Higher-Order Orthogonal Causal Learning for Treatment Effect

Yiyan Huang 1 Cheuk Hang Leung *1 Xing Yan 2 Qi Wu 1

Abstract
Most existing studies on the double/debiased machine learning method concentrate on the causal parameter estimation recovering from the first-order orthogonal score function. In this paper, we will construct the $k^{th}$-order orthogonal score function for estimating the average treatment effect (ATE) and present an algorithm that enables us to obtain the debiased estimator recovered from the score function. Such a higher-order orthogonal estimator is more robust to the misspecification of the propensity score than the first-order one does. Besides, it has the merit of being applicable with many machine learning methodologies such as Lasso, Random Forests, Neural Nets, etc. We also undergo comprehensive experiments to test the power of the estimator we construct from the score function using both the simulated datasets and the real datasets.

1. Introduction
The estimation of the treatment effects from the observational data is essential in causal learning. Traditional methods of estimating the treatment effects include, for instance, the regression adjustment and the inverse probability weighting (IPW). The regression adjustment that focuses on the estimation of features-outcome relation ignores the probabilistic impact of the features-treatment relation, and hence is easy to lead a biased estimation of the treatment effects once the relation is not well inferred. The covariate balancing method IPW infers the features-treatment relation with the inverse propensity score as the weight to make a synthetic randomized controlled trial, but it omits the features-outcome relation when estimating the treatment effects. Heuristically, such estimators are unbiased when either the features-outcome relation or the features-treatment relation is estimated well, but not necessarily both in general.

Since the appearance of DML, researchers apply the estimators in different fields. Examples include the use of the DML estimators when the data is of panel type in Semenova et al. (2018), and the study of the action-response effects under the credit risk context in Huang et al. (2020). Besides, researchers elaborate and investigate the DML estimators theoretically. For example, Tibshirani et al. (2016), Berk et al. (2013), and the references therein investigate the post-selection inference. Some researches focus on the confidence intervals of the causal parameters (see, for instance, Zhang & Zhang (2014), Van de Geer et al. (2014), and the references therein). Besides, authors in Oprescu et al. (2019) combine the DML estimators with the generalized random forest given in Athey et al. (2019) to estimate the heterogeneous effect (or the conditional treatment effect (CATE)). Finally, authors in Shi et al. (2019) adapt the neural networks to estimate the average treatment effect. They improve the network architecture proposed by Shalit et al. (2017) and introduce a novel loss using the DML estimators.

In the literature, most studies on DML focus on the first-order orthogonal score functions. Naturally, it is reasonable to extend from the first-order orthogonal condition to the higher-order one, and investigate the advantages of consulting the higher-order one. Mackey et al. (2018) apply the theories of the higher-order orthogonal condition with an example of constructing a score function satisfying the second-order orthogonal condition for estimating the causal parameters under the partially linear model. However, the constructions of any-order orthogonal score functions for the treatment effects under the fully non-linear model are missing, which is our goal of this paper.

The rest of the paper is organized as follows. Section 2 gives the mathematical background, including the notational
conventions and the model for the upcoming investigations. In Section 3, we introduce the basic concepts related to the conditions a score function should satisfy. In Section 4, we summarize the main results of our paper: the score function and the estimator we construct. In Section 5, we undergo comprehensive experiments using the simulated datasets and the benchmark real datasets.

1.1. Contributions

The contributions of our paper are four-fold:

1. We consider a fully non-linear model with multiple treatments. More importantly, we are the first to propose a higher-order orthogonal score function in a fully non-linear model and use it to recover an estimator for the average treatment effect (ATE) estimation.

2. We present an algorithm to construct the higher-order estimator from the observational data using the established score function which satisfies the $k^{th}$-order orthogonal condition, where the value of $k$ is an arbitrary integer. Such an algorithm can also be used to recover the higher-order estimator of other prevalent treatment effects. Besides, our higher-order estimator has proved unbiased and consistent.

3. Our higher-order orthogonal estimator can correct the error of the regression adjustment method, and is less sensitive to the propensity score estimation than DML method.

4. Our higher-order orthogonal estimator can work with any statistical ML methods that are used for training the nuisance parameters. We test the power of our estimator in comprehensive experiments, combined with many ML methods such as Lasso, Random Forests, Multi-layer Perception, and the neural nets for causal learning such as TARNET (Shalit et al. (2017)) and Dragonnet (Shi et al. (2019)).

2. Background

If we want the estimated causal parameter to be insensitive to the nuisance parameters, the constructed score function should not only satisfy the moment condition, but also satisfy the first-order orthogonal condition or even higher-order orthogonal condition (see Chernozhukov et al. (2018) and Mackey et al. (2018)). In this section, we present the notations and the related mathematical backgrounds for the discussions in the upcoming sections.

2.1. Notational Conventions

For any two random variables $\mathcal{X}$ and $\mathcal{Y}$, we would use $\mathcal{X} \perp \perp \mathcal{Y}$ to represent that $\mathcal{X}$ and $\mathcal{Y}$ are independent of each other. If $\mathcal{X}$ and $\mathcal{Y}$ have the same distribution, then we denote the relation as $\mathcal{X} \overset{d}{=} \mathcal{Y}$. The variable $Y$ is the response variable. $D$ is the intervention/treatment variable which takes $d$ different treatments, namely $\{d^1, \ldots, d^n\}$. $Z$ is the confounders/covariates which affect $Y$ and $D$ simultaneously. $W$ is the random vector such that it equals $(Y, D, Z)$. We assume that $g$ and $m$ are $\mathbb{P}$-integrable functions and $\mathbb{E}[\cdot]$ represents the expectation over a probability space $(\Omega, \mathcal{F}, \mathbb{P})$. $\xi$ and $\nu$ are the noise terms. Finally, we denote the causal parameter as $\theta$, while the authentic causal parameter is represented as $\theta_0$, and they lie in a convex set $\Theta$. The nuisance parameters are denoted as $\rho$, while the authentic nuisance parameters are represented as $\rho$, and they lie in a convex set $\mathcal{F}$. $\psi$ is the score function which maps $(W, \vartheta, \varrho)$ to $\mathbb{R}$.

2.2. Related Works

When studying the treatment effects under the unconfoundedness assumption of Rosenbaum & Rubin (1983), we usually consider the random vector $(Y, D, Z)$ satisfying

\[
\begin{align*}
Y &= g(D, Z) + \xi, \quad \mathbb{E}[\xi | D, Z] = 0 \quad a.s., \\
D &= m(Z) + \nu, \quad \mathbb{E}[\nu | Z] = 0 \quad a.s.,
\end{align*}
\]

where $\xi \perp \perp \nu$, $\nu \perp \perp Z$, and $\xi \perp \perp (D, Z)$. According to Chernozhukov et al. (2018), since the classical estimator is derived from the score function that only satisfies the moment condition but violates the orthogonal condition, the perturbation of the nuisance parameters will easily bring the biasedness to the causal parameter estimation. We should construct the score function which satisfies both the moment condition and the orthogonal condition such that the recovered estimator is unbiased and consistent. In this paper, we concentrate on the discussion of the ATE-related quantity $\theta^i$ such that

\[
\theta^i := \mathbb{E}[g(d^i, Z)].
\]

The discussion of another prevalent treatment effect, the average treatment effect on the treated (ATTE), is similar and hence is omitted due to the limitation of pages.

Initially, Chernozhukov et al. (2018) propose an orthogonal score function for binary treatment effect estimation. Huang et al. (2020) extend the orthogonal score function to estimate the quantity $\theta^i$ for multiple treatments in credit lending business based on the model (1a) and (1b). The score function $\psi^i(W, \vartheta, \varrho)$ which can be used to estimate $\theta^i$ is

\[
\vartheta - g(d^i, Z) - \frac{1_{\{D=d^i\}}}{\alpha_i(Z)}(Y - g(d^i, Z)),
\]

where $g(d^i, Z)$ and $\alpha_i(Z)$ are the nuisance parameters, and $g(d^i, Z)$ and $\pi^i(Z)$ are the authentic ones. Note that $\pi^i(Z) = \mathbb{E}[1_{\{D=d^i\}} | Z]$ is also called the propensity score. Then one can recover an estimator of $\theta^i$ from Equa-


\[ 
\frac{1}{N} \sum_{m=1}^{N} \hat{g}(d^{i}, Z_{m}) + \frac{1}{N} \sum_{m=1}^{N} \frac{1_{\{D_{m}=d^{i}\}} (Y_{m} - \hat{g}(d^{i}, Z_{m}))}{\pi^{i}(Z_{m})}, 
\]

where \( N \) is the number of individuals in an observational dataset and \( (Y_{m}, D_{m}, Z_{m}) \) is the vector of the \( m \)th individual in the observational dataset, and \( \hat{g}(d^{i}, \cdot) \) and \( \pi^{i}(\cdot) \) are the estimated functions of \( g(d^{i}, \cdot) \) and \( \pi(\cdot) \) respectively. It has been proven that this estimator satisfies both the moment condition and the orthogonal condition of the first order only. Our aim in this paper is to develop an estimator of \( \theta^{i} \) satisfying the higher-order orthogonal condition.

2.3. Model Setup

Instead of considering Equation (1a) and Equation (1b), we consider a more general model setting. To start with, we first consider Equation (1b). Since \( D = \sum_{i=1}^{n} d^{i} 1_{\{D=d^{i}\}} \) and 
\[ m(Z) = \sum_{i=1}^{n} d^{i} \pi^{i}(Z), \]
we can replace Equation (1b) with

\[ 1_{\{D=d^{i}\}} = \pi^{i}(Z) + \nu^{i}, \]

where \( \mathbb{E} [\nu^{i} | Z] = 0 \) for all \( i \in \{1, \cdots, n\} \). On the other hand, Equation (1a) describes the relation between the response variable \( Y \) and the features \( Z \) when \( D \) takes different intervention assignments. Similarly, we can therefore replace Equation (1a) with

\[ Y^{i} = g(d^{i}, Z) + \xi^{i}, \quad i \in \{1, \cdots, n\}, \]

where \( \mathbb{E} [\xi^{i} | Z] = 0 \). Here \( Y^{i} \) is the outcome variable under the treatment \( d^{i} \).

In reality, we can characterize an individual based on its factual treatment. The set \( D_{i} \) contains all the individuals whose factual treatment is \( d^{i} \), while the set \( \bar{D}_{i} \) contains all the individuals whose factual treatment is not \( d^{i} \). Hence, if an individual comes from \( D_{i} \), Equation (6) can be recast as

\[ Y^{i:F} = g(d^{i}, Z) + \xi^{i:F}, \quad \mathbb{E} [\xi^{i:F} | Z] = 0, \]

while if an individual comes from \( \bar{D}_{i} \), Equation (6) can be recast as

\[ Y^{i:CF} = g(d^{i}, Z) + \xi^{i:CF}, \quad \mathbb{E} [\xi^{i:CF} | Z] = 0. \]

Similar to the assumptions about the noise terms in Chernozhukov et al. (2018), we impose some assumptions about \( \xi^{i:F}, \xi^{i:CF}, \) and \( \nu^{i} \) such that \( \xi^{i:F} \overset{d}{=} \xi^{i:CF}, \xi^{i:F} \perp \perp Z, \xi^{i:CF} \perp \perp Z, \) and \( \nu \perp \perp Z \). Moreover, for arbitrary two intervention indices \( i \neq j \), any two of \( \nu^{i}, \nu^{j}, \xi^{i:F}, \xi^{j:F}, \xi^{i:CF}, \) and \( \xi^{j:CF} \) are independent of each other. Besides, we assume that all feature vectors are drawn independently and identically from the underlying distribution of \( Z \).

3. Moment Condition and Higher-Order Orthogonal Condition

In this section, we present the definitions of the two conditions which guide us to design score functions and recover estimators for the causal parameters. To start with, the score function we construct should satisfy the moment condition, which is defined in the following Definition 1.

**Definition 1 (Moment Condition).** Suppose the causal parameter \( \vartheta \) and the authentic causal parameter \( \theta \) lie in a convex set \( \Theta \) while the nuisance parameters \( g \) and the authentic nuisance parameters \( \rho \) lie in a convex set \( \mathcal{F} \). We say that a score function \( \psi(W, \vartheta, g) \) satisfies the moment condition if

\[ \mathbb{E} [\psi(W, \vartheta, g)] |_{\vartheta=\theta, g=\rho} = 0. \]

Mathematically, the moment condition guarantees that the estimator recovered from the score function is unbiased if the nuisance parameters equal the authentic ones. However, the estimator can still be biased if some nuisance parameters are misspecified, e.g., the estimator can be regularization biased if the misspecification is caused by the regularization term (see Chernozhukov et al. (2018)). To remove the bias due to the misspecification of some nuisance parameters, one can recover the estimator from the score function satisfying the (higher-order) orthogonal condition, which is defined in the following Definition 2.

**Definition 2 (Higher-Order Orthogonal Condition).** Suppose the causal parameter \( \vartheta \) and the authentic causal parameter \( \theta \) are in the convex set \( \Theta \). Furthermore, suppose that the nuisance parameters \( g \) and the authentic nuisance parameters \( \rho \) are \( \gamma \)-tuples such that

\[ g = (h_{1}, \cdots, h_{\gamma}) \text{ and } \rho = (h_{1}, \cdots, h_{\gamma}). \]

Let \( \alpha = (\alpha_{1}, \cdots, \alpha_{\gamma}) \) such that each entry is a non-negative integer. The \( \alpha \)-differential of a score function \( \psi(W, \vartheta, g) \) w.r.t. the nuisance parameters, denoted as \( D^{\alpha} \psi(W, \vartheta, g) \), is defined as

\[ D^{\alpha} \psi(W, \vartheta, g) = \partial_{\alpha_{1}} \partial_{\alpha_{2}} \cdots \partial_{\alpha_{\gamma}} \psi(W, \vartheta, g) = \partial_{\alpha_{1}} \partial_{\alpha_{2}} \cdots \partial_{\alpha_{\gamma}} \psi(W, \vartheta, h_{1}, \cdots, h_{\gamma}). \]

Furthermore, the score function \( \psi(W, \vartheta, g) \) is said to be \( S \)-orthogonal w.r.t. \( (h_{1}, \cdots, h_{\gamma}) \) for some set \( S \subseteq \mathbb{N}^{\gamma} \) if for any \( \alpha \in S \), we have

\[ \mathbb{E} [D^{\alpha} \psi(W, \vartheta, g)] |_{\vartheta=\theta, g=\rho} | Z | = 0. \]

We demonstrate the meaning of \( D^{\alpha} \psi(W, \vartheta, g) \) by taking the score function in Equation (3) as an example. Before the demonstration, we define several symbols for notational simplicity which are used in the sequel. They are

\[ g'(\cdot) := g(d^{i}, \cdot), \quad g^{i}(\cdot) := g(d^{i}, \cdot). \]
Now, the nuisance parameters in Equation (3) can be rewritten as $g = (\theta_1, \theta_2) = (g^i, a_i)$ for notational simplicity. Suppose $\alpha = (1, 1)$, then $D^\alpha \psi(W, \vartheta, g)$ is the first partial derivative of $\psi(W, \vartheta, g)$ w.r.t. $g^i$ and $a_i$ such that

$$D^\alpha \psi(W, \vartheta, g) = \partial_\vartheta \partial_{g^i} \psi(W, \vartheta, g) = \partial_\vartheta \partial_{a_i} \psi(W, \vartheta, \theta_1, \theta_2) = \partial_\vartheta \{ \vartheta - g^i - \frac{1}{a_i}(Y - g^i) \} = \partial_\vartheta \{ \frac{1}{a_i}(Y - g^i) \} = \frac{1}{a_i^2} a_i$$

Furthermore, if the set $S$ equals $\{ \alpha \in \mathbb{N}^7 \mid \| \alpha \|_1 \leq k \}$ and Equation (11) holds for all $\alpha \in S$, then we say that the score function $\psi(W, \vartheta, g)$ satisfies the $k^{th}$-order orthogonal condition. When the set $S = \{ \alpha \in \mathbb{N}^7 \mid \| \alpha \|_1 \leq 1 \}$, we have the (first-order) orthogonal condition which is given in Chernozhukov et al. (2018).

Intuitively, Definition 2 states that the expectations of the Gateaux derivatives of the score function w.r.t. the nuisance parameters are zero, implying that the score function is insensitive to the estimation of the nuisance parameters. Indeed, any estimators which are constructed from the orthogonal score functions are regularization unbiased (see Chernozhukov et al. 2018), Mackey et al. (2018), and Neyman (1979) for more details. Now we are ready to present the methodology of constructing a score function such that its $k^{th}$-order orthogonality and one can recover an estimator of $\theta^i$ from the score function. The main result is summarized in the following Theorem 1. Moreover, we also present an algorithm which allows us to obtain the estimator when given the data set in the upcoming section.

### 4. Theoretical Results

In this section, we are going to present the theoretical results and the algorithm of this paper. First of all, an iterative approach is used to construct a score function satisfying the higher-order orthogonal condition as summarized in Theorem 1. Then we use the score function to recover an estimator as summarized in Corollary 2. At last, we describe an algorithm to construct such an estimator given the observational dataset.

**Theorem 1.** We are given the positive integers $r$ and $k$ such that $2 \leq k \leq r$, and furthermore, we assume that $\mathbb{E}[(\nu^i)^q]$ are finite for $1 \leq q \leq r$ and $\mathbb{E}[(\nu^i)^{r+1}] \neq 0$. Suppose the nuisance parameters $\vartheta$ and the authentic nuisance parameters $\rho$ are tuples of $(g^i(\cdot), a_i(\cdot))$ and $(g^i(\cdot), \pi^i(\cdot))$ respectively, then the score function $\psi^i(W, \vartheta, g)$ we construct in the following satisfies the $k^{th}$ orthogonal condition:

$$\vartheta - g^i(Z) - (Y^i - g^i(Z))A(D, Z; a_i), \quad \text{for} \quad i = 1, \ldots, k$$

where

$$A(D, Z; a_i) = \hat{b}_r \left[ (1_{D=d^i} - a_i(Z))^r \right] + \sum_{q=1}^{k-1} b_q \left[ (1_{D=d^i} - a_i(Z))^{q+1} - \mathbb{E}[(\nu^i)^q] \right]. \quad (13)$$

The coefficient $\hat{b}_r = \frac{1}{\mathbb{E}[(\nu^i)^r]}$. Meanwhile, the coefficients $b_q$ in the sum in Equation (13) are computed in the descending order, i.e., we start with computing $b_{k-1}$, followed by computing $b_{k-2}, b_{k-3}, \ldots$, until we compute all the coefficients. For each $q \in \{1, \ldots, k \}$, $b_q$ is computed as follows:

$$b_q = -\sum_{u=1}^{k-1-q} b_{q+u} \left( \frac{q + u}{q} \right) \mathbb{E}[(\nu^i)^u] - \hat{b}_r \left( \frac{r}{q} \right) \mathbb{E}[(\nu^i)^{r-q}]. \quad (14)$$

It is not difficult to see that, when $k = r - 1$ or $k = r$, we have the same score functions. For example, when $(r, k) = (3, 2)$ or $(r, k) = (3, 3)$, the score functions are the same. Besides, from Equation (13), we know that the score function which is used to recover the estimation of the causal parameter $\theta^i$ requires the knowledge of the terms $\mathbb{E}[(\nu^i)^q]$ for all $q \in \{1, \ldots, k \}$. In this paper, we infer $\mathbb{E}[(\nu^i)^q]$ from the estimated function $\hat{\pi}^i$ and do not treat these terms as nuisance parameters.

It is not difficult to prove that the score function in Theorem 1 satisfies the moment condition. Moreover, the $k^{th}$ orthogonal condition is also satisfied, which can be proven too. We leave the proof in the supplementary. Using this score function, our recovered estimator for the causal parameter is given in Corollary 2. In addition, under the mild assumptions on the estimation of the nuisance parameters, Chernozhukov et al. (2018) and Mackey et al. (2018) show that their recovered estimators for the causal parameter are consistent. Following the same assumptions and procedure, we can show that our recovered estimator is consistent too.

**Corollary 2.** Suppose the observational dataset can be divided into the sets $\mathcal{I}'$ and $\mathcal{I}$ such that $\mathcal{I} \cap \mathcal{I}' = \emptyset$. Let $\hat{\pi}^i(\cdot)$ and $\hat{g}^i(\cdot)$ be the trained functions of $\pi^i(\cdot)$ and $g^i(\cdot)$ respectively using the observations in $\mathcal{I}'$. If $N$ represents the size of $\mathcal{I}$, then the estimator $\hat{\theta}_N^i$ of $\theta^i$ using the score function in Theorem 1 is

$$\frac{1}{N} \sum_{m \in \mathcal{I}} \hat{g}^i(Z_m) \quad (15a)$$

$$+ \frac{1}{N} \sum_{m \in \mathcal{I}} (Y_m^i - \hat{g}^i(Z_m))A(D_m, Z_m; \hat{\pi}^i), \quad (15b)$$

where the definition of the quantity $A(\cdot, \cdot; \cdot)$ can be found in (12) and (13). And under mild conditions on the estimated functions $\hat{\pi}^i(\cdot)$ and $\hat{g}^i(\cdot)$, the estimator $\hat{\theta}_N^i$ is consistent.
Let’s investigate the term given in (15b). The quantity which is given in (15b) can be decomposed into the sum of two quantities, which are

\[
\frac{1}{N} \sum_{m \in R \cap I} (Y_m^{i,F} - \hat{g}^i(Z_m)) A(D_m, Z_m; \hat{\pi}^i) \tag{16a}
\]

and

\[
\frac{1}{N} \sum_{m \in D_i \cap I} (Y_m^{i,F} - \hat{g}^i(Z_m)) A(D_m, Z_m; \hat{\pi}^i). \tag{16b}
\]

The quantity given in (16a) can be computed directly by running through those observations whose observed treatment is \( d^i \) in \( I \). On the other hand, the quantity given in (16b) cannot be computed directly from the observational data. Recall that \( \xi^{i,CF} := Y^{i,CF} - g^i(Z) \), then (16b) is an estimator of

\[
\frac{1}{N} \sum_{m \in D_i \cap I} \xi^{i,CF} A(D_m, Z_m; \hat{\pi}^i).
\]

In reality, since the counterfactuals cannot be observed, direct estimate of \( \xi^{i,CF} \) is not available for any individual in \( D_i \cap I \). However, we can use the information of those individuals in \( D_i \cap I \) to estimate \( \xi^{i,F} \) which can be treated as indirect estimate of \( \xi^{i,CF} \), under the assumption that \( \xi^{i,CF} = \xi^{i,F} \). Recall that \( \xi^{i,F} \perp \perp Z \) and \( \xi^{i,CF} \perp \perp Z \) such that \( \xi^{i,F} \perp \perp A(D, Z; \hat{\pi}^i) \) and \( \xi^{i,CF} \perp \perp A(D, Z; \hat{\pi}^i) \), so it is reasonable to replace \( \xi^{i,CF} \) with \( \xi^{i,F} \) such that (16c) has the same distribution as

\[
\frac{1}{N} \sum_{m \in D_i \cap I} \xi^{i,F} A(D_m, Z_m; \hat{\pi}^i). \tag{16d}
\]

We remark that in Equation (16d), the quantity \( \xi^{i,F} A(D_m, Z_m; \hat{\pi}^i) \) means that for the \( m^{th} \)-individual in \( D_i \cap I \), we multiply the estimate of \( A(D_m, Z_m; \hat{\pi}^i) \) by an estimate of \( \xi^{i,F} \) which can be inferred based on the observations in the set \( D_i \cap I \). The difference between (16c) and (16d) converges to 0 in probability when \( N \) tends to infinity.

Hence, we can use the quantity \( \hat{\theta}^i_N \) such that

\[
\hat{\theta}^i_N = \frac{1}{N} \sum_{m \in I} \hat{g}^i(Z_m)
\]

\[
+ \frac{1}{N} \sum_{m \in D_i \cap I} (Y_m^{i,F} - \hat{g}^i(Z_m)) A(D_m, Z_m; \hat{\pi}^i)
\]

\[
+ \frac{1}{N} \sum_{m \in D_i \cap I} \xi^{i,F} A(D_m, Z_m; \hat{\pi}^i)
\]

as an estimator of the causal parameter \( \theta^i \) where the definition of \( A(\cdot, \cdot, \cdot) \) is stated in (12) and (13).

We discuss how to give an estimate of (17c) in detail. We first construct the set \( \mathcal{A} \) such that

\[
\mathcal{A} = \left\{ y_m^{i,F} - g^i(Z_m) \mid m \in D_i \cap I \right\},
\]

(18) means that, after obtaining the estimated function \( \hat{g}^i \) from the set \( I \), we compute \( y - g^i(z) \) for each observation \((y, z) \in D_i \cap I \) and store the results in the set \( \mathcal{A} \). To obtain an estimate of (17c), we compute the estimated value of \( A(D_m, Z_m; \hat{\pi}^i) \) for the \( m^{th} \)-individual in the set \( D_i \cap I \). We then compute the average and obtain an estimate of (17c) according to the given formula.

It is also essential to eliminate the extra randomness of the estimate in the proposed methodology. We can reduce the randomness by repeating the procedure for \( R \) times and average the obtained \( R \) results as the final estimate. Mathematically, we use

\[
\frac{1}{R} \sum_{u=1}^{R} \left( \frac{1}{N} \sum_{m \in D_i \cap I} \xi^{i,F} A(D_m, Z_m; \hat{\pi}^i) \right)
\]

(19) as an estimator of (17c). Here, the index \( u \) of \( \{ \xi^{i,F}_{m,u} \}_{u=1}^{R} \) represents the \( u \)th element picked by us. We show that the estimator, given in (17a), (17b), and (19), is a consistent and unbiased estimator of the causal parameter \( \theta^i \). We defer the detailed derivations and proofs of all the theoretical results to the supplementary. Before we move to the next section, we outline the algorithm of estimating \( \theta^i \) based on the observational data in Algorithm 1.

5. Experiments

In this section, we compare our higher-order estimator with the DML estimator as well as the regression adjustment/direct regression (DR) estimator through simulated datasets and benchmark causal inference datasets. In the simulation experiment, we consider three types of machine learning methods: i) linear: Lasso and Logistic Regression (LR); ii) tree-based: Random Forests (RF); iii) non-linear neural network: Multi-layer Perceptron (MLP). In addition to these methods, we consider two more state-of-art neural network architectures: TARNET (Shalit et al. (2017)) and Dragonnet (Shi et al. (2019)) in the benchmark experiments.

5.1. Experiment on Simulated Data

We simulate the data as follows. First, we generate i.i.d. observations of the covariates \( Z = (Z_1, \ldots, Z_p)^T \) which follow a standard multivariate Gaussian distribution. For each
Algorithm 1 Algorithm of obtaining an estimate of $\theta^i$ using (17a), (17b), and (17c).

1: Input: Observational dataset $\{(y_m, d_m, z_m)\} = \mathcal{D} \cup \mathcal{F}^c$, and $\mathcal{F} \cap \mathcal{F}^c = \emptyset$.
2: Train $g^i(\cdot)$ and $\pi^i(\cdot)$ using the observed data in the set $\mathcal{F}^c$ and obtain the estimated functions $\hat{g}^i(\cdot)$ and $\hat{\pi}^i(\cdot)$.
3: For each observational data point $(y, d, z) \in \mathcal{F}$, relabel it as $(\hat{y}, \hat{d}, \hat{z})$ such that $\hat{d} = 1$ if the observed treatment is $d^i$ and $\hat{d} = 0$ if the observed treatment is not $d^i$. Compute $\hat{d} - \hat{\pi}^i(z)$ for each observation in $\mathcal{F}$. Then we estimate $\mathbb{E}[\nu^i]^\theta$ for each $q$ by the mean of all $(\hat{d} - \hat{\pi}^i(z))^q$ in $\mathcal{F}$.
4: Compute the realizations of the estimated residual $\hat{\nu}^{i,F}$ with $y - \hat{g}^i(z)$ for each observation in $\mathcal{F}$ and store the realizations in $\mathcal{D}^i$.
5: Compute (17a) and (17b) using the observational data.
6: For the $m$th-individual in $\mathcal{D}^i \cap \mathcal{F}$, we randomly pick a value from the set $\mathcal{D}^i$ and multiply it to the realization of $A(D, z, \hat{\pi}^i)$. Run through the calculations in $\mathcal{D}^i \cap \mathcal{F}$ and compute an estimate using the formula in (17c).
7: Repeat Step 6 for $R$ times and find the average value according to (19) which is an estimate of (17c).
8: Return: Return the sum of the values in Step 5 and 7.

For each fixed combination of machine learning methods and causal estimator, we repeat the full simulation $M$ times, denote the estimated ATE and the true ATE in the $m$th simulation as $\hat{\theta}^{i,k,m}$ and $\hat{\theta}^{i,k,m}$ respectively, and report the average relative error $\epsilon_{ATE}$ for comparisons:

$$\epsilon_{ATE} = \frac{1}{M} \sum_{m=1}^{M} \sum_{i \neq k} \sum_{1 \leq i,k \leq n} \frac{|\hat{\theta}^{i,k,m} - \theta^{i,k,m}|}{\theta^{i,k,m}},$$

where $n$ is the number of treatments (in the simulated dataset $n = 3$ while in the benchmark dataset $n = 2$). We generate 100 datasets ($M = 100$, and $Q = 10000$ in each dataset) for every simulation experiment, and split every dataset by the ratio 56%/14%/30% as training/validation/test sets such that $\mathcal{F}$ is the test set and $\mathcal{F}^c$ is the union of the training and validation sets. Besides, we choose 4 higher-order estimators as illustrations, i.e., $(r, k) = (2, 2), (3, 3), (4, 2)$, and $(4, 4)$ in Equation (13) for comparisons.

Varying $r_c$. We plot $\epsilon_{ATE}$ produced by every method versus different $r_c$ in Figure 1. We notice that the DML estimator is sensitive to the change of $r_c$, especially when the classifier is MLP. Neural network models, such as MLP, can bring a big variance to the estimated function due to big model complexity. As a consequence, the DML estimator which includes $\frac{1}{\pi^i(\cdot)}$ in Equation (4) will give extreme values at some of the data points, and hence magnify the estimation error of ATE. Nevertheless, our higher-order estimators are less volatile to the variation of $r_c$ regardless of the choice of classifiers.

Varying $p$. We plot $\epsilon_{ATE}$ produced by every method versus different $p$ with $r_c = 1$ in Figure 2. When $p$ increases, the classifiers will be more difficult to be well-fitted and give accurate propensity score estimations. Any ATE estimator that involves the propensity score will face the challenge, but we find that most of our higher-order estimators are still robust in ATE estimation, even $p$ varies dramatically.

In summary, most situations of Figure 1 and Figure 2 show that the higher-order estimator of $(r, k) = (2, 2)$ case performs better than the DML estimator and always gives a robust estimation.

Consistency of higher-order estimators. In this part, we set $r_c = 1$, $p = 2$, and let the number of observations $Q$ vary in $\{1, 2, 4, 8, 16\} \times 10000$. We check the consistency of higher-order estimators through simulations and report $\epsilon_{ATE}$ in Figure 3, which shows that the error reduces when the sample size increases for all higher-order estimators.
5.2. Experiment on Benchmark Datasets

**Models.** Similarly, we choose Lasso, RF, and MLP as the regressors for learning $q^i(\cdot)$, and choose LR, RF, and MLP as the classifiers for learning $\pi^i(\cdot)$. Besides, we use TARNET and Dragonnet as additional models for learning both of the nuisance parameters simultaneously. TARNET, a neural network architecture to estimate the outcome $Y$ with the representation of the covariates $Z$, which can be jointly trained with a logistic regression such that the whole architecture can incorporate the estimations of both $Y$ and $D$ (Shi et al. (2019)). Dragonnet uses the representation of $Z$ not only to estimate $Y$ as TARNET does, but also to estimate $D$ instead of using the covariates $Z$ itself.

**Settings.** We implement the above methods on two benchmark datasets for causal inference: IHDP and ACIC, followed by three estimators adopted: DR, DML, and higher-order estimator. We take the $2^{nd}$-order estimator $((r, k) = (2, 2))$ in Equation (13)) as a representative of the higher-order estimator because for real datasets with relatively small sample size and large feature dimension, the estimation of the second moment of $\nu^i$ is more reliable compared to higher moment estimations. We use grid search to adjust the hyperparameters for those general machine learning models, and for TARNET and Dragonnet, we use the same network structures (layers, units, regularization, batch size, learning rate, and stopping criterion) as Shi et al. (2019) did.

**IHDP.** This is a commonly adopted benchmark dataset for causal inference introduced by Hill (2011). IHDP dataset is constructed based on the randomized controlled experiment conducted by Infant Health and Development Program. The collected 25-dimensional confounders from the 747 samples are associated with the properties of infants and their mothers such as birth weight and mother’s age, which can be used to study the effect of the specialist visits (treatment) on the cognitive scores (outcome). The selection bias in the IHDP dataset is simulated by removing a subset of the treated group. The authors in Shalit et al. (2017) generated 1000 IHDP datasets, and we adopt the same 1000 datasets and the same sample split ratio with training/validation/test being $63\%/27\%/10\%$ such that $I$ is the test set and $I_c$ is the union of the training and validation sets.

**ACIC.** The Atlantic Causal Inference Conference (ACIC) provides data for a specific causal inference challenge annually since 2016. In 2019, the ACIC focused on the estimation of ATE. It includes 1600 low-dimensional (ACIC-low) datasets with the dimension being 22-31 and 1600 high-dimensional (ACIC-high) datasets with the dimension being 200, each with a binary treatment and a continuous outcome. We split every dataset by the ratio of $56\%/14\%/30\%$ as training/validation/test sets such that $I$ is the test set and $I_c$ is the union of the training and validation sets.

![Figure 1. Plots of $\epsilon_{ATE}$ versus the confounder ratio $r_c$ which compare different higher-order estimators for different $(r,k)$ with the DML estimator using different ML methods.](image1)

![Figure 2. Plots of $\epsilon_{ATE}$ versus the confounder dimension $p$ which compare different higher-order estimators for different $(r,k)$ with the DML estimator using different ML methods.](image2)

![Figure 3. Plots of $\epsilon_{ATE}$ versus the total sample size $Q$ (in ten thousand) which demonstrate the consistency of different higher-order estimators for different $(r,k)$ using different ML methods.](image3)
We report the performance of every method measured by $\epsilon_{ATE}$ in every experiment in Table 1, 2, and 3. Compared to DR and DML, we also report the relative error reduction produced by our 2nd-order estimator, denoted as $R_{DR}$ and $R_{DML}$. For those datasets which may violate the overlap assumption or have very small sample size, machine learning models can easily fail to converge although the model parameters have been tuned. In this situation, there may exist individuals whose estimated propensity score can be very close to 1 or 0. Consequently, the DML estimator which incorporates the inverse propensity score term will give a very large or infinity estimation. We defer IHDP and ACIC-low experimental results on the whole datasets to the supplementary. In the main paper, we delete those datasets where the DML estimator gives infinite value and conducts comparisons on the remaining datasets. To be specific, the IHDP experiment remains 987 datasets and the ACIC-low experiment remains 1053 datasets.

Table 1. The $\epsilon_{ATE}$ reported on test set w.r.t. different models and estimators in the IHDP experiment with 987 datasets (with infinite DML estimation deleted).

| Model + Estimator | DR   | DML  | $2^{nd}$-order | $R_{DR}$ | $R_{DML}$ |
|-------------------|------|------|----------------|---------|---------|
| Lasso+LR          | 9.5% | 10.5%| 9.3%           | 3.8%    | 11.5%   |
| Lasso+RF          | 9.6% | 11.0%| 9.2%           | 4.2%    | 16.0%   |
| Lasso+MLP         | 9.6% | 10.3%| 9.4%           | 2.7%    | 8.5%    |
| RF+LR             | 9.6% | 12.6%| 8.9%           | 6.9%    | 29.5%   |
| RF+RF             | 9.6% | 12.5%| 9.1%           | 4.9%    | 27.4%   |
| RF+MLP            | 9.6% | 12.3%| 9.1%           | 5.2%    | 26.0%   |
| MLP+LR            | 18.3%| 28.6%| 18.1%          | 1.0%    | 36.9%   |
| MLP+RF            | 18.3%| 35.4%| 18.0%          | 1.3%    | 49.1%   |
| MLP+MLP           | 18.3%| 29.2%| 18.1%          | 1.0%    | 38.1%   |
| TARNET            | 9.5% | 10.5%| 9.4%           | 1.6%    | 10.5%   |
| Dragonnet         | 9.1% | 10.6%| 9.0%           | 1.5%    | 15.3%   |

Table 2. The $\epsilon_{ATE}$ reported on test set w.r.t. different models and estimators in the ACIC experiment with 1053 low-dimensional datasets (with infinite DML estimation deleted).

| Model + Estimator | DR   | DML  | $2^{nd}$-order | $R_{DR}$ | $R_{DML}$ |
|-------------------|------|------|----------------|---------|---------|
| Lasso+LR          | 21.4%| 44.1%| 20.5%          | 4.5%    | 53.6%   |
| Lasso+RF          | 24.1%| 17.0%| 20.4%          | 4.7%    | 30.2%   |
| Lasso+MLP         | 21.4%| 106.0%| 20.2%        | 5.6%    | 80.9%   |
| RF+LR             | 14.7%| 43.9%| 14.1%          | 4.1%    | 68.0%   |
| RF+RF             | 14.7%| 20.1%| 14.0%          | 4.4%    | 30.2%   |
| RF+MLP            | 14.7%| 114.8%| 13.9%        | 5.5%    | 87.9%   |
| MLP+LR            | 30.9%| 63.1%| 29.6%          | 4.0%    | 53.1%   |
| MLP+RF            | 30.9%| 32.6%| 29.7%          | 3.8%    | 8.9%    |
| MLP+MLP           | 30.9%| 149.0%| 29.4%        | 4.7%    | 80.3%   |
| TARNET            | 25.6%| 287.0%| 24.2%        | 5.6%    | 91.6%   |
| Dragonnet         | 27.2%| 55.5%| 25.8%          | 5.2%    | 53.5%   |

Table 3. The $\epsilon_{ATE}$ reported on test set w.r.t. different models and estimators in the ACIC experiment with the whole 1600 high-dimensional datasets.

| Model + Estimator | DR   | DML  | $2^{nd}$-order | $R_{DR}$ | $R_{DML}$ |
|-------------------|------|------|----------------|---------|---------|
| Lasso+LR          | 20.4%| inf  | 19.8%          | 3.1%    | \     |
| Lasso+RF          | 20.4%| 23.4%| 19.8%          | 3.0%    | 15.4%   |
| Lasso+MLP         | 20.4%| 23.5%| 19.9%          | 2.7%    | 15.6%   |
| RF+LR             | 32.9%| inf  | 32.0%          | 2.7%    | \     |
| RF+RF             | 32.9%| 33.3%| 32.2%          | 2.2%    | 3.5%    |
| RF+MLP            | 32.9%| 36.5%| 32.4%          | 1.6%    | 11.2%   |
| MLP+LR            | 199.0%| inf  | 186.8%         | 6.1%    | \     |
| MLP+RF            | 199.0%| 39.4%| 187.8%         | 5.6%    | -376.2%|
| MLP+MLP           | 199.0%| 44.1%| 187.4%         | 5.8%    | -325.5%|
| TARNET            | 1019.1%| inf  | 760.0%         | 25.4%   | \     |
| Dragonnet         | 965.2%| inf  | 765.2%         | 20.7%   | \     |

Due to the misspecification on $g^i(\cdot)$, the DML estimator can reduce the biasedness if the propensity score is well estimated (e.g., Lasso+RF case in Table 2; MLP+RF and MLP+MLP cases in Table 3). However, the advantages of DML are not easy to achieve in practice because 1) we always try to train $g^i(\cdot)$ as good as possible, and hence the DML estimator will not improve the DR estimator much even if the propensity score is well estimated, 2) sometimes the propensity score estimated by the classifier will be very close to 1 or 0 for some individual, especially when we encounter the high-dimensional and complex data, and in this situation the DML estimator will give an infinite estimation. From these perspectives, our higher-order estimator is more practical since it corrects the error for the DR estimator both theoretically and numerically, and is more robust to the estimation of propensity score than the DML estimator.

6. Conclusion

This paper constructs a general higher-order orthogonal score function to recover a debiased estimator for the ATE. We also give an algorithm to compute our higher-order estimator with observational data. Theoretically, we prove that the higher-order estimator is unbiased and consistent. Numerically, our estimator has improved the DR and DML estimators significantly in a simulation experiment and a real-data experiment containing two benchmark datasets.
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Appendix

7. Tables

In this section, two tables are presented. Table 4 reported $\epsilon_{ATE}$ on test set w.r.t. different models and estimators using all the 1000 datasets from the IHDP database. Table 5 reported $\epsilon_{ATE}$ on test set w.r.t. different models and estimators using all the 1600 datasets from the ACIC-low dimensional database. The $\epsilon_{ATE}$ is defined such that

$$
\epsilon_{ATE} = \frac{1}{M} \sum_{m=1}^{M} \sum_{1 \leq i, k \leq n} \left| \frac{\hat{\theta}_{i,k;m} - \theta_{i,k;m}}{\sum_{i \neq k} |\theta_{i,k;m}|} \right|
$$

Here, $n = 2$ while $M = 1000$ and $M = 1600$ when we consider IHDP database and ACIC-low dimensional database, respectively.

Table 4. The $\epsilon_{ATE}$ reported on test set w.r.t. different models and estimators in the IHDP experiment with the whole 1000 datasets.

| Model | Estimator | DR | DML | 2nd-order | $R_{DR}$ | $R_{DML}$ |
|-------|-----------|----|-----|-----------|---------|---------|
| Lasso+LR | 9.6 % | 10.6 % | 9.2 % | 3.8 % | 12.9 % |
| Lasso+RF | 9.6 % | inf | 9.2 % | 4.2 % | \   |
| Lasso+MLP | 9.6 % | 10.3 % | 9.3 % | 2.7 % | 9.6 % |
| RF+LR | 9.5 % | 12.7 % | 8.8 % | 6.8 % | 30.1 % |
| RF+RF | 9.5 % | inf | 9.0 % | 4.8 % | \   |
| RF+MLP | 9.5 % | 12.3 % | 9.0 % | 5.2 % | 26.6 % |
| MLP+LR | 18.2 % | 28.8 % | 18.0 % | 1.1 % | 37.5 % |
| MLP+RF | 18.2 % | inf | 17.9 % | 1.4 % | \   |
| MLP+MLP | 18.2 % | 29.2 % | 18.0 % | 1.0 % | 38.3 % |
| TARNET | 9.5 % | 10.6 % | 9.3 % | 1.6 % | 11.8 % |
| Dragonnet | 9.1 % | 10.7 % | 8.9 % | 1.5 % | 16.4 % |

Table 5. The $\epsilon_{ATE}$ reported on test set w.r.t. different models and estimators in the ACIC experiment with the whole 1600 low-dimensional datasets.

| Model | Estimator | DR | DML | 2nd-order | $R_{DR}$ | $R_{DML}$ |
|-------|-----------|----|-----|-----------|---------|---------|
| Lasso+LR | 24.3 % | inf | 23.6 % | 3.0 % | \   |
| Lasso+RF | 24.3 % | inf | 23.5 % | 3.4 % | \   |
| Lasso+MLP | 24.3 % | inf | 23.4 % | 3.7 % | \   |
| RF+LR | 16.2 % | inf | 15.7 % | 3.3 % | \   |
| RF+RF | 16.2 % | inf | 15.7 % | 3.4 % | \   |
| RF+MLP | 16.2 % | inf | 15.6 % | 4.1 % | \   |
| MLP+LR | 37.1 % | inf | 36.0 % | 3.0 % | \   |
| MLP+RF | 37.1 % | inf | 36.0 % | 3.0 % | \   |
| MLP+MLP | 37.1 % | inf | 35.8 % | 3.5 % | \   |
| TARNET | 31.7 % | inf | 29.0 % | 8.5 % | \   |
| Dragonnet | 32.1 % | inf | 30.5 % | 5.1 % | \   |

8. Proofs

In this section, we are going to present the theoretical proofs of the theorems and corollaries given in the main paper.

Proof of Theorem 1.

To find out the score function $\psi^i(W, \vartheta, \varrho)$ which can be used to recover the causal parameter $\hat{\theta}^i = \mathbb{E} [g^i(Z)]$, we try an ansatz of $\psi^i(W, \vartheta, \varrho)$ such that

$$
\psi^i(W, \vartheta, \varrho) = \vartheta - g^i(Z) - (Y^i - g^i(Z))A(D, Z; a_i),
$$

where

$$
A(D, Z; a_i) = \bar{b}_r \left[ \mathbb{1}_{\{D=d^i\}} - a_i(Z) \right]^r + \sum_{q=1}^{b-1} b_q \left[ \mathbb{1}_{\{D=d^q\}} - a_i(Z) \right]^q - \mathbb{E} \left[ \nu^i \right].
$$
We then compute $\partial A_0$ for any $q \geq 0$ and $b_r$ compute the coefficients $\partial E_g b_r$ of the moment condition, i.e., $E \left[ \psi^i(W, \vartheta, \varrho) \right]_{\vartheta = \vartheta', \varrho = \rho} = 0$. Indeed, we have

$$\begin{align*}
E \left[ \psi^i(W, \vartheta, \varrho) \right]_{\vartheta = \vartheta', \varrho = \rho} &= 0 \\
&= E \left[ \theta^i - g^i(Z) - (Y^i - g^i(Z))A(D, Z; \pi^i) \right] \\
&= E \left[ \theta^i - g^i(Z) \right] - E \left[ (Y^i - g^i(Z))A(D, Z; \pi^i) \right] \\
&= - E \left[ \xi^i \times A(D, Z; \pi^i) \right] \\
&= - E \left[ \xi^i \times A(D, Z; \pi^i) \right] = 0.
\end{align*}$$

The second last equality comes from the fact that $A(D, Z; \pi^i)$ is a function of $Z$ and $\nu^i$ only such that $A(D, Z; \pi^i)$ is independent of $\xi^i$.

Now, we aim to find out the coefficients of $b_1, \cdots, b_{k-1}, \bar{b}_r$ such that the score function (23) satisfies the $k^{th}$ order orthogonal condition, provided that the nuisance parameters are $\tilde{g}^i(\cdot)$ and $a_i(\cdot)$ only. Indeed, we need to have

$$E \left[ \partial g^i_{\alpha_1} \partial g^i_{\alpha_2} \psi^i(W, \vartheta, \varrho) \right]_{\vartheta = \vartheta', \varrho = \rho} = 0 \text{ for all } \alpha_1 \text{ and } \alpha_2 \text{ which are non-negative integers such that } 1 \leq \alpha_1 + \alpha_2 \leq k.$$

Since $\partial g^i_{\alpha_1} \partial g^i_{\alpha_2} \psi^i(W, \vartheta, \varrho) = 0$ when $\alpha_1 \geq 2$ and $\alpha_2$ is arbitrary, we only need to formulate the equality relations of

$$E \left[ \partial g^i_{\alpha_1} \psi^i(W, \vartheta, \varrho) \right]_{\vartheta = \vartheta', \varrho = \rho} = 0 \text{ and } E \left[ \partial g^i_{\alpha_1} \partial g^i_{\alpha_2} \psi^i(W, \vartheta, \varrho) \right]_{\vartheta = \vartheta', \varrho = \rho} = 0 \text{ for } q = 0, \cdots, k-1 \text{ such that we can compute the coefficients } b_1, \cdots, b_{k-1}, \bar{b}_r \text{ in (24). In addition, note that}

$$\begin{align*}
E \left[ \partial g^i_{\alpha_1} \psi^i(W, \vartheta, \varrho) \right]_{\vartheta = \vartheta', \varrho = \rho} &= 0 \\
&= E \left[ (Y^i - g^i(Z)) \times \partial g^i_{\alpha_1} A(D, Z; a_i) \right]_{a_i = \pi^i} | Z \\
&= E \left[ (Y^i - g^i(Z)) \times \partial g^i_{\alpha_1} A(D, Z; a_i) \right]_{a_i = \pi^i} | Z \\
&= 0.
\end{align*}$$

Consequently, we only need to consider the equality relations of

$$E \left[ \partial g^i_{\alpha_1} \partial g^i_{\alpha_2} \psi^i(W, \vartheta, \varrho) \right]_{\vartheta = \vartheta', \varrho = \rho} = 0 \text{ for } q = 0, \cdots, k-1. \text{ Generally, the } k \text{ unknowns could be solved uniquely.}

We then compute $\partial g^i_{\alpha_1} \partial g^i_{\alpha_2} \psi^i(W, \vartheta, \varrho)$ for $q = 0, \cdots, k-1$. We have

$$\partial g^i_{\alpha_1} \partial g^i_{\alpha_2} \psi^i(W, \vartheta, \varrho) = -1 + A(D, Z; a_i)$$

for $q = 0$ and

$$\partial g^i_{\alpha_1} \partial g^i_{\alpha_2} \psi^i(W, \vartheta, \varrho) = \bar{b}_r r! (-1)^q \left( 1 - \alpha_i(Z) \right)^{r-q}
\begin{align*}
&\frac{}{(r-q)!} \\
&+ \sum_{u=q}^{k-1} b_u (-1)^q \left( 1 - \alpha_i(Z) \right)^{u-q}
\end{align*}
\begin{align*}
&\frac{}{(u-q)!}
\end{align*}$$

for any $1 \leq q \leq k-1$. Recall that a score function $\psi^i(W, \vartheta, \varrho)$ which satisfies the higher order orthogonal conditions is equivalent to

$$E \left[ \partial g^i_{\alpha_1} \partial g^i_{\alpha_2} \psi^i(W, \vartheta, \varrho) \right]_{\vartheta = \vartheta', \varrho = \rho} = 0$$

for any $0 \leq q \leq k-1$. Consequently, we need to solve for $b_1, \cdots, b_{k-1}$ and $\bar{b}_r$ simultaneously from

$$\begin{align*}
1 &= E \left[ A(D, Z; \pi^i) \right] | Z \\
0 &= E \left[ \bar{b}_r r! (-1)^q \left( 1 - \pi_i(Z) \right)^{r-q} \right] | Z \\
&+ \sum_{u=q}^{k-1} b_u (-1)^q \left( 1 - \pi_i(Z) \right)^{u-q} | Z.
\end{align*}$$

(25a)
From (25a), we have
\[
1 = \bar{b}_r \mathbb{E} \left[ \left( \mathbf{1}_{(D = d^i)} - \pi^i(Z) \right)^r | Z \right] \\
+ \sum_{q=1}^{k-1} b_q \mathbb{E} \left[ \left( \mathbf{1}_{(D = d^i)} - \pi^i(Z) \right)^q | Z \right] \\
- \sum_{q=1}^{k-1} b_q \mathbb{E} \left[ (\nu^q) r | Z \right] \\
\Rightarrow 1 = \bar{b}_r \mathbb{E} \left[ (\nu^r) r | Z \right] + \sum_{q=1}^{k-1} b_q \mathbb{E} \left[ (\nu^q) q - \mathbb{E} \left[ (\nu^q) r | Z \right] \right] | Z \\
\Rightarrow 1 = \bar{b}_r \mathbb{E} \left[ (\nu^r) r | Z \right] + \sum_{q=1}^{k-1} b_q \left( \mathbb{E} \left[ (\nu^q) r | Z \right] \right) \\
\Rightarrow 1 = \bar{b}_r \mathbb{E} \left[ (\nu^r) r | Z \right].
\]
Clearly, we can solve \( \bar{b}_r \) by
\[
\bar{b}_r = \frac{1}{\mathbb{E} \left[ (\nu^r) r | Z \right]} = \frac{1}{\mathbb{E} \left[ (\nu^r) r \right]},
\]
where the last equality holds from the assumption that \( \nu \) is independent of \( Z \). It remains to find out \( b_1, \ldots, b_{k-1} \) from (25b).
Indeed, we can simplify (25b) as
\[
\bar{b}_r \mathbb{E} \left[ \frac{r!(\nu^r) r - q}{(r - q)!} | Z \right] + \sum_{u=q}^{k-1} b_u \mathbb{E} \left[ \frac{u!(\nu^u) u - q}{(u - q)!} | Z \right] = 0 \\
\Rightarrow \bar{b}_r \left( \frac{r}{q} \right) \mathbb{E} \left[ (\nu^r) r - q | Z \right] + \sum_{u=q}^{k-1} b_u \left( \frac{u}{q} \right) \mathbb{E} \left[ (\nu^u) u - q | Z \right] = 0 \\
\Rightarrow \bar{b}_r \left( \frac{r}{q} \right) \mathbb{E} \left[ (\nu^r) r - q \right] + \sum_{u=q}^{k-1} b_u \left( \frac{u}{q} \right) \mathbb{E} \left[ (\nu^u) u - q \right] = 0
\]
which holds for \( 1 \leq q \leq k-1 \). Now, we solve \( b_1, \ldots, b_{k-1} \). We start with finding out \( b_{k-1} \), followed by \( b_{k-2}, b_{k-3}, \ldots, b_1 \).
When \( q = k-1 \), (26) becomes
\[
0 = \bar{b}_r \left( \frac{r}{k-1} \right) \mathbb{E} \left[ (\nu^r) r - k+1 \right] + b_{k-1} \left( \frac{k-1}{k-1} \right) \mathbb{E} \left[ (\nu^r) 0 \right] \\
\Rightarrow b_{k-1} = -\bar{b}_r \left( \frac{r}{k-1} \right) \mathbb{E} \left[ (\nu^r) r - k+1 \right].
\]
Now, when \( q = k-2 \), (26) becomes
\[
0 = \bar{b}_r \left( \frac{r}{k-2} \right) \mathbb{E} \left[ (\nu^r) r - k+2 \right] \\
+ b_{k-1} \left( \frac{k-1}{k-2} \right) \mathbb{E} \left[ (\nu^r) r - k+1 \right] \mathbb{E} \left[ (\nu^r) 0 \right] \\
\Rightarrow b_{k-2} = -\bar{b}_{k-1} \left( \frac{k-1}{k-2} \right) \mathbb{E} \left[ (\nu^r) 1 \right] - \bar{b}_r \left( \frac{r}{k-2} \right) \mathbb{E} \left[ (\nu^r) r - k+2 \right].
\]
Iteratively, suppose we have \( b_{q+1}, \ldots, b_{k-1} \) and we want to find what \( b_q \) is, we have to solve it from
\[
\mathbb{E} \left[ (\nu^r) r - q \right] + \sum_{u=q+1}^{k-1} b_u \left( \frac{u}{q} \right) \mathbb{E} \left[ (\nu^u) u - q \right] + b_q \mathbb{E} \left[ (\nu^r) 0 \right] = 0
\]
We can obtain $b_q$ from the above equation, which gives

$$b_q = - \sum_{u=q+1}^{k-1} b_u \left( \frac{u}{q} \right) E \left[ \left( \nu^u \right)^{u-q} \right] - \tilde{b}_q \left( \frac{r}{q} \right) E \left[ \left( \nu^r \right)^{r-q} \right].$$

$$\Rightarrow b_q = - \sum_{u=1}^{k-1} b_{q+u} \left( \frac{q + u}{q} \right) E \left[ \left( \nu^u \right)^u \right] - \tilde{b}_r \left( \frac{r}{q} \right) E \left[ \left( \nu^r \right)^{r-q} \right].$$

The proof is completed. □

**Proof of Corollary 2.**
Before presenting the proof of Corollary 2, we need to use the consistency result of the estimators given in Mackey et al. (2018) (In Chernozhukov et al. (2018), the authors give a general consistent result). We restate here as the Proposition 3:

**Proposition 3.**
Given a score function $\psi_i(W, \theta_i, \rho_i)$ such that the authentic causal parameters and the authentic nuisance parameters are $\theta^i$ and $\rho$ respectively. Suppose that the observational dataset is divided into the sets $\mathcal{I}^c$ and $\mathcal{I}$ such that $\mathcal{I} \cap \mathcal{I}^c = \emptyset$. Let $\hat{\rho}$ be the estimated nuisance parameter using the observational data in $\mathcal{I}^c$. If $N$ represents the size of $\mathcal{I}$ and $\hat{\theta}_i$ be an estimator of $\theta^i$ which is obtained by solving

$$\frac{1}{N} \sum_{m \in \mathcal{I}} \psi(W_m, \hat{\theta}_i, \hat{\rho}) = 0, \quad (27)$$

then under the mild conditions, the estimator $\hat{\theta}_i$ is a consistent estimator of $\theta^i$.

The assumptions given in Mackey et al. (2018) are the mild conditions. In particular, it is essential to impose the conditions for the nuisance parameters for the assertion holds.

Based on the Proposition 3, we only need to construct the desired estimator according to the methodology using the score function given in (12) of the main paper.

We introduce some notations used in our derivations. Denoting the $\hat{\pi}^i(\cdot)$ and $\hat{g}^i(\cdot)$ be the trained functions of $\pi^i(\cdot)$ and $g^i(\cdot)$ respectively. Then, using (12) in the main paper and (27), we can obtain an estimator $\hat{\theta}_N^i$ of the quantity $\theta^i = E[\hat{g}^i(Z)]$ such that

$$\hat{\theta}_N^i = \frac{1}{N} \sum_{m \in \mathcal{I}} \hat{g}^i(Z_m) \quad (28)$$

$$+ \frac{1}{N} \sum_{m \in \mathcal{I}} (Y_m^i - \hat{g}^i(Z_m))A(D_m, Z_m; \hat{\pi}^i).$$

Now, the proof is completed. □

**9. Discussions about the estimator (17a), (17b) and (17c) given in the main paper**

Our estimator of $\theta^i$ is the sum of three quantities, which are (17a), (17b) and (17c) in the main paper. We restate our estimator $\hat{\theta}_N^i$ here, which is

$$\hat{\theta}_N^i = \frac{1}{N} \sum_{m \in \mathcal{I}} \hat{g}^i(Z_m) \quad (29a)$$

$$+ \frac{1}{N} \sum_{m \in \mathcal{I} \setminus \mathcal{I}} (Y_m^i - \hat{g}^i(Z_m))A(D_m, Z_m; \hat{\pi}^i) \quad (29b)$$

$$+ \frac{1}{R} \sum_{u=1}^{R} \left[ \frac{1}{N} \sum_{m \in \mathcal{I} \setminus \mathcal{I}} \hat{\xi}^{u,F}_{m,u}A(D_m, Z_m; \hat{\pi}^i) \right]. \quad (29c)$$
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It is essential to compare our estimator $\hat{\theta}_N$ with $\tilde{\theta}_N$. To start with, we reformulate the $\tilde{\theta}_N$ as

$$
\tilde{\theta}_N = \frac{1}{N} \sum_{m \in \mathcal{I}} \hat{g}(Z_m) + \frac{1}{N} \sum_{m \in \mathcal{D}_i \cap \mathcal{I}} (Y_i^{CF} - \hat{g}(Z_m)) A(D_m, Z_m; \hat{\pi}^i)
$$

(30a)

$$
+ \frac{1}{N} \sum_{m \in \mathcal{D}_c \cap \mathcal{I}} (Y_i^{CF} - \hat{g}(Z_m)) A(D_m, Z_m; \hat{\pi}^i).
$$

(30b)

The Equation (30c) is an estimator of

$$
\frac{1}{N} \sum_{m \in \mathcal{D}_i \cap \mathcal{I}} (Y_i^{CF} - \hat{g}(Z_m)) A(D_m, Z_m; \hat{\pi}^i)
$$

(30c)

In reality, since the counterfactuals can never be observed, direct estimate of $\xi_i^{CF}$ is not available for any individual in $\mathcal{D}_i \cap \mathcal{I}$. However, we can use the information of those individuals in $\mathcal{D} \cap \mathcal{I}$ to estimate $\xi_i^{CF}$ which can be treated as indirect estimate of $\xi_i^{CF}$ under the assumption that $\xi_i^{CF} \perp \perp Z$ and $\xi_i^{CF} \perp \perp Z$ such that $\xi_i^{CF} \perp \perp A(D, Z, \pi^i)$, so it is reasonable to replace $\xi_i^{CF}$ with $\xi_i^F$ such that (30d) has the same distribution as

$$
\frac{1}{N} \sum_{m \in \mathcal{D}_i \cap \mathcal{I}} \xi_i^F A(D_m, Z_m; \hat{\pi}^i).
$$

(30d)

Consequently, we have another estimator such that

$$
\tilde{\theta}_N = \frac{1}{N} \sum_{m \in \mathcal{I}} \hat{g}(Z_m)
$$

(30f)

$$
+ \frac{1}{N} \sum_{m \in \mathcal{D}_i \cap \mathcal{I}} (Y_i^{CF} - \hat{g}(Z_m)) A(D_m, Z_m; \hat{\pi}^i)
$$

(30g)

$$
+ \frac{1}{N} \sum_{m \in \mathcal{D}_c \cap \mathcal{I}} \xi_i^F A(D_m, Z_m; \hat{\pi}^i).
$$

(30h)

which are (17a), (17b) and (17c) given in the main paper. It is necessary to eliminate the extra randomness of the estimate if $\tilde{\theta}_N$ is used, resulting in using the estimator $\hat{\theta}_N$.

To summarize, we have to investigate:

1. What is the statistical difference between (30d) and (30e)? Equivalently, how “close” it is between the two quantities which allows us to replace (30d) with (30e)?

2. Is $\hat{\theta}_N$ the unbiased estimator of $\theta^i$ when the $\hat{g}^i$ and $\hat{\pi}^i$ in (29a), (29b) and (29c) are set to be $g^i$ and $\pi^i$ respectively?

3. What is the asymptotic property of $\hat{\theta}_N$ as an estimator of $\theta^i$?
9.1. Statistical difference between (30d) and (30e)

(30d) and (30e) are closed in the probability sense, i.e., the probability that (30d) and (30e) are different from each other becomes smaller. Before stating the result, we define two quantities which simplifies our notations in the later discussions:

\[
\hat{\kappa}_N^i := \frac{1}{N} \sum_{m \in \mathcal{D}_i \cap \mathcal{F}} \xi_m^{i,C,F} A(D_m, Z_m; \pi^i) \tag{30d}
\]

\[
\hat{\kappa}_N^i := \frac{1}{N} \sum_{m \in \mathcal{D}_i \cap \mathcal{F}} \xi_m^{i,F} A(D_m, Z_m; \pi^i). \tag{30e}
\]

The result is summarized in the Proposition 4.

**Proposition 4.** \(\hat{\kappa}_N^i - \hat{\kappa}_N^i\) converges to 0 in probability as \(N \to \infty\).

**Proof.** For any \(\epsilon > 0\), considering \(P \{ |\hat{\kappa}_N^i - \hat{\kappa}_N^i| \geq \epsilon \} \) and we have

\[
P \{ |\hat{\kappa}_N^i - \hat{\kappa}_N^i| \geq \epsilon \} \leq \frac{E \left( (\hat{\kappa}_N^i - \hat{\kappa}_N^i)^2 \right)}{\epsilon^2}.
\]

Denoting \(\xi_m^{i,C,F} - \xi_m^{i,F}\) and \(A(D_m, Z_m; \pi^i)\) as \(\Xi_m^i\) and \(A_m^i\) respectively, we have

\[
E \left( \sum_{m \in \mathcal{D}_i \cap \mathcal{F}} (\xi_m^{i,C,F} - \xi_m^{i,F}) A(D_m, Z_m; \pi^i) \right)^2 = \sum_{m, m' \in \mathcal{D}_i \cap \mathcal{F}} E \left( \Xi_m^i \Xi_{m'}^i \right) E \left( A_m^i A_{m'}^i \right) \leq 2\sigma^i \sum_{m \in \mathcal{D}_i \cap \mathcal{F}} E \left( A_m^i \right)^2,
\]

where \(\sigma^i = E \left( (\xi_m^{i,C,F})^2 \right) = E \left( (\xi_m^{i,F})^2 \right)\). The derivations are valid since \(\xi_m^{i,C,F} \perp \perp Z\) and \(\xi_m^{i,F} \perp \perp Z\). As a consequence, we have

\[
P \{ |\hat{\kappa}_N^i - \hat{\kappa}_N^i| \geq \epsilon \} \leq \frac{2\sigma^i \sum_{m \in \mathcal{D}_i \cap \mathcal{F}} E \left( A_m^i \right)^2}{N^2 \epsilon^2}.
\]

Since \(2\sigma^i \sum_{m \in \mathcal{D}_i \cap \mathcal{F}} E \left( (A_m^i)^2 \right) < 2\sigma^i N E \left( (A_m^i)^2 \right)\), we know that \(P \{ |\hat{\kappa}_N^i - \hat{\kappa}_N^i| \geq \epsilon \}\) converges to 0 as \(N \to \infty\). The proof is completed.

From the Proposition 4, it is reasonable to replace \(\hat{\theta}_N^i\) with \(\tilde{\theta}_N^i\), in particular when the number of observations is numerous since the probability of obtaining significant difference between (30d) and (30e) is rare for large \(N\).

9.2. Unbiasedness of \(\tilde{\theta}_N^i\)

Good estimators should be unbiased and it is essential to check the unbiased condition. Naturally, we need to investigate if the estimator \(\tilde{\theta}_N^i\) is unbiased when \(\hat{\theta}_N^i\) and \(\hat{\pi}_N^i\) are set to be \(g^i(\cdot)\) and \(\pi^i(\cdot)\) respectively. The estimator \(\tilde{\theta}_N^i\), after setting
The first equality holds using the assumption that \( \xi \). Next, we prove that
\[
\bar{\theta}_N \rightarrow \theta^i.
\]
In the section 9.1, we consider if we can replace \( \hat{\theta}_N \) with \( \bar{\theta}_N \) when \( N \) is large. We also discuss how to obtain an estimate based on \( \bar{\theta}_N \). As stated before, it is essential of repeating the estimation procedure for \( R \) times and obtain the average value. Therefore, we consider the statistical difference between (30e) and
\[
\tilde{\kappa}_N := \frac{1}{R} \sum_{u=1}^{R} \left[ \frac{1}{N} \sum_{m \in \mathcal{D}_i \setminus \mathcal{F}} \xi^{i,F}_{m,u} A(D_m, Z_m; \pi^i) \right].
\] (33)

9.3. Asymptotic property of \( \hat{\theta}_N^i \)

In the section 9.1, we consider if we can replace \( \hat{\theta}_N^i \) with \( \bar{\theta}_N \) when \( N \) is large. We also discuss how to obtain an estimate based on \( \hat{\theta}_N^i \). As stated before, it is essential of repeating the estimation procedure for \( R \) times and obtain the average value. Therefore, we consider the statistical difference between (30e) and
\[
\tilde{\kappa}_N := \frac{1}{R} \sum_{u=1}^{R} \left[ \frac{1}{N} \sum_{m \in \mathcal{D}_i \setminus \mathcal{F}} \xi^{i,F}_{m,u} A(D_m, Z_m; \pi^i) \right].
\] (33)

9.3.1. Statistical difference between (30e) and (33)

In this section, we study the statistical difference between (30e) and (33). The results are summarized in the Proposition 6.

**Proposition 6.** Denoting (30e) as \( \hat{\kappa}_N^i \). Using the notation given (33), we have \( \mathbb{E} \left[ \hat{\kappa}_N^i - \tilde{\kappa}_N^i \right] = 0 \) and \( \tilde{\kappa}_N^i - \hat{\kappa}_N^i \) converges to 0 in probability as \( N \rightarrow \infty \).

**Proof.** First, we prove \( \mathbb{E} \left[ \tilde{\kappa}_N^i - \hat{\kappa}_N^i \right] = 0 \). We consider \( \mathbb{E} \left[ \tilde{\kappa}_N^i \right] \), which gives
\[
\mathbb{E} \left[ \tilde{\kappa}_N^i \right] = \frac{1}{R} \sum_{u=1}^{R} \mathbb{E} \left[ \frac{1}{N} \sum_{m \in \mathcal{D}_i \setminus \mathcal{F}} \xi^{i,F}_{m,u} A(D_m, Z_m; \pi^i) \right]
\]
\[
= \frac{1}{R} \sum_{u=1}^{R} \mathbb{E} \left[ \hat{\kappa}_N^i \right] = \mathbb{E} \left[ \hat{\kappa}_N^i \right].
\]

Next, we prove that \( \tilde{\kappa}_N^i - \hat{\kappa}_N^i \) converges to 0 in probability. Note that we can rewrite (33) as
\[
\frac{1}{N} \sum_{m \in \mathcal{D}_i \setminus \mathcal{F}} \left( \frac{1}{R} \sum_{u=1}^{R} \xi^{i,F}_{m,u} \right) A(D_m, Z_m; \pi^i)
\] (34)
Now, denoting $\frac{1}{N} \sum_{u=1}^{R} \xi_{m,u}^{i,F}$ and $A(D_m, Z_m; \pi)$ as $\delta_m^{i}$ and $A_m^{i}$ respectively for the purpose of simplifying the notations, for $\epsilon > 0$, we have

$$\Pr \left\{ \left| \tilde{\kappa}_N - \kappa_N \right| \geq \epsilon \right\} \leq \frac{\mathbb{E} \left[ \left( \frac{1}{N} \sum_{m \in D_m \cap \mathcal{f}} \left[ \delta_m^{i} - \xi_{m}^{i,F} \right] A_m^i \right)^2 \right]}{\epsilon^2}.$$ 

Considering $\mathbb{E} \left[ \left( \frac{1}{N} \sum_{m \in D_m \cap \mathcal{f}} \left[ \delta_m^{i} - \xi_{m}^{i,F} \right] A_m^i \right)^2 \right]$, we have

$$\mathbb{E} \left[ \left( \frac{1}{N} \sum_{m \in D_m \cap \mathcal{f}} \left[ \delta_m^{i} - \xi_{m}^{i,F} \right] A_m^i \right)^2 \right] = \frac{1}{N^2} \sum_{m,m\in D_m \cap \mathcal{f}} \mathbb{E} \left[ \left( \delta_m^{i} - \xi_{m}^{i,F} \right) \left( \delta_m^{i} - \xi_{m}^{i,F} \right) A_m A_m^i \right] = \frac{1}{N^2} \sum_{m \in D_m \cap \mathcal{f}} \mathbb{E} \left[ \left( \delta_m^{i} - \xi_{m}^{i,F} \right)^2 \right] \mathbb{E} \left[ \left( A_m^i \right)^2 \right].$$

The second last equality follows from the fact that $\delta_m^{i} - \xi_{m}^{i,F}$ and $\delta_m^{i} - \xi_{m}^{i,F}$ are independent of $A_m^i$ and $A_m^i$ as well as the fact that $\mathbb{E} \left[ \left( \delta_m^{i} - \xi_{m}^{i,F} \right)^2 \right] = 0$. In addition, we simplify the quantity $\mathbb{E} \left[ \left( \delta_m^{i} - \xi_{m}^{i,F} \right)^2 \right]$. Note that

$$\mathbb{E} \left[ \left( \sum_{u=1}^{R} \xi_{m,u}^{i,F} - \xi_{m}^{i,F} \right)^2 \right] = \mathbb{E} \left[ \sum_{u=1}^{R} \mathbb{E} \left[ \left( \xi_{m,u}^{i,F} - \xi_{m,u}^{i,F} \right) \left( \xi_{m,u}^{i,F} - \xi_{m,u}^{i,F} \right) \right] \right] = \sum_{u=1}^{R} \mathbb{E} \left[ \left( \xi_{m,u}^{i,F} - \xi_{m}^{i,F} \right)^2 \right] = R^2 + \mathbb{E} \left[ \mathbb{E} \left[ \left( \xi_{m,u}^{i,F} \right)^2 \right] - \left( \mathbb{E} \left[ \mathbb{E} \left[ \left( \xi_{m,u}^{i,F} \right)^2 \right] \right] \right) \right] = R^2 + \mathbb{E} \left[ \mathbb{E} \left[ \left( \xi_{m,u}^{i,F} \right)^2 \right] \right].$$

Consequently, we have

$$\mathbb{E} \left[ \left( \delta_m^{i} - \xi_{m}^{i,F} \right)^2 \right] = \left( 1 + \frac{1}{R} \right) \mathbb{E} \left[ \left( \xi_{m}^{i,F} \right)^2 \right]$$

and

$$\Pr \left\{ \left| \tilde{\kappa}_N - \kappa_N \right| \geq \epsilon \right\} \leq \frac{\frac{1}{N^2} \sum_{m \in D_m \cap \mathcal{f}} \left( 1 + \frac{1}{R} \right) \sigma^i}{\epsilon^2},$$

where $\sigma^i := \mathbb{E} \left[ \left( \xi_{m}^{i,F} \right)^2 \right]$. We notice that no matter we set $R \to \infty$ followed by $N \to \infty$ or vice versa, or we fix $R$ but letting $N \to \infty$, we see that $\Pr \left\{ \left| \tilde{\kappa}_N - \kappa_N \right| \geq \epsilon \right\}$ converges to 0.
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From the Proposition 6, we notice that it is reasonable to consider \( \hat{\theta}^i_N \) instead of \( \bar{\theta}^i_N \). Furthermore, \( \hat{\theta}^i_N \) should be a better estimator when \( R \) in (29c) increases.

9.3.2. CONSISTENCY OF \( \hat{\theta}^i_N \)

In this section, we investigate if the estimator \( \hat{\theta}^i_N \) is a consistent estimator. First, we will introduce a Lemma summarized in the lemma 7 to assist the proof of consistency.

Lemma 7. Given two sequences of random variables \((X_N)_{N=1}^\infty\) and \((Y_N)_{N=1}^\infty\) such that \( X_N \overset{d}{=} Y_N \). If \( X_N \overset{p}{\to} c \) for some constant \( c \), then \( Y_N \overset{p}{\to} c \).

Proof. Let \( f_{X_N}(\cdot) \) and \( f_{Y_N}(\cdot) \) be the density functions of the random variables \( X_N \) and \( Y_N \) respectively. Since \( X_N \overset{d}{=} Y_N \), \( f_{X_N}(\cdot) = f_{Y_N}(\cdot) \). Hence, \( \mathbb{P}\{|X_N - c| \geq \epsilon\} = \mathbb{P}\{|f_{X_N}(z)dz \geq \epsilon\} = \mathbb{P}\{|Y_N - c| \geq \epsilon\} \). Consequently, \( X_N \overset{p}{\to} c \) implies \( Y_N \overset{p}{\to} c \).

Using the Lemma 7 and the assumptions given in Mackey et al. (2018), we can summarize the result \( \hat{\theta}^i_N \) is a consistent estimator of \( \theta^i \) in the Proposition 8.

Proposition 8. Under the mild conditions, the estimator \( \hat{\theta}^i_N \) is a consistent estimator of \( \theta^i \).

Proof. For \( \epsilon > 0 \), we have

\[
\mathbb{P}\left\{ \left| \hat{\theta}^i_N - \theta^i \right| \geq \epsilon \right\} = \mathbb{P}\left\{ \left| \hat{\theta}^i_N - \bar{\theta}^i_N + \bar{\theta}^i_N - \theta^i \right| \geq \epsilon \right\} \\
\leq \mathbb{P}\left\{ \left| \hat{\theta}^i_N - \bar{\theta}^i_N \right| \geq \frac{\epsilon}{2} \right\} + \mathbb{P}\left\{ \left| \bar{\theta}^i_N - \theta^i \right| \geq \frac{\epsilon}{2} \right\}.
\]

The assumptions given in Mackey et al. (2018) are our mild conditions. Since \( \hat{\theta}^i_N \) is a consistent estimator of \( \theta^i \) under the mild conditions, we know that \( \lim_{N \to \infty} \mathbb{P}\left\{ \left| \hat{\theta}^i_N - \theta^i \right| \geq \frac{\epsilon}{2} \right\} = 0 \) by the definition of consistency. Since \( \bar{\theta}^i_N \overset{d}{=} \bar{\theta}^i_N \), we can get the result \( \lim_{N \to \infty} \mathbb{P}\left\{ \left| \bar{\theta}^i_N - \theta^i \right| \geq \frac{\epsilon}{2} \right\} = 0 \) by the Lemma 7. We need to consider the quantity \( \mathbb{P}\left\{ \left| \hat{\theta}^i_N - \bar{\theta}^i_N \right| \geq \frac{\epsilon}{2} \right\} \). For notational simplicity, let’s define

\[
\hat{K}_N := \frac{1}{R} \sum_{u=1}^{R} \left[ \frac{1}{N} \sum_{m \in \mathcal{D}^i_N \cap \mathcal{F}} \tilde{\xi}^i_{m,u} A(D_m, Z_m; \hat{\pi}^i) \right]
\]

\[
\bar{K}_N := \frac{1}{N} \sum_{m \in \mathcal{D}^i_N \cap \mathcal{F}} \tilde{\xi}^i_{m} A(D_m, Z_m; \hat{\pi}^i).
\]

Using our definitions on \( \hat{K}_N, \bar{K}_N \) and \( \hat{K}_N \), we have

\[
\mathbb{P}\left\{ \left| \hat{\theta}^i_N - \hat{\theta}^i_N \right| \geq \frac{\epsilon}{2} \right\} = \mathbb{P}\left\{ \left| \hat{K}_N - \bar{K}_N \right| \geq \frac{\epsilon}{2} \right\} \\
\leq \mathbb{P}\left\{ \left| \hat{K}_N - \bar{K}_N \right| \geq \frac{\epsilon}{8} \right\} + \mathbb{P}\left\{ \left| \bar{K}_N - \bar{K}_N \right| \geq \frac{\epsilon}{8} \right\} \\
+ \mathbb{P}\left\{ \left| \bar{K}_N - \hat{K}_N \right| \geq \frac{\epsilon}{8} \right\} + \mathbb{P}\left\{ \left| \hat{K}_N - \hat{K}_N \right| \geq \frac{\epsilon}{8} \right\}.
\]

The convergence of \( \mathbb{P}\left\{ \left| \hat{K}_N - \bar{K}_N \right| \geq \frac{\epsilon}{8} \right\} \) and \( \mathbb{P}\left\{ \left| \bar{K}_N - \bar{K}_N \right| \geq \frac{\epsilon}{8} \right\} \) as \( N \to \infty \) are proven in the Proposition 4 and the Proposition 6. It suffices to consider \( \mathbb{P}\left\{ \left| \hat{K}_N - \bar{K}_N \right| \geq \frac{\epsilon}{8} \right\} \) and \( \mathbb{P}\left\{ \left| \bar{K}_N - \hat{K}_N \right| \geq \frac{\epsilon}{8} \right\} \). Consider \( \mathbb{P}\left\{ \left| \hat{K}_N - \bar{K}_N \right| \geq \frac{\epsilon}{8} \right\} \). Denoting \( A(D_m, Z_m; \hat{\pi}^i) \) and \( A(D_m, Z_m; \hat{\pi}^i) \) as \( A_{\hat{\pi}^i} \) and \( A_{\hat{\pi}^i} \) respectively, then we can
simplify $P \left\{ |\hat{K}_N^i - \tilde{K}_N^i| \geq \frac{\epsilon}{8} \right\}$ as

$$P \left\{ \frac{1}{N} \sum_{m \in D^i \cap J} (\xi_{m}^{i,CF} A_m^i - \xi_{m}^{i,F} A_m^i) \geq \frac{\epsilon}{24} \right\}$$

(35a)

$$P \left\{ \frac{1}{N} \sum_{m \in D^i \cap J} (\xi_{m}^{i,CF} A_m^i - \hat{\xi}_{m}^{i,F} A_m^i) \geq \frac{\epsilon}{24} \right\}$$

(35b)

$$P \left\{ \frac{1}{N} \sum_{m \in D^i \cap J} (\hat{\xi}_{m}^{i,F} A_m^i - \hat{A}_m^i) \geq \frac{\epsilon}{24} \right\}$$

(35c)

The convergence of (35a) when $N \to \infty$ is guaranteed from the Proposition 4. We investigate the quantities (35b) and (35c).

(35b) can be further bounded by three terms, which are

$$P \left\{ \frac{1}{N} \sum_{m \in D^i \cap J} \xi_{m}^{i,F} A_m^i - \mathbb{E} \left[ \xi_{i,F} A^i \right] \geq \frac{\epsilon}{72} \right\}$$

(36a)

$$P \left\{ | \mathbb{E} \left[ \xi_{i,F} A^i \right] - \mathbb{E} \left[ \hat{\xi}_{i,F} A^i \right] | \geq \frac{\epsilon}{72} \right\}$$

(36b)

$$P \left\{ | \mathbb{E} \left[ \hat{\xi}_{i,F} A^i \right] - \frac{1}{N} \sum_{m \in D^i \cap J} \hat{\xi}_{m}^{i,F} A_m^i | \geq \frac{\epsilon}{72} \right\}$$

(36c)

Recalling the assumptions that $\xi_{i,F} \sim d \xi_{i,CF}$, $\xi_{i,F} \perp \perp Z$ and $\hat{\xi}_{i,F} \perp \perp Z$, we have

$$\frac{1}{N} \sum_{m \in D^i \cap J} \xi_{m}^{i,F} A_m^i = \frac{1}{N} \sum_{m \in D^i \cap J} \xi_{m}^{i,CF} A_m^i$$

and $\mathbb{E} \left[ \xi_{i,F} A^i \right]$ is a constant, we know that (36a) converges to 0. Due to the fact that the $\hat{\xi}_{i,F}$ is consistent to $\xi_{i,F}$ (Assumption 1.5 of Mackey et al. (2018)), $\mathbb{E} \left[ \xi_{i,F} A^i \right] - \mathbb{E} \left[ \hat{\xi}_{i,F} A^i \right]$ converges to 0 in probability. Finally, under the assumptions of Mackey et al. (2018), the uniform law of large number holds, meaning that the supremum of

$$\mathbb{E} \left[ \hat{\xi}_{i,F} A^i \right] - \frac{1}{N} \sum_{m \in D^i \cap J} \hat{\xi}_{m}^{i,F} A_m^i$$

over a set which contains all the estimated nuisance parameters $(\hat{g}_i, \hat{\pi}_i)$ such that each $(\hat{g}_i, \hat{\pi}_i)$ is close to $(g_i, \pi_i)$ (indeed, we only need to use the fact that $\hat{g}_i$ is close to $g_i$ since we do not consider estimating $\pi_i$ this time) converges to 0 in probability. (36c) would converge to 0 when $N \to \infty$.

Simultaneously, (35c) can be further bounded by three terms, which are

$$P \left\{ \frac{1}{N} \sum_{m \in D^i \cap J} \hat{\xi}_{m}^{i,F} A_m^i - \mathbb{E} \left[ \hat{\xi}_{i,F} A^i \right] \geq \frac{\epsilon}{24} \right\}$$

(37a)

$$P \left\{ | \mathbb{E} \left[ \hat{\xi}_{i,F} A^i \right] - \mathbb{E} \left[ \hat{\xi}_{i,F} \hat{A}^i \right] | \geq \frac{\epsilon}{24} \right\}$$

(37b)

$$P \left\{ | \mathbb{E} \left[ \hat{\xi}_{i,F} \hat{A}^i \right] - \frac{1}{N} \sum_{m \in D^i \cap J} \hat{\xi}_{m}^{i,F} \hat{A}_m^i | \geq \frac{\epsilon}{24} \right\}$$

(37c)

Using the same ideas in considering (36c), we can argue that (37a) and (37c) converge to 0 when $N \to \infty$. Besides, (37b) converges to 0 when $N \to \infty$ since $\mathbb{E} \left[ \hat{\xi}_{i,F} A^i \right] - \mathbb{E} \left[ \hat{\xi}_{i,F} \hat{A}^i \right] = \mathbb{E} \left[ (\hat{\xi}_{i,F} - \xi_{i,F}) (A^i - \hat{A}^i) \right]$, which implies that it converges to 0 in probability due to the fact that $\hat{g}_i$ and $\hat{\pi}_i$ are consistent to $g_i$ and $\pi_i$ respectively (Assumption 1.5 of Mackey et al. (2018)).
We turn to consider the quantity $P\left\{ \left| K_N^i - \hat{K}_N^i \right| \geq \frac{\varepsilon}{8} \right\}$. In fact, we have

$$
\begin{align*}
P\left\{ \left| K_N^i - \hat{K}_N^i \right| \geq \frac{\varepsilon}{8} \right\} & \leq P\left\{ \left| \frac{1}{N} \sum_{m \in D^i \cap \mathcal{I}} \frac{1}{R} \sum_{u=1}^{R} (\hat{\xi}_{m,u}^i F_m - \hat{\xi}_{m,u}^i) \left( \hat{A}_m^i - A_m^i \right) \right| \geq \frac{\varepsilon}{16} \right\} \\
& \quad + P\left\{ \left| \frac{1}{N} \sum_{m \in D^i \cap \mathcal{I}} A_m^i \frac{1}{R} \sum_{u=1}^{R} \left[ (\hat{\xi}_{m,u}^i F_m - \hat{\xi}_{m,u}^i) \right] \right| \geq \frac{\varepsilon}{16} \right\} 
\end{align*}
$$

(38a)

We can apply similar arguments in considering the quantity (35b) to prove that (38a) tends to 0 when $N \to \infty$. Similarly, we can apply similar arguments in considering the quantity (35c) to prove that (38b) tends to 0 when $N \to \infty$. Consequently, we have $K_N^i - \hat{K}_N^i$ converges to 0 in probability.

The proof is completed. \qed