified the data generation process to explore the performance of our method under correlated covariates by sampling the covariate $Z \sim \mathcal{N}(0, \Sigma_m)$, where the ρ_{ij} in Σ_m is $\max(0.01, \rho^{|i-j|})$. The results are shown in Table 2. The results show that our method still outperforms the baseline methods. Moreover, we further explore the effect of heterogeneity degrees on the performance of the proposed method, as shown in Figure 1, where one can see that as the heterogeneity degree increases, our method stably outperforms the Quantile-Reg in terms of PEHE. Finally, we examine the effect of different kernels and bandwidths,

Table 3: The experiment results on the IHDP dataset and JOBS dataset. The best result is bolded.

	IHDP				JOBS			
	In-sample		Out-sample		In-sample		Out-sample	
Methods	$\sqrt{\epsilon_{\text{PEHE}}}$	ϵ_{ATE}	$\sqrt{\epsilon_{\text{PEHE}}}$	ϵ_{ATE}	R_{Pol}	ϵ_{ATT}	R_{Pol}	ϵ_{ATT}
T-learner	1.49 ± 0.03	0.37 ± 0.05	1.81 ± 0.04	0.49 ± 0.04	0.31 ± 0.06	0.16 ± 0.10	0.27 ± 0.08	0.20 ± 0.07
X-learner	1.50 ± 0.02	0.21 ± 0.05	1.73 ± 0.03	0.36 ± 0.07	0.16 ± 0.04	0.07 ± 0.05	0.16 ± 0.03	0.10 ± 0.09
BNN	2.09 ± 0.16	1.00 ± 0.23	2.37 ± 0.15	1.18 ± 0.19	0.15 ± 0.01	0.08 ± 0.03	0.16 ± 0.02	0.13 ± 0.07
TARNet	1.52 ± 0.07	0.22 ± 0.13	1.78 ± 0.07	0.34 ± 0.18	0.17 ± 0.06	0.06 ± 0.08	0.18 ± 0.09	0.10 ± 0.06
CFRNet	1.46 ± 0.06	0.17 ± 0.15	1.77 ± 0.06	0.32 ± 0.20	0.17 ± 0.03	$\mathbf{0.05 \pm 0.03}$	0.19 ± 0.07	0.10 ± 0.04
CEVAE	4.08 ± 0.88	3.67 ± 1.23	4.12 ± 0.91	3.75 ± 1.23	0.18 ± 0.05	0.09 ± 0.03	0.22 ± 0.08	0.10 ± 0.09
DragonNet	1.49 ± 0.08	0.22 ± 0.14	1.80 ± 0.06	0.29 ± 0.19	0.17 ± 0.06	0.07 ± 0.07	0.20 ± 0.08	0.11 ± 0.09
DeRCFR	1.48 ± 0.06	0.25 ± 0.14	1.69 ± 0.06	0.25 ± 0.14	0.15 ± 0.02	0.14 ± 0.04	0.16 ± 0.04	0.15 ± 0.11
DESCN	2.08 ± 0.98	0.74 ± 1.00	2.67 ± 1.45	1.04 ± 1.46	0.15 ± 0.02	0.21 ± 0.14	0.22 ± 0.16	0.16 ± 0.04
ESCFR	1.46 ± 0.09	0.16 ± 0.16	1.73 ± 0.08	0.27 ± 0.16	0.14 ± 0.02	0.10 ± 0.03	0.15 ± 0.02	0.10 ± 0.08
Quantile-Reg	1.43 ± 0.05	0.14 ± 0.09	1.56 ± 0.03	0.18 ± 0.09	0.14 ± 0.01	0.06 ± 0.01	0.15 ± 0.01	0.07 ± 0.04
CFQP	1.47 ± 0.10	0.18 ± 0.17	1.48 ± 0.05	0.15 ± 0.08	0.15 ± 0.02	0.23 ± 0.15	0.16 ± 0.03	0.15 ± 0.07
Ours	$\mathbf{1.41 \pm 0.02}$	$\mathbf{0.11 \pm 0.10}$	$\mathbf{1.50 \pm 0.06}$	$\mathbf{0.13 \pm 0.08}$	$\mathbf{0.08 \pm 0.04}$	0.06 ± 0.02	$\mathbf{0.11 \pm 0.05}$	$\mathbf{0.05 \pm 0.05}$

as shown in Figure 2, our method stably outperforms the Quantile-Reg and ESCFR methods with different kernels and bandwidths.

6.2 Real-World Experiment

Dataset and Preprocessing. Following previous studies [47, 48, 53, 54], we conduct experiments on semi-synthetic dataset IHDP and real-world dataset JOBS. The IHDP dataset [55] is constructed from the Infant Health and Development Program (IHDP) with 747 individuals and 25 covariates. The JOBS dataset [56] is based on the National Supported Work program with 3,212 individuals and 17 covariates. We follow [47] to split the data into training/validation/testing set with ratios 63/27/10 and 56/24/20 with 100 and 10 repeated times on the IHDP and the JOBS datasets, respectively.

Evaluation Metrics. Following previous studies [47, 48, 54], besides ϵ_{PEHE}, we also use the absolute error in *Average Treatment Effect* (ATE) for evaluation, which is defined as $\epsilon_{\text{ATE}} = \frac{1}{N}|\sum_{i=1}^{N}((\hat{Y}_i(1)-\hat{Y}_i(0))-(Y_i(1)-Y_i(0)))|$. We use $\sqrt{\epsilon_{\text{PEHE}}}$ and ϵ_{ATE} to evaluate performance on the IHDP dataset. For the JOBS dataset, since one of the potential outcomes is not available, we evaluate the performance using the absolute error in *Average Treatment effect on the Treated* (ATT) as $\epsilon_{\text{ATT}} = |\text{ATT} - \frac{1}{|T|}\sum_{i\in T}(\hat{Y}_i(1) - \hat{Y}_i(0)|$ with $\text{ATT} = |\frac{1}{|T|}\sum_{i\in T} Y_i - \frac{1}{|C\cap E|}\sum_{i\in C\cap E} Y_i|$. We also use the policy risk $R_{\text{Pol}} = 1-(\mathbb{E}[Y(1) \mid \hat{Y}(1)-\hat{Y}(0) > 0, X = 1]\cdot\mathbb{P}(\hat{Y}(1)-\hat{Y}(0) > 0)+\mathbb{E}[Y(0) \mid \hat{Y}(1)-\hat{Y}(0) \leq 0, X = 0] \cdot \mathbb{P}(\hat{Y}(1) - \hat{Y}(0) \leq 0))$, where T, C, E are the indexes of treatment sample set, control sample set, and randomized sample set, respectively.

Performance Comparison. The experiment results are shown in Table 3. Similar to the synthetic experiment, the Quantile-Reg method still achieves the most competitive performance compared to the other baselines. Our method stably outperforms all the baselines on both the semi-synthetic dataset IHDP and the real-world dataset JOBS, especially in the out-sample scenario. This provides the empirical evidence of the effectiveness of our method.

7 Related Work

Conditional Average Treatment Effect (CATE). CATE also referred to as heterogeneous treatment effect, represents the average treatment effects on subgroups categorized by covariate values, and plays a central role in areas such as precision medicine [57, 58, 59, 60], policy learning [61, 62], and recommender systems [63, 64, 65]. Benefiting from recent advances in machine learning, many methods have been proposed for estimating CATE, including matching methods [66, 67, 54, 68], tree-based methods [69, 70], representation learning methods [46, 47, 49, 50, 52], and generative methods [48, 53]. Unlike the existing work devoted to estimating CATE at the intervention level for subgroups, our work focuses on counterfactual inference at the more challenging and fine-grained individual level.

Counterfactual Inference. Counterfactual inference involves the identification and estimation of counterfactual outcomes. For identification, [71] provided an algorithm leveraging counterfactual graphs to identify counterfactual queries. In addition, [72] discussed the identifiability of nested counterfactuals within a given causal graph. More relevant to our work, [19] and [24] studied the identifiability assumptions in the setting of backdoor criterion under homogeneity and strict monotonicity assumptions. Several methods focus on determining its bounds with less stringent assumptions, such as [10, 13, 73, 74]. In addition, [11] proposed a method for identifying the joint distribution of potential outcomes using multiple experimental datasets.

For estimation, [8] introduced a three-step procedure for counterfactual inference. Many machine learning methods estimate counterfactual outcomes in this framework, such as [6, 18, 24, 25, 75, 76, 77]. Recently, [19] employed quantile regression to estimate the counterfactual outcomes, effectively circumventing the need for SCM estimation. In our work, we extend the above methods in both identification and estimation. Recently, counterfactual inference methods have been extensively applied across various application scenarios, such as counterfactual fairness [78, 79, 80, 81, 82, 83], policy evaluation and improvement [14, 84, 85, 86], reinforcement learning [24, 87, 88, 89, 90, 91, 92], imitation learning [93, 94], counterfactual generation [76, 95, 96, 97], counterfactual explanation [98, 99, 100, 101, 102], counterfactual harm [13, 14, 103, 15], physical audiovisual commonsense reasoning [104], interpretable time series prediction [105], classification and detection in medical imaging [106], data valuation [107], etc. Therefore, developing novel counterfactual inference methods holds significant practical implications.

8 Conclusion

This work addresses the fundamental challenge of counterfactual inference in the absence of a known SCM and under heterogeneous endogenous variables. We first introduce the rank preservation assumption to identify counterfactual outcomes, showing that it is slightly weaker than the homogeneity and monotonicity assumptions. Then, we propose a novel ideal loss for unbiased learning of counterfactual outcomes and develop a kernel-based estimator for practical implementation. The convexity of the ideal loss and the unbiased nature of the proposed estimator contribute to the robustness and reliability of our method. A potential limitation arises when the propensity score is extremely small in certain data sparsity scenarios, which may cause instability in the estimation method. Further investigation is warranted to address and overcome this challenge.

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A Proofs in Sections 3 and 4

One can show Lemma 3.3 by a similar argument of the proof of Theorem 1 in [19]. For the sake of self-containedness, we provide a novel proof of it.

Lemma 3.3 *Under Assumptions 3.1-3.2, $y_{x'}$ is identifiable.*

Proof of Lemma 3.3. First, the distributions $\mathbb{P}(Y_x|Z = z)$ and $\mathbb{P}(Y_{x'}|Z = z)$ can be identified as $\mathbb{P}(Y|X = x, Z = z)$ and $\mathbb{P}(Y|X = x', Z = z)$, respectively, by the backdoor criterion (i.e., $(Y_x, Y_{x'}) \perp\!\!\!\perp X|Z)$ of the setting.

Then, according to the model (1), we can equivalently write

$$Y_x = f_Y(x, z, U_x),\ Y_{x'} = f_Y(x', z, U_{x'}),$$

and Y and U_X in model (1) can be expressed as $Y = \sum_{x\in\mathcal{X}} \mathbb{I}(X = x)\cdot Y_x$ and $U_X = \sum_{x\in\mathcal{X}} \mathbb{I}(X = x)\cdot U_x$, where $\mathcal{X}$ is the support set of X and $\mathbb{I}(\cdot)$ is an indicator function. Assumption 3.1 implies that $U_X = U_x = U_{x'}$ conditional on Z, i.e., $Y_x = f_Y(x, z, U_X),\ Y_{x'} = f_Y(x', z, U_X)$.

Finally, for the individual with observation $(X = x, Z = z, Y = y)$, we denote $(y_x, y_{x'})$ as the true values of $(Y_x, Y_{x'})$ for this individual. For this individual, we can identify the quantile of y_x in the distribution of $\mathbb{P}(Y_x|Z = z) = \mathbb{P}(Y|X = x, Z = z)$, denoted by τ^*. Let u_{τ^*} be the true value of U_X for this individual, it is the τ^*-quantile in the distribution $\mathbb{P}(U_X|Z = z)$, then we have

$$\begin{aligned}
\tau^* &= \mathbb{P}(Y_x \le y_x|Z = z) && \text{(by the definition of } \tau) \\
&= \mathbb{P}(U_x \le u_\tau|Z = z) && \text{(by Assumption 3.2)} \\
&= \mathbb{P}(U_{x'} \le u_\tau|Z = z) && \text{(by Assumption 3.1)} \\
&= \mathbb{P}(Y_{x'} \le f_Y(x', z, u_{\tau^*})|Z = z) && \text{(by Assumption 3.2)} \\
&= \mathbb{P}(Y_{x'} \le y_{x'}|Z = z) && \text{(by the definition of } y_{x'}),
\end{aligned}$$

which implies that for this individual, its rankings of y_x and $y_{x'}$ are the same in the distributions of $\mathbb{P}(Y_x|Z = z)$ and $\mathbb{P}(Y_{x'}|Z = z)$, resepcctively. Thus, $y_{x'}$ is identified as the τ^*-quantile of the distribution $\mathbb{P}(Y_{x'}|Z = z) = \mathbb{P}(Y|X = x', Z = z)$.

□

Proposition 4.3 *Under Assumption 4.2, $y_{x'}$ is identified as the τ^*-th quantile of $\mathbb{P}(Y|X = x', Z = z)$, where τ^* is the quantile of y in the distribution of $\mathbb{P}(Y|X = x, Z = z)$.*

Proof of Proposition 4.3. For the individual with observation $(X = x, Z = z, Y = y)$, we denote $(y_x, y_{x'})$ as the true values of $(Y_x, Y_{x'})$. Assumption 4.2 implies that for this individual, its rankings of y_x and $y_{x'}$ are the same in the distributions of $\mathbb{P}(Y_x|Z = z)$ and $\mathbb{P}(Y_{x'}|Z = z)$, respectively. Therefore,

$$\mathbb{P}(Y_x \le y_x|Z = z) = \mathbb{P}(Y_{x'} \le y_{x'}|Z = z). \tag{3}$$

Since $y_x = y$ is observed and the distributions $\mathbb{P}(Y_x|Z = z)$ and $\mathbb{P}(Y_{x'}|Z = z)$ can be identified as $\mathbb{P}(Y|X = x, Z = z)$ and $\mathbb{P}(Y|X = x', Z = z)$, respectively, by the backdoor criterion (i.e., $(Y_x, Y_{x'}) \perp\!\!\!\perp X|Z)$, we can identify the quantile of y_x in the distribution of $\mathbb{P}(Y|X = x, Z = z)$, denoted by τ^*. Then

$$\mathbb{P}(Y_{x'} \le y_{x'}|Z = z) = \tau^*,$$

which yields that θ is identified as the τ^*-quantile of $\mathbb{P}(Y|X = x', Z = z)$.

□

The following Proposition 4.4* serves as a complement to Proposition 4.4.

Proposition 4.4* Under Assumption 3.1, or more generally, if U_x is a strictly monotone increasing function of $U_{x'}$, Assumption 4.2 is equivalent to Assumption 3.2.

Proof of Proposition 4.4. According to the model (1), we can equivalently write

$$Y_x = f_Y(x, z, U_x),\ Y_{x'} = f_Y(x', z, U_{x'}).$$

Suppose that U_x is a strictly monotone increasing function of $U_{x'}$ (Assumption 3.1, i.e., $U_x = U_{x'}$, is a special case of it). Under this condition, we next prove sufficiency and necessity, respectively.

First, we show that Assumption 3.2 implies Assumption 4.2. If Assumption 3.2 holds, then Y_x is a strictly monotonic function of U_x, and $Y_{x'}$ is a strictly monotonic function of $U_{x'}$. Since U_x is a strictly monotone increasing function of $U_{x'}$, then Y_x is a strictly increasing monotonic function of $Y_{x'}$, which leads to Assumption 4.2.

Second, we show that Assumption 4.2 implies Assumption 3.2. If Assumption 4.2 holds, then given $Z = z$, Y_x is a strictly increasing function of $Y_{x'}$. When U_x is a strictly monotone increasing function of $U_{x'}$ and note that

$$Y_x = f_Y(x, z, U_X),\ Y_{x'} = f_Y(x', z, U_X),$$

which implies that f_Y is a strictly monotonic function of U_X, i.e., Assumption 3.2 holds.

This finishes the proof.

□

Proposition 4.7 *Under Assumption 4.6, the conclusion in Proposition 4.3 also holds.*

Proof of Proposition 4.7. This can be shown through a proof analogous to that of Proposition 4.3.

□

B Proofs in Section 5

Recall that $l_\tau(\xi) = \tau\xi \cdot \mathbb{I}(\xi \geq 0) + (\tau - 1)\xi \cdot \mathbb{I}(\xi < 0)$, and

$$\begin{aligned}
q(x, z; \tau) &\triangleq \inf_y \{y : \mathbb{P}(Y \leq y | X = x, Z = z) \geq \tau\} \\
q_0(z; \tau) &\triangleq \inf_y \{y : \mathbb{P}(Y_0 \leq y | Z = z) \geq \tau\} \\
q_1(z; \tau) &\triangleq \inf_y \{y : \mathbb{P}(Y_1 \leq y | Z = z) \geq \tau\}.
\end{aligned}$$

Lemma 5.1 We have that

(i) $q_x(Z; \tau) = \arg\min_f \mathbb{E}[l_\tau(Y_x - f(Z))]$ *for any given* x*;*

(ii) $q(X, Z; \tau) = \arg\min_f \mathbb{E}[l_\tau(Y - f(X, Z))]$.

Proof of Lemma 5.1. We prove $q_x(Z; \tau) = \arg\min_f \mathbb{E}[l_\tau(Y_x - f(Z))]$, and $q(X, Z; \tau) = \arg\min_f \mathbb{E}[l_\tau(Y - f(X, Z))]$ can be derived by an exactly similar manner. We write

$$\mathbb{E}[l_\tau(Y_x - f(Z))] = \mathbb{E}[\mathbb{E}\{l_\tau(Y_x - f(Z)) \mid Z\}].$$

To obtain the conclusion, note that $l_\tau(Y_x - f(Z))$ is always positive, it suffices to show that

$$q_x(z; \tau) = \arg\min_f \mathbb{E}[l_\tau(Y_x - f(Z)) \mid Z = z] \tag{4}$$

for any given $Z = z$. Next, we focus on analyzing the term $\mathbb{E}[l_\tau(Y_x - f(Z)) \mid Z = z]$. Given $Z = z$, $f(Z)$ is a constant and we denote it by c, then

$$\begin{aligned}
&\mathbb{E}[l_\tau(Y_x - f(Z)) \mid Z = z] \\
&= \mathbb{E}[l_\tau(Y_x - c) \mid Z = z] \\
&= \mathbb{E}\Big[\tau(Y_x - c)\mathbb{I}(Y_x \geq c) + (\tau - 1)(Y_x - c)\mathbb{I}(Y_x < c) \mid Z = z\Big] \\
&= \tau \int_c^\infty (y_x - c) g(y_x|z) dy_x + (\tau - 1) \int_{-\infty}^c (y_x - c) g(y_x|z) dy_x,
\end{aligned}$$

where $g(y_x|z)$ denotes the probability density function of Y_x given $Z = z$.

Since the check function is a convex function, differentiating $\mathbb{E}[l_\tau(Y_x - c) \mid Z = z]$ with respect to c and setting the derivative to zero will yield the solution for the minimum

$$\begin{aligned}
&\frac{\partial}{\partial c}\mathbb{E}[l_\tau(Y_x - c) \mid Z = z] \\
&= \tau \int_c^\infty \frac{\partial}{\partial c}[(y_x - c)g(y_x|z)]dy_x + (\tau - 1)\int_{-\infty}^c \frac{\partial}{\partial c}[(y_x - c)g(y_x|z)]dy_x \\
&= -\tau\Big(1 - \int_{-\infty}^c g(y_x|z)dy_x\Big) + (1-\tau)\int_{-\infty}^c g(y_x|z)dy_x.
\end{aligned}$$

Then let $\frac{\partial}{\partial c}\mathbb{E}[l_\tau(Y_x - c) \mid Z = z] = 0$ leads to that

$$\int_{-\infty}^c g(y_x|z)dy_x = \tau,$$

that is, $c = q_x(z;\tau)$. This completes the proof of Proposition 5.1.

□

Theorem 5.2 (Validity of the Proposed Ideal Loss). *The loss $R_{x'}(t; x, z, y)$ is minimized uniquely at t^*, where t^* is the solution satisfying*

$$\mathbb{P}(Y_{x'} \le t^*|Z = z) = \mathbb{P}(Y_x \le y|Z = z).$$

Proof of Theorem 5.2. Recall that

$$R_{x'}(t|x,z,y) = \mathbb{E}\left[|Y_{x'} - t| \;\Big|\; Z = z\right] + \mathbb{E}\left[\text{sign}(Y_x - y) \;\Big|\; Z = z\right] \cdot t.$$

Let $g(y_x|z)$ be the probability density function of Y_x given $Z = z$. By calculation,

$$\mathbb{E}\left[|Y_{x'} - t| \;\Big|\; Z = z\right] = \int_t^\infty (y_{x'} - t)g(y_{x'}|z)dy_{x'} + \int_{-\infty}^t (t - y_{x'})g(y_{x'}|z)dy_{x'},$$

$$\frac{\partial}{\partial t}\mathbb{E}\left[|Y_{x'} - t| \;\Big|\; Z = z\right] = -\Big(1 - \int_{-\infty}^t g(y_{x'}|z)dy_{x'}\Big) + \int_{-\infty}^t g(y_{x'}|z)dy_{x'} = 2\mathbb{P}(Y_{x'} \le t|Z = z) - 1,$$

and

$$\mathbb{E}\left[\text{sign}(Y_x - y) \;\Big|\; Z = z\right] = \mathbb{E}\left[-2\mathbb{I}(Y_x \le y) + 1 \;\Big|\; Z = z\right] = -2\mathbb{P}(Y_x \le y|Z = z) + 1,$$

we have

$$\begin{aligned}
\frac{\partial}{\partial t}R_{x'}(t|x,z,y) &= 2\mathbb{P}(Y_{x'} \le t|Z = z) - 1 + \mathbb{E}\left[\text{sign}(Y - y) \;\Big|\; Z = z\right] \\
&= 2\mathbb{P}(Y_{x'} \le t|Z = z) - 1 - 2\mathbb{P}(Y_x \le y|Z = z) + 1 \\
&= 2\Big\{\mathbb{P}(Y_{x'} \le t|z) - \mathbb{P}(Y_x \le y|z)\Big\}.
\end{aligned}$$

Since

$$\frac{\partial^2}{\partial t^2}R_{x'}(t|x,z,y) = 2\partial\mathbb{P}(Y_{x'} \le t|z)/\partial t = 2g(y_{x'} = t|z) \ge 0,$$

$R_{x'}(t|x,z,y)$ is a convex function with respect to t. Letting $\frac{\partial}{\partial t}R_{x'}(t|x,z,y) = 0$ yields that

$$\mathbb{P}(Y_{x'} \le t|z) - \mathbb{P}(Y_x \le y|z) = 0.$$

That is, $R_{x'}(t|x,z,y)$ attains its minimum at $t = q_{x'}(z;\tau^*)$, where τ^* is the quantile of y in the distribution $\mathbb{P}(Y_x|Z = z)$.

□

Proposition 5.3. *If $h \to 0$ as $N \to \infty$, $\hat{p}_x(z)$ and $\hat{p}_{x'}(z)$ are consistent estimates of $p_x(z)$ and $p_{x'}(z)$, and the density function of Z is differentiable, then*

$$\hat{R}_{x'}(t; x, z, y) \xrightarrow{\mathbb{P}} R_{x'}(t; x, z, y),$$

where $\xrightarrow{\mathbb{P}}$ means convergence in probability.

Proof of Proposition 5.3. For analyzing the theoretical properties of $\hat{R}_{x'}(t; x, z, y)$, we rewritten $\hat{R}_{x'}(t; x, z, y)$ as

$$\hat{R}_{x'}(t; x, z, y) = \frac{\sum_{k=1}^{N} K_h(Z_k - z) \frac{\mathbb{I}(X_k = x')}{\hat{p}_{x'}(Z_k)} |Y_k - t|}{\sum_{k=1}^{N} K_h(Z_k - z)} + \frac{\sum_{k=1}^{N} K_h(Z_k - z) \frac{\mathbb{I}(X_k = x)}{\hat{p}_x(Z_k)} \cdot \text{sign}(Y_k - y)}{\sum_{i=1}^{N} K_h(Z_k - z)} \cdot t,$$

where the capital letters denote random variables and lowercase letters denote their realizations. This is slightly different from that used in the main text.

When $\hat{p}_x(z)$ and $\hat{p}_{x'}(z)$ are consistent estimates of $p_x(z)$ and $p_{x'}(z)$, to show the conclusion, it is sufficient to prove that

$$\frac{\sum_{k=1}^{N} K_h(Z_k - z) \frac{\mathbb{I}(X_k = x')}{p_{x'}(Z_k)} |Y_k - t|}{\sum_{k=1}^{N} K_h(Z_k - z)} \xrightarrow{\mathbb{P}} \mathbb{E}\left[\frac{\mathbb{I}(X = x')}{p_{x'}(z)} |Y - t| \,\Big|\, Z = z \right] = \mathbb{E}\left[|Y_{x'} - t| \,\Big|\, Z = z \right], \tag{5}$$

$$\frac{\sum_{k=1}^{N} K_h(Z_k - z) \frac{\mathbb{I}(X_k = x)}{p_x(Z_k)} \cdot \text{sign}(Y_k - y)}{\sum_{i=1}^{N} K_h(Z_k - z)} \xrightarrow{\mathbb{P}} \mathbb{E}\left[\frac{\mathbb{I}(X = x)}{p_x(z)} \cdot \text{sign}(Y - y) \,\Big|\, Z = z \right] = \mathbb{E}\left[\text{sign}(Y_x - y) \,\Big|\, Z = z \right]. \tag{6}$$

We prove equation (5) only, as equation (6) can be addressed similarly.

Note that

$$\frac{\sum_{k=1}^{N} K_h(Z_k - z) \frac{\mathbb{I}(X_k = x')}{p_{x'}(Z_k)} |Y_k - t|}{\sum_{k=1}^{N} K_h(Z_k - z)} = \frac{\frac{1}{N} \sum_{k=1}^{N} K_h(Z_k - z) \frac{\mathbb{I}(X_k = x')}{p_{x'}(Z_k)} |Y_k - t|}{\frac{1}{N} \sum_{k=1}^{N} K_h(Z_k - z)},$$

we analyze the denominator and numerator on the right side of the equation separately. For the denominator, it is an average of N independent random variables and converges to its expectation $\mathbb{E}[K_h(Z_k - z)]$ almost surely. Let $g(z_k)$ be the probability density function of Z_k, and $g^{(1)}(z_k)$ is its first derivative. Since

$$\begin{aligned}
\mathbb{E}[K_h(Z_k - z)] &= \int \frac{1}{h} K(\frac{z_k - z}{h}) g(z_k) dz_k \\
&= \int K(u) g(z + hu) du \qquad (\text{let } z_k = z + hu) \\
&= \int K(u) \cdot \{g(z) + g^{(1)}(z) hu + o(h)\} du \qquad (\text{by Taylor Expansion}) \\
&= g(z) \int K(u) du + g^{(1)}(z) h \int K(u) u du + o(h) \\
&= g(z) + o(h) \qquad (\text{by the definition of kernel function}),
\end{aligned} \tag{7}$$

when $h \to 0$ as $N \to \infty$, the denominator converges to $g(z)$ in probability.

Next, we focus on dealing with the numerator, which also converges to its expectation.

$$\begin{aligned}
&\mathbb{E}[K_h(Z_k - z) \frac{\mathbb{I}(X_k = x')}{p_{x'}(Z_k)} |Y_k - t|] \\
= &\mathbb{E}\Big[K_h(Z_k - z) \mathbb{E}\Big\{ \frac{\mathbb{I}(X_k = x')}{p_{x'}(Z_k)} |Y_k - t| \Big| Z_k \Big\} \Big] \qquad (\text{by the law of iterated expectations}) \\
= &\mathbb{E}\Big[K_h(Z_k - z) \mathbb{E}\Big\{ \frac{\mathbb{I}(X_k = x')}{p_{x'}(Z_k)} |Y_{x',k} - t| \Big| Z_k \Big\} \Big] \qquad (\text{write } Y_k \text{ as the form of potential outcome}) \\
= &\mathbb{E}\Big[K_h(Z_k - z) \mathbb{E}\Big\{ |Y_{x',k} - t| \Big| Z_k \Big\} \Big] \qquad (\text{by backdoor criterion } Y_{x',k} \perp\!\!\!\perp X_k | Z_k).
\end{aligned} \tag{8}$$

Define $m(Z) = \mathbb{E}[|Y_{x'} - t| \big| Z]$ and $m^{(1)}(Z)$ is its first derivative, then the right side of equation (5) is $m(z)$, and

$$\mathbb{E}\Big[K_h(Z_k - z) \cdot \mathbb{E}\Big\{|Y_{x',k} - t|\Big|Z_k\Big\}\Big] = \mathbb{E}\Big[K_h(Z_k - z) \cdot m(Z_k)\Big]$$
$$= \int \frac{1}{h}K(\frac{z_k - z}{h}) \cdot m(z_k) \cdot g(z_k)dz_k$$
$$= \int K(u) \cdot m(z + hu) \cdot g(z + hu)du \qquad \text{(let } z_k = z + hu\text{)}$$
$$= \int K(u) \cdot \{m(z) + m^{(1)}(z)hu + o(h)\} \cdot \{g(z) + g^{(1)}(z)hu + o(h)\}du \qquad \text{(by Taylor Expansion)}$$
$$= m(z)g(z) + o(h). \tag{9}$$

Thus, when $h \to 0$ as $N \to \infty$, the numerator converges to $g(z)$ in probability.

Combining equations (7), (8), and (9) yields the equality (5). This completes the proof.

□

C Extension to Continuous Outcome

When the treatment is continuous, we can estimate the ideal loss with the following estimator

$$\tilde{R}_{x'}(t|x, z, y) = \frac{\sum_{k=1}^{N} K_h(z_k - z)\frac{K_h(x_k - x')}{p_{x'}(z_k)}|y_k - t|}{\sum_{k=1}^{N} K_h(z_k - z)} + \frac{\sum_{k=1}^{N} K_h(z_k - z)\frac{K_h(x_k - x)}{p_x(z_k)} \cdot \text{sign}(y_k - y)}{\sum_{k=1}^{N} K_h(z_k - z)} \cdot t,$$

which is a smoothed version of the estimator

$$\hat{R}_{x'}(t|x,z,y) = \frac{\sum_{k=1}^{N} K_h(z_k - z)\frac{\mathbb{I}(x_k = x')}{p_{x'}(z_k)}|y_k - t|}{\sum_{k=1}^{N} K_h(z_k - z)} + \frac{\sum_{k=1}^{N} K_h(z_k - z)\frac{\mathbb{I}(x_k = x)}{p_x(z_k)} \cdot \text{sign}(y_k - y)}{\sum_{k=1}^{N} K_h(z_k - z)} \cdot t,$$

defined in Section 5. In addition, by a proof similar to that of Proposition 5.3, we also can show that $\tilde{R}_{x'}(t; x, z, y) \xrightarrow{\mathbb{P}} R_{x'}(t; x, z, y)$.