Efficient Estimation of General Treatment Effects using Neural Networks with A Diverging Number of Confounders

XIAOHONG CHEN??, YING LIU??, SHUJIE MA??,* and ZHENG ZHANG??

Xiaohong Chen
Department of Economics
Yale University
New Haven, CT 06520, USA
e-mail: xiaohong.chen@yale.edu

Ying Liu
Department of Statistics
University of California at Riverside
Riverside, CA 92521, USA
e-mail: yliu364@ucr.edu

Shujie Ma
Department of Statistics
University of California at Riverside
Riverside, CA 92521, USA
e-mail: shujie.ma@ucr.edu

Zheng Zhang
Institute of Statistics and Big Data
Renmin University of China
Beijing 100872, China
e-mail: zhengzhang@ruc.edu.cn

Abstract: The estimation of causal effects is a primary goal of behavioral, social, economic and biomedical sciences. Under the unconfounded treatment assignment condition, adjustment for confounders requires estimating the nuisance functions relating outcome and/or treatment to confounders. The conventional approaches rely on either a parametric or a nonparametric modeling strategy to approximate the nuisance functions. Parametric methods can introduce serious bias into casual effect estimation due to possible mis-specification, while nonparametric estimation suffers from the “curse of dimensionality”. This paper proposes a unified approach for efficient estimation of treatment effects using feedforward artificial neural networks with the number of covariates allowed to increase with the sample size. We consider a general optimization framework that includes the average, quantile and asymmetric least squares treatment effects as special cases. Under this unified setup, we develop a generalized optimization estimator for the treatment effect with the nuisance function estimated by neural networks. We further establish the consistency and asymptotic normality

*The research of Liu and Ma is supported in part by the U.S. NSF grants DMS-17-12558 and DMS-20-14221 and the UCR Academic Senate CoR Grant.
of the proposed estimator and show that it attains the semiparametric efficiency bound. The proposed methods are illustrated via simulation studies and a real data application.

**MSC2020 subject classifications:** Primary 62G08; secondary 62G10, 62G20, 62J07.

**Keywords and phrases:** Treatment effects, Propensity score, Artificial neural networks, Semiparametric efficiency.

1. Introduction

The estimation of causal effects is a primary goal of behavioral, social, economic and biomedical sciences. Recent technological advances have created numerous large-scale observational studies, which bring unprecedented opportunities for evaluating the treatment effectiveness. Examples of such data include patient registries, electronic health records, pharmacy and health insurance claims and user-generated social media platforms, all of which are increasingly available in large volumes. The increase occurs not only in the number of sample observations, but also in the number of variables measured for each subject.

A major difficulty in causal inference from observational studies is how to control the bias caused by the confounding variables that influence both the outcome and treatment assignment. To overcome this difficulty, under the unconfounded treatment assignment condition (Rosenbaum and Rubin, 1983), one often needs an intermediate estimate of unknown nuisance functions that relate outcome and/or treatment to confounders (Heckman, Ichimura, and Todd, 1998; Hirano, Imbens, and Ridder, 2003; Chan, Yam, and Zhang, 2016; Ai, Linton, Motegi, and Zhang, 2018; Ding and Li, 2018; Han, 2018). The conventional estimation methods may no longer be well suited to handle large-scale data. The mis-specification of the parametric approaches can introduce serious bias into causal effect estimation (Kang and Schafer, 2007; Freedman and Berk, 2008), which is a big concern in the context of large-scale data. Although the classical nonparametric methods such as kernels or splines are flexible for recovering unknown functions, they suffer from the “curse of dimensionality” (Bellman, 1961). On the other hand, the unconfounded treatment assignment requires that all observed confounders be included in the analysis, as we often have no prior knowledge of which variables are important confounders. Thus, there is a pressing need to apply a data-driven method that can provide effective protection against mis-specification bias as well as achieving dimension reduction. Some proposals have made initial attempts to solve this problem using the sufficient dimension reduction (Huang and Chan, 2017; Luo, Zhu, and Ghosh, 2017; Ma, Zhu, Zhang, Tsai, and Carroll, 2019). This technique requires the dependence of treatment assignment on confounders through a few linear combinations of them.

Thanks to the rapid development of scalable computing and optimization techniques in recent years (Kingma and Ba, 2014; Abadi, Agarwal, Barham, and et al., 2016), it becomes appealing to use artificial neural networks (ANNs) to approximate the nuisance functions. Similar as splines, ANNs are also a class of
approximation bases, but they can contain multilayers. ANNs are universal approximators of a wide variety of functions (White, 1992; Hornik, Stinchcombe, White, and Auer, 1994; Chen and White, 1999; Yarotsky, 2018; Bauer and Kohler, 2019; Schmidt-Hieber, 2020), so they are robust to mis-specification. It is shown in Chen and White (1999) that their approximation rate to a smooth function can be smaller than $n^{-1/4}$, where $n$ is the sample size, no matter how large the dimension of covariates is, indicating that ANNs have the potential to overcome the “curse of dimensionality” that typically arises in classical non-parametric estimation approaches. ANNs are shown to be particularly useful for classification and prediction from large datasets (Anthony and Bartlett, 2009).

However, how do we go one step further to conduct causal inference using ANNs? It needs careful thought, and research on this topic is still in its infancy.

One recent work (Farrell, Liang, and Misra, 2019) estimates the average treatment effects (TEs) using a doubly robust (DR) method with the nuisance functions approximated by ANNs, and provides a sound theoretical justification for their method. It is worth noting that DR estimators of TEs are constructed based on efficient influence functions, so they arise naturally for pursuing asymptotic normality and efficiency, which are of critical importance for conducting causal inference (e.g. van der Laan and Robins, 2003; Bang and Robins, 2005; Cao, Tsiatis, and Davidian, 2009; Tan, 2010; van der Laan and Rose, 2011; Rotnitzky, Lei, Sued, and Robins, 2012; Chan and Yam, 2014; Farrell, 2015; Kennedy, Ma, McHugh, and Small, 2017; Tan, 2020; Ning, Peng, and Imai, 2020). Despite its popularity, the DR method is mainly applied for average TEs estimation, as in order to use this method, one needs to first work out the influence functions that are unlike for different types of TEs. Estimation of the influence functions for the average TE is straightforward, but it can be complicated for other types of TEs, such as quantile TEs.

In this paper, we propose a new ANN-based estimator of general TEs. Different from Farrell, Liang, and Misra (2019), our TE estimator is directly obtained through optimizing a generalized objective function that only involves the propensity score (PS) function (Rosenbaum and Rubin, 1983), which is approximated by ANNs. As a result, it can be naturally used to estimate general TEs, including the average, quantile and asymmetric least squares TEs. Our work differs from Farrell, Liang, and Misra (2019) in several aspects: first, we present a general optimization estimation framework that can be applied to various types of TEs, while their estimator obtained from the inference function is specifically for the average TE; second, we allow the number of confounders to grow with the sample size, but they treat it to be fixed; third, our procedure only needs to estimate the PS function rather than the influence functions. It is worth noting that if our interest focuses on the average TE specifically, we also propose an ANN-based estimator obtained from the outcome regression (OR) function. This estimator can be more robust than the PS based estimator in case that the estimated PS function has very small values. However, it is difficult to apply this OR based estimator to other types of TEs such as quantile TEs. In the context of average TE, our proposed PS and OR estimators which involve only one nuisance function have the same asymptotic distribution and efficiency.
as the DR-based estimator considered in Farrell, Liang, and Misra (2019).

Theoretically, we derive a desirable convergence rate of the ANN estimator for the nuisance function under mild conditions. We also show that the number of the confounders is allowed to grow with the sample size with a rate no greater than \( \log(n) \) in order to ensure root-n consistency of the TE estimator. Moreover, our proposed TE estimator possesses asymptotic normality, and it also attains the semiparametric efficiency bound given in Chen (2007), Chen, Hong, Tarozzi, et al. (2008) and Ai, Linton, Motegi, and Zhang (2018). To the best of our knowledge, our work is the first one that investigates how fast the dimension of the covariates can grow with the sample size for conducting casual inference when the nuisance function is approximated by ANNs without assuming sparsity, and proposes a generalized optimization approach that can efficiently estimate different types of TEs without estimating the efficient influence function in the presence of high-dimensional covariates. While the development of credible theories for the ANN-based estimator of TEs, including root-n asymptotic normality and semiparametric efficiency, is essential to test causal relationships, it is also a daunting task because of the complex nonlinear structure of the ANNs. To better illustrate our TE estimation procedure, we focus on using the ANNs with one-hidden layer to construct the TE estimator, and discuss the extension of our method to ANNs with multiple hidden layers and its statistical properties in Section 8.2. It is worth mentioning that random forests are another attractive machine learning tool that enjoys flexibility for unknown function approximation, and have been applied by pioneer works (Wager and Athey, 2018; Athey, Tibshirani, and Wager, 2019) for causality analysis. They proposed random forest estimators for conditional TEs localizing around given values of confounders, while we study efficient estimation of population TEs. Their estimators are locally asymptotic normal, but do not possess the semiparametric efficiency.

The paper is organized as follows. Section 2 sets up the basic framework, Section 3 gives a review of artificial feedforward neural networks and related approximation results, Section 4 describes our proposed inverse probability weighting estimator for TEs, Section 5 establishes the large sample properties of the proposed estimator, Section 6 studies the estimation of asymptotic variance, Section 7 proposes a regression estimator for average TEs, Section 8 discusses some extensions, Section 9 reports the numerical results of simulation studies, and Section 10 illustrates the proposed method using a data example, followed by some concluding remarks in Section 11. All the technical proofs are provided in the on-line Appendices.

2. Basic framework and notation

Let \( D \) denote a multivalued treatment variable taking value in \( D = \{0, 1, ..., J\} \), where \( J \geq 1 \) is a positive integer. Let \( Y^*(d) \) denote the potential outcome when the treatment status \( D = d \) is assigned. Let \( L(\cdot) \) denote a known convex loss function whose derivative, denoted by \( L'(\cdot) \), exists almost everywhere. Let
$\beta^* = (\beta^*_0, \beta^*_1, \ldots, \beta^*_J)^\top \in \mathbb{R}^{J+1}$ be the parameter of interest which is identified through the following optimization problem:

$$\beta^* := \arg \min_{\beta} \sum_{d=0}^J E [L(Y^*(d) - \beta_d)],$$  \hspace{1cm} (1)

where $\beta = (\beta_0, \beta_1, ..., \beta_J)^\top \in \mathbb{R}^{J+1}$. The formulation (1) permits the following important already considered models and much more:

- $L(v) = v^2$ and $J = 1$, then $\beta^*_0 = E[Y^*(0)]$ and $\beta^*_1 = E[Y^*(1)]$, and $\beta^*_1 - \beta^*_0$ is the average treatment effects (ATE) studied by Hahn (1998), Hirano, Imbens, and Ridder (2003) and Chan, Yam, and Zhang (2016). When $J \geq 2$, then $\beta^*_d = E[Y^*(d)]$ is the multi-valued treatment effects studied by Cattaneo (2010).

- $L(v) = v \cdot \{\tau - I(v \leq 0)\}$ for some $\tau \in (0, 1)$ and $J = 1$, then $\beta^*_0 = F_{Y^*(0)}^{-1}(\tau)$ and $\beta^*_1 = F_{Y^*(1)}^{-1}(\tau)$, and $\beta^*_1 - \beta^*_0$ is the quantile treatment effects (QTE) Firpo, 2007; Han, Kong, and Zhao, 2019).

- $L(v) = v^2 \cdot |\tau - I(v \leq 0)|$ is the asymmetric least square effects (Yao and Tong, 1996).

The problem with (1) is that the potential outcomes $(Y^*(0), Y^*(1), ..., Y^*(J))$ cannot all be observed. The observed outcome is denoted by $Y := Y^*(D)$. One may attempt to solve the problem:

$$\min_{\beta} \sum_{d=0}^J E [L(Y - \beta_d)].$$

However, due to the selection in treatment, the true value $\beta^*$ is not the solution of above minimization problem. To address this problem, most of literature impose unconfoundedness treatment assignment condition (Rosenbaum and Rubin, 1983; Cattaneo, 2010). Specifically, let $X_i = (X_{i1}, \ldots, X_{ip})^\top$ denote a $p$-dimensional vector of covariates with $p \in \mathbb{N}$. The observed data, denoted by $\{D_i, Y_i, X_i\}_{i=1}^n$, are independent and identically distributed (i.i.d.). The following condition shall be maintained through this article:

**Assumption 1.** For each $d \in D$, $Y^*_i(d) \perp D_i | X_i$.

Under Assumption 1, the causal parameters $\beta^*$ can be identified by

$$\beta^* := \arg \min_{\beta} \sum_{d=0}^J \mathbb{E} \left[ \frac{D_{di}}{\pi_d^*(X_i)} L(Y_i - \beta_d) \right],$$  \hspace{1cm} (2)

where $D_{di} := I(D_i = d)$, and

$$\pi_d^*(X_i) := P(D_i = d | X_i) = P(D_{di} = 1 | X_i)$$

is the propensity score function which is unknown in practice.
Based on (2), existing approaches rely on parametric or nonparametric estimation of the PS function $\pi^*_d(X_i)$. Parametric methods suffer from model misspecification problem, while conventional nonparametric methods, such as linear sieve or kernel regression, fail to work if the dimension of covariates $p$ is large which is known as the curse of dimensionality (Li and Racine, 2007). The goal of this article is to efficiently estimate $\beta^*$ under this general framework when the dimension of covariates $p$ is large, and it possibly increases as the sample size $n$ grows. We propose to estimate the PS function $\pi^*_d(X_i)$ using feedforward ANNs with one hidden layer described in Section 3.

3. Artificial neural networks and sieve extremum estimates

Feedforward ANNs are effective tools for solving the classification and prediction problems for “big data”. The basic idea is to extract linear combinations of the inputs as features, and then model the target as a nonlinear function of these features. This section presents ANNs with one hidden layer and the related results which are used in this article.

As given in Hornik, Stinchcombe, White, and Auer (1994), let the target function $f: \mathbb{R}^p \to \mathbb{R}$ have a Fourier representation such that $f \in F_p$, where

$$F_p := \left\{ f: \mathbb{R}^p \to \mathbb{R} : f(x) = \int \exp (ia^T x) d\sigma_f(a), ||\sigma_f||_1 := \int l(a)d||\sigma_f||_{tv}(a) < \infty \right\},$$

(3)

where $\sigma_f(\cdot)$ is a complex measure on $\mathbb{R}^p$, $||\sigma_f||_{tv}$ denotes the total variation of $\sigma_f$, and $l(a) := \max\{(a^T a)^{1/2}, 1\}$. If $\sigma_f(\cdot)$ is absolutely continuous with respect to Lebesgue measure, its density has the Fourier transform

$$\frac{d\sigma_f(a)}{da} = \tilde{f}(a) = \frac{1}{(2\pi)^p} \int_{\mathbb{R}^p} \exp (-ia^T x) f(x) dx.$$ 

Hence, $F_p$ contains a broad class of functions whose Fourier transform and inverse Fourier transform exist, for example $f \in L^1(dx)$ and $\tilde{f} \in L^1(dx)$.

We approximate any target function $f \in F_p$ using the ANN class

$$G_p(\psi, B, r_n) = \left\{ g: g(x) = \gamma_0 + \sum_{j=1}^{r_n} \gamma_j \psi(a_j^T x + a_{j0}), \sum_{j=0}^{r_n} |\gamma_j| \leq B, \sup_{1 \leq j \leq r_n} \sum_{k=0}^{p} |a_{jk}| \leq B \right\},$$

where $a_j = (a_{j1}, ..., a_{jp})^T$ and $B$ is a fixed constant. $G_p(\psi, B, r_n)$ is the collection of output functions for neural networks with $p$-dimensional input feature $x$, a single hidden layer with $r_n$ hidden units and a common activation function $\psi$, real-valued input-to-hidden unit weights ($a_j$), bias ($a_{j0}$), and hidden-to-output weights ($\gamma_j$).

Following Chen and White (1999), we impose the Hölder condition on the activation function:
Assumption 2. There exists an $\alpha \in (0, 1]$ such that
\[ \|\psi(a^\top X + \theta) - \psi(a^\top X + \theta_1)\|_{L^2} \leq \text{const} \times \left\{ (a - a_1)^\top (a - a_1) \right\}^{1/2} + |\theta - \theta_1|^{\alpha}. \]

Under Assumption 2, Chen and White (1999, Theorem 2.1) establishes the $L_2$-approximation rate by ANN estimates, which is stated as follows:

**Proposition 1.** Let $f_0 \in \mathcal{F}_p$. Suppose that $dF_X$ and $\psi(\cdot)$ are compactly supported, and that $\psi$ satisfies Assumption 2. Let $B > \text{const} \times \|f\|_1$. Then
\[ \inf_{f \in \mathcal{G}_p(\psi, B, r_n)} \|f_0 - f\|_{L^2} \leq B \cdot r_n^{-\frac{1}{2} - \frac{\alpha}{p+1}}. \]

Proposition 1 shows that the approximation rate based on ANNs is always faster than $O(n^{-1/2})$, no matter how large the dimension of $X$ is. Hence, it overcomes the “curse of dimensionality” problem that typically arises in nonparametric kernel and linear sieve estimation. To facilitate our subsequent statistical applications, we allow $r_n$ to depend on sample size $n$, and denote the resulting ANN sieve as $\mathcal{G}_n := \mathcal{G}_p(\psi, B, r_n)$. We denote the $L_2$-projection of $f(X)$ on the ANN sieve space $\mathcal{G}_n$ by $\text{Proj}_{\mathcal{G}_n} f(X)$. Let $f_0(\cdot) \in \mathcal{F}_p$ be defined by $E[L_n(f_0(\cdot))] \geq E[L_n(f(\cdot))|$ for all $f(\cdot) \in \mathcal{F}_p$, where $L_n(f(\cdot)) := n^{-1} \sum_{i=1}^n \ell(X_i; f(\cdot))$ with $\ell(\cdot; \cdot) : \mathbb{R}^p \times \mathcal{F}_p \to \mathbb{R}$ being the empirical criterion based on a single observation. The sieve extremum estimates (Chen and Shen, 1998) of $f_0(\cdot)$, denoted by $\hat{f}(\cdot) \in \mathcal{G}_n$, is defined by
\[ \hat{f}(\cdot) := \arg \max_{f \in \mathcal{G}_n} L_n(f(\cdot)). \tag{4} \]

The following result establishes the approximation rate of $f_0$ by $\hat{f}$. The proof of Proposition 2 is presented in Supplement ??.

**Proposition 2.** Let $f_0 \in \mathcal{F}_p$. Suppose the conditions imposed in Proposition 1 hold. Assume
\[ p = O(\log r_n) \text{ and } r_n^{2(1+\frac{\alpha}{p})} \cdot \{\log r_n\}^2 = O(n). \tag{5} \]

Then
\[ \|\hat{f} - f_0\|_{L^2} = O_P \left( \frac{n}{(\log n)^{\frac{1+2\alpha/(p+1)}{2(1+\alpha/(p+1))}}} \right). \]

**Remark:**
1. The convergence rate established in Proposition 2 is slightly slower than that given in Chen and White (1999), i.e. $O_P \left( \left\{ \frac{n}{\log n} \right\}^{-\frac{1+2\alpha/(p+1)}{2(1+\alpha/(p+1))}} \right)$. The slower convergence rate is caused by the increasing dimension of $X$ with the sample size (i.e., we allow $p \to \infty$ as $n \to \infty$), while the dimension of $X$ is considered as fixed in Chen and White (1999).
2. To ensure that the $L_2$-approximation rate of the ANN estimate $\hat{f}(\cdot)$ achieves $o_P(n^{-1/4})$, i.e.
\[
\|\hat{f} - f_0\|_{L_2} = o_P(n^{-1/4}), \tag{6}
\]
which is critical to establish the $\sqrt{n}$-asymptotic normality of the TE estimator, the growing speed of $p$ cannot be too fast; indeed, the rate in Proposition 2 can be written as
\[
[n/(\log n)^2]^{-1+2\alpha/(p+1)}/[4(1+\alpha/(p+1))]
\]
\[
=n^{-1/4} \cdot n^{-\alpha/(p+1)/(4+\alpha/(p+1))} \cdot \{\log n\}^{1/2+\alpha/(p+1)/[2(1+\alpha/(p+1))]}.
\]
To ensure the above rate to be $o_P(n^{-1/4})$, it is equivalent to require that
\[
n^{-\alpha/(p+1)/(4+\alpha/(p+1))} \cdot \{\log n\}^{1/2+\alpha/(p+1)/[2(1+\alpha/(p+1))]} \rightarrow 0
\]
\[
\Leftrightarrow \log n^{1/2} \cdot \left[\frac{\{\log n\}^2}{n}\right]^{-\alpha/(p+1)/(4+\alpha/(p+1))} \rightarrow 0
\]
\[
\Leftrightarrow \frac{1}{2} \log \log n + \frac{\alpha/(p+1)}{4(1+\alpha/(p+1))} \cdot [2 \log \log n - \log n] \rightarrow -\infty
\]
\[
\Leftrightarrow 2 \cdot \log \log n + \frac{\alpha}{(p + 1) + \alpha} \cdot [2 \log \log n - \log n] \rightarrow -\infty
\]
\[
\Leftrightarrow \frac{(p + 1) + 2\alpha}{(p + 1) + \alpha} \cdot \log \log n - \frac{1}{2} \cdot \frac{\alpha}{(p + 1) + \alpha} \cdot \log n \rightarrow -\infty
\]
\[
\Leftrightarrow \{1 + O(p^{-1})\} \log \log n - \frac{1}{2} \cdot \frac{\alpha}{(p + 1) + \alpha} \cdot \log n \rightarrow -\infty \text{ [since } p \rightarrow +\infty\].
\]
Therefore, the growth rate of $p$ shall be restricted to
\[
p = p(n) \leq C \cdot \alpha \cdot \frac{\log n}{\log \log n} \text{ for } 0 < C < \frac{1}{2}. \tag{7}
\]
For example, let $p = O((\log n)^\nu)$ for any $0 < \nu < 1$, Condition (7) holds.

4. Inverse probability weighting estimation

We first apply ANN sieve extremum estimation derived in Section 3 to estimate the propensity score function $\pi_d^*(X)$, then use the empirical version of (2) to construct the estimates of $\beta^*$. The log-likelihood function of the observation $(D_{di}, X_i)$ is:
\[
\ell_d(D_{di}, X_i; \pi_d(\cdot)) := D_{di} \log \pi_d(X_i) + \{1 - D_{di}\} \log(1 - \pi_d(X_i)),
\]
and the true propensity score $\pi_d^*(X)$ satisfies $\mathbb{E}[\ell_d(D_{di}, X_i; \pi_d^*(\cdot))] \geq \mathbb{E}[\ell_d(D_{di}, X_i; \pi_d(\cdot))]$ for all $\pi_d(\cdot)$. Let

$$L_{d,n}(\pi_d(\cdot)) := \frac{1}{n} \sum_{i=1}^{n} \ell_d(D_{di}, X_i; \pi_d(\cdot)).$$

The sieve extremum estimator of $\pi_d^*(\cdot)$ based on ANN is defined by

$$\hat{\pi}_d(\cdot) := \arg \max_{\pi_d(\cdot) \in \mathcal{G}_n} L_{d,n}(\pi_d(\cdot)). \quad (8)$$

where

$$\mathcal{G}_n := \left\{ g : g(x) = \frac{\exp(f(x))}{1 + \exp(f(x))}, \quad f(x) = \gamma_0 + \sum_{j=1}^{r_n} \gamma_j \psi(a_j^\top x + a_{j0}), \quad \max_{1 \leq j \leq r_n} \sum_{k=0}^{p} |a_{jk}| \leq B, \quad \sum_{j=1}^{r_n} |\gamma_j| \leq B \right\}.$$ 

Here we use a logit transformed ANN to ensure the estimated propensity score lies between 0 and 1. The estimates of $\beta^*$, denoted by $\hat{\beta}_d = \{\hat{\beta}_j\}_{j=0}^J$, are defined to be

$$\hat{\beta}_d = \arg \min_{\beta_d} \frac{1}{n} \sum_{i=1}^{n} \frac{D_{di}}{\hat{\pi}_d(X_i)} L(Y_i - \beta_d), \quad d \in \{0, 1, ..., J\}. \quad (9)$$

5. Large sample properties

**Assumption 3.** (i) Let $\Theta$ be a compact set of $\mathbb{R}^{J+1}$. The parameter space $\Theta \times \mathcal{F}_p$ contains the true parameters $(\beta^*, \{\pi_d^*(\cdot)\}_{d=0}^J)$. (ii) The propensity scores are uniformly bounded away from zero and one, i.e., there exist two constants $\underline{\pi}$ and $\overline{\pi}$ such that

$$0 < \underline{\pi} \leq \pi_d^*(x) \leq \overline{\pi} < 1,$$

for all $x \in \mathcal{X}$ and $d \in \{0, 1, ..., J\}$. (iii) The random variable $\mathbb{E}[\ell'(Y - \beta_d^*)|X]$ is bounded.

**Assumption 4.**

1. The dimension of $X$ is denoted by $p \in \mathbb{N}$, and it possibly grows to infinity as the sample size $n$ increases, with the rate

$$p \leq C \cdot \alpha \cdot \log n / \log \log n, \quad \text{for any } 0 < C < 1/2,$$

where $\alpha$ is the degree of smoothness of activation function defined in Assumption 2.
2. The number of hidden units is denoted by \( r_n \), and it grows to infinity as the sample size \( n \) increases, with the rate 

\[
\sqrt{n} \cdot r_n^{2(1+\frac{1}{p}+\alpha)} \to 0 \quad \text{and} \quad r_n^2 \left( 1+\frac{1}{p}+\alpha \right)^n \{\log r_n\}^2 = O(n).
\]

Assumption 3 (i) is a regular condition on the parameter space that is typically imposed in the nonparametric estimation literature. Assumption 3 (ii) is the overlap condition ensuring the existence of participants at all treatment levels, which is commonly assumed in the literature. Assumption 4 (i) imposes restrictions on the growth rate of the dimension of covariates to ensure that the \( L^2 \)-convergence rate of estimated propensity score is of \( o_P(n^{-1/4}) \), see remark 2 in Section 3. Assumption 4 (ii) imposes restrictions on the smoothing parameters. Both of them are needed for the \( \sqrt{n} \)-consistency of the TE estimator. It is worth noting that Assumption 4 implies Condition (5).

The following lemma is critical for establishing the efficiency of the proposed estimator \( \hat{\beta} \), see the discussion in the end of this section. The proof of Lemma 3 is presented in Supplement ??.

Lemma 3. Let \( E_d(X) := \mathbb{E}[L'(Y^*(d) - \beta_j^*)|X] \) for \( d \in \{0, 1, ..., J\} \). Under Assumptions 1-4, we have

\[
\sqrt{n} \cdot \mathbb{E} \left[ \left\{ \frac{\hat{\pi}_d(X) - \pi_j^*(X)}{\pi_j^*(X)} \right\} E_d(X) \right] = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left\{ \frac{D_{di} - \pi_j^*(X_i)}{\pi_j^*(X_i)} \right\} E_d(X_i) + o_p(1).
\]

In order to establish the \( \sqrt{n} \)-normality of the proposed estimator \( \hat{\beta} \), we impose the following conditions:

Assumption 5. We assume \( \hat{\beta} = (\hat{\beta}_j)_{j=0}^J \) satisfies the stochastic first order condition, i.e. for every \( d \in \{0, 1, ..., J\} \):

\[
\frac{1}{n} \sum_{i=1}^{n} \frac{D_{di}}{\hat{\pi}_d(X_i)} L' \left( Y_i - \hat{\beta}_d \right) = o_P(n^{-1/2}).
\]

Assumption 6. \( L(Y - \beta) \) is continuous in \( \beta \), \( \sup_{\beta \in \Theta} \mathbb{E}[L(Y - \beta)] < \infty \) and \( \mathbb{E}[\sup_{\beta \in \Theta} |L(Y - \beta)|] < \infty \).

Assumption 7.

1. There exists a finite positive constants \( C \) such that for any \( \beta \in \Theta \) and any \( \delta > 0 \) in a neighborhood of 0,

\[
\mathbb{E} \left[ \sup_{\beta:|\beta - \beta_\delta|<\delta} \{L'(Y - \beta) - L'(Y - \beta_\delta)\}^2 \right] \leq C \cdot \delta.
\]

2. \( \mathbb{E} \left[ \sup_{\beta \in \Theta} |L'(Y - \beta)|^{2+\delta} \right] < \infty \) for some \( \delta > 0 \).

Assumption 8. Let \( q(Y, \beta) := \{L'(Y - \beta) - L'(Y - \beta^*_y)\}^2 \),
1. there exist some finite positive constants $C$ and $\gamma$ such that for any $\beta \in \Theta$ and any $\delta > 0$ in a neighborhood of 0,

$$
\mathbb{E} \left[ \sup_{\tilde{\beta} : |\tilde{\beta} - \beta| < \delta} \left\{ q(Y, \tilde{\beta}) - q(Y, \beta) \right\} \right] \leq C \cdot \delta^\gamma.
$$

2. $\mathbb{E} \left[ \sup_{\beta \in \Theta} |q(Y, \beta)|^{2+\delta} \right] < \infty$ for some $\delta > 0$.

Assumption 5 is the first order condition, similar to the one imposed in $Z$-estimation. This first order condition is satisfied by popular nonsmooth loss functions, see Pakes and Pollard (1989). Assumption 6 is an envelope condition that is sufficient for the applicability of the uniform law of large numbers. A similar condition is also imposed in Newey and McFadden (1994, Lemma 2.4). Assumptions 7 and 8 concern $L^2$ continuity and envelope conditions, which are needed for establishing stochastic equicontinuity and weak convergence, see Andrews (1994, Theorems 4 and 5). Again, they are satisfied by widely used loss functions such as $L(v) = v^2$, $L(v) = v\{\tau - I(v \leq 0)\}$, and $L(v) = v^2 \cdot |\tau - I(v \leq 0)|$ discussed in Section 2.

The following theorem shows that the proposed estimator $\hat{\beta}$ is $\sqrt{n}$-consistent and attains the semiparametric efficiency bound. The proof of Theorem 4 is presented in Supplement ??.

**Theorem 4.** Under Assumptions 1-8, for any $d \in \{0, 1, \ldots, J\}$, we have

1. $\hat{\beta}_d \overset{P}{\rightarrow} \beta^*_d$;
2. $\sqrt{n}(\hat{\beta}_d - \beta^*_d)$ has the following influence representation:

$$
\sqrt{n}(\hat{\beta}_d - \beta^*_d) = H_d^{-1} \cdot \frac{1}{\sqrt{n}} \sum_{i=1}^{n} S_d(Y_i, D_{di}, X_i) + o_P(1),
$$

where $H_d := -\partial_{\beta_d} \mathbb{E}[L'(Y^*(d) - \beta^*_d)]$, and

$$
S_d(Y_i, D_{di}, X_i) := \frac{D_{di}}{\pi^*_d(X_i)} L'(Y_i - \beta^*_d) - \left\{ \frac{D_{di}}{\pi^*_d(X_i)} - \mathbb{E}[L'(Y^*(d) - \beta^*_d)] \right\} \varepsilon_d(X_i) - \mathbb{E}[L'(Y^*(d) - \beta^*_d)].
$$

Hence the estimator $\hat{\beta}$ attains the semiparametric efficiency bound of $\beta^*$ derived by Ai, Linton, Motegi, and Zhang (2018).

Let $\hat{\beta}_{d, true}$ be the estimator of $\beta^*_d$ using the true propensity score $\pi^*_d(X)$, assuming that it is known. By applying Delta method, we can show that $\sqrt{n}(\hat{\beta}_{d, true} - \beta^*_d)$ has the following influence representation

$$
\sqrt{n}(\hat{\beta}_{d, true} - \beta^*_d) = H_d^{-1} \cdot \frac{1}{\sqrt{n}} \sum_{i=1}^{n} S_{d, true}(Y_i, D_{di}, X_i) + o_P(1),
$$
where
\[
S_{d,\text{true}}(Y_i, D_{di}, X_i) := \frac{D_{di}}{\pi_d^*(X_i)} L'\{Y_i - \beta_d^*\} - \mathbb{E}[L'\{Y_i^*(d) - \beta_d^*\}]
\]
\[
= S_d(Y_i, D_{di}, X_i) + \left\{ \frac{D_{di} - \pi_d^*(X_i)}{\pi_d^*(X_i)} \right\} \mathcal{E}_d(X_i).
\]

It can be shown that
\[
\mathbb{E}\left[\left\{ S_{d,\text{true}}(Y_i, D_{di}, X_i) \right\}^2 \right] > \mathbb{E}\left[\left\{ S_d(Y_i, D_{di}, X_i) \right\}^2 \right],
\]
which implies the asymptotic variance of the estimated \(\beta_d^*\) obtained from the true propensity score \(\pi_d^*(X)\) is larger than that obtained from the estimated one \(\hat{\pi}_d(X)\). This phenomenon is also noticed by Hahn (1998) and Hirano, Imbens, and Ridder (2003). The additional term
\[
\left\{ \frac{D_{di} - \pi_d^*(X_i)}{\pi_d^*(X_i)} \right\} \mathcal{E}_d(X_i)
\]
in the efficient influence function \(S_d(Y_i, D_{di}, X_i)\) comes from Lemma 3.

6. Variance estimation

A consistent variance estimator is needed to conduct statistical inference. Theorem 4 gives that the efficient covariance matrix of \(\beta^*\) is
\[
V = H^{-1} \mathbb{E}[S(Y, D, X)S^\top(Y, D, X)]H^{-1},
\]
where \(H = \text{Diag}\{H_0, ..., H_J\}\) and \(S(Y, D, X) = (S_0, ..., S_J)^\top\). Hence a consistent covariance estimates can be obtained by replacing \(\{H_d\}_{d=0}^J\) and \(\{S_d\}_{d=0}^J\) with some consistent estimates.

Since the nonsmooth loss function may invalidate the exchangeability between the expectation and derivative operator, some care in the estimation of \(H_d\) is warranted. Using the tower property of conditional expectation, we rewrite \(H_d\) as:
\[
H_d = -\partial_{\beta_d} \mathbb{E} \left[ \frac{D_{di}}{\pi_d^*(X)} \cdot \mathbb{E} [L'(Y - \beta_d)|D, X] \right]_{\beta_d = \beta_d^*}
\]
\[
= -\mathbb{E} \left[ \frac{D_{di}}{\pi_d^*(X)} \cdot \partial_{\beta_d} \mathbb{E} [L'(Y - \beta_d)|D, X] \right]_{\beta_d = \beta_d^*}.
\]

Applying integration by parts (see Supplement ??), we obtain
\[
\partial_{\beta_d} \mathbb{E} [L'(Y - \beta_d)|D = d, X = x] \big|_{\beta_d = \beta_d^*}
\]
\[
= \mathbb{E} \left[ L'(Y - \beta_d^*) \frac{\partial}{\partial y} \log f_{Y,X|D}(Y,X|d) \big| D = d, X = x \right] (10)
\]
and consequently
\[
H_d = -E \left[ \frac{D_d}{\pi_d(X)} L'(Y - \beta^*_d) \frac{\partial}{\partial y} \log f_{Y,X|D}(Y, X | d) \right].
\]

The log density \( \log f_{Y,X|D}(y, x | d) \) can be estimated via the widely used sieve extremum estimator (Chen, 2007, Example 2.6, page 5565):
\[
\hat{f}_{Y,X|D}(y, x | d) := \frac{\exp \left( \hat{a}_{d,K_0}^T r_{K_0}(y, x) \right)}{\int_{Y \times X} \exp \left( \hat{a}_{d,K_0}^T r_{K_0}(y, x) \right) dy dx},
\]
where \( \hat{a}_{K_0} \in \mathbb{R}^{K_0} \) (\( K_0 \in \mathbb{N} \)) maximizes the following concave objective function:
\[
\hat{a}_{d,K_0} := \arg \max_{a \in \mathbb{R}^{K_0}} \frac{1}{n} \sum_{i=1}^{n} D_{di} \left[ a^T r_{K_0}(Y_i, X_i) - \log \int_{Y \times X} \exp (a^T r_{K_0}(y, x)) dy dx \right],
\]
and \( r_{K_0}(y, x) \) is a \( K_0 \)-dimensional sieve basis. Then \( H_d \) can be estimated by
\[
\hat{H}_d := \frac{1}{n} \sum_{i=1}^{n} \frac{D_{di}}{\hat{\pi}_d(X_i)} L'(Y_i - \hat{\beta}_d) \cdot \left\{ \hat{a}_{d,K_0}^T \frac{\partial}{\partial y} r_{K_0}(Y_i, X_i) \right\}. \tag{11}
\]

Under Assumption 1, \( E_d(X) = E[L'(Y - \beta^*_d)|X, D = d] \), hence \( E_d(X) \) can be estimated by using ANN extremum estimates:
\[
\hat{E}_d(\cdot) := \arg \min_{g(\cdot) \in G_n} \frac{1}{n} \sum_{i=1}^{n} D_{di} \left\{ L' \left( Y_i - \hat{\beta}_d \right) - g(X_i) \right\}^2.
\]

Therefore, the plug-in estimates of \( S_d(Y, D, d, X) \) is
\[
\hat{S}_d(Y_i, D_{di}, X_i) = \frac{D_{di}}{\hat{\pi}_d(X_i)} L'(Y_i - \hat{\beta}_d) - \frac{D_{di} - \hat{\pi}_d(X_i)}{\hat{\pi}_d(X_i)} \hat{E}_d(X_i) - \frac{1}{n} \sum_{j=1}^{n} \frac{D_{dj}}{\hat{\pi}_d(X_j)} L'(Y_j - \hat{\beta}_d).
\tag{12}
\]

Finally, by (11) and (12), the asymptotic covariance matrix of the estimator is estimated by
\[
\hat{V} := \hat{H}^{-1} \left\{ \frac{1}{n} \sum_{i=1}^{n} \hat{S}(Y_i, D_i, X_i) \hat{S}(Y_i, D_i, X_i)^\top \right\} (\hat{H}^\top)^{-1}.
\]

where \( \hat{H} = \text{Diag}\{\hat{H}_0, ..., \hat{H}_J\} \) and \( \hat{S}(Y, D, X) = (\hat{S}_0, ..., \hat{S}_J)^\top \). Since \( |\hat{\beta}_d - \beta^*_d| \xrightarrow{P} 0 \), \( \hat{\pi}_d(\cdot) \xrightarrow{L^2} \pi_0(\cdot) \) and \( \hat{E}_d(\cdot) \xrightarrow{L^2} E_d(\cdot) \) for all \( d \in \{0, 1, ..., J\} \). Based on these results, the consistency of \( \hat{V} \), i.e., \( \hat{V} \xrightarrow{P} V \) follows from standard arguments.

The asymptotic normality of \( \hat{\beta} = (\hat{\beta}_0, \hat{\beta}_1, ..., \hat{\beta}_J)^\top \) established in Theorem 4 together with the consistency of \( \hat{V} \) provides a theoretical support for conducting statistical inference of the TE parameter vector \( \beta^* = (\beta^*_0, \beta^*_1, ..., \beta^*_J)^\top \). For
instance, based on these results, we can construct a $100(1 - \alpha)\%$ confidence interval for each $\beta^*_d$, $0 \leq d \leq J$, given by
$$\left[ \hat{\beta}_d - n^{-1/2}z_{\alpha/2}\hat{\mathbf{V}}_{\mathbf{d}}^{1/2}, \quad \hat{\beta}_d + n^{-1/2}z_{\alpha/2}\hat{\mathbf{V}}_{\mathbf{d}}^{1/2} \right],$$
where $\hat{\mathbf{V}}_{\mathbf{d}}$ is the $(d, d)$-element of the estimated covariance matrix $\hat{\mathbf{V}}$, and $z_{\alpha/2}$ is the $100(1 - \alpha/2)$ percentile of the standard normal. We can also construct confidence intervals for a contrast of $\beta^*$ for a comparison of different TE parameters. That is, for any given $\mathbf{a} \in \mathbb{R}^{J+1}$, a $100(1 - \alpha)\%$ confidence interval for $\mathbf{a}^T\beta^*$ is given by
$$\left[ \mathbf{a}^T\hat{\beta} - n^{-1/2}z_{\alpha/2}(\mathbf{a}^T\hat{\mathbf{V}}\mathbf{a})^{1/2}, \quad \mathbf{a}^T\hat{\beta} + n^{-1/2}z_{\alpha/2}(\mathbf{a}^T\hat{\mathbf{V}}\mathbf{a})^{1/2} \right].$$

### 7. Outcome regression estimation

Using Assumption 1 and the property of conditional expectation, we can rewrite (13) as follows:
$$\beta^* = \arg\min_{\beta} \sum_{d=0}^J \mathbb{E}[L(Y - \beta_d)|X, D = d].$$

Based on above expression, an alternative estimation strategy is to first estimate the conditional expectation $\mathbb{E}[L(Y - \beta_d)|X, D = d]$ (with $\beta_d$ being fixed), then estimate $\beta^*$ by minimizing the empirical version of (13) with estimated $\mathbb{E}[L(Y - \beta_d)|X, D = d]$. However, unlike the linear sieve estimation, there may not exist a closed form for ANN estimator of $\mathbb{E}[L(Y - \beta_d)|X, D = d]$, hence the outcome regression estimation for a general $L(\cdot)$ is difficult to obtain. In this section, we consider a particular but important parameter ATE which corresponds to $L(\nu) = \nu^2$. In this case, $\beta^*_d = \mathbb{E}[Y^*(d)] = \mathbb{E}[g^*_d(X)]$, where $g^*_d(X) := \mathbb{E}[Y|X, D = d]$ is the outcome regression function. We can estimate $g^*_d(X)$ through neural networks:
$$\hat{g}_d(\cdot) = \arg\min_{g(\cdot) \in \mathcal{G}_d} \frac{1}{2n} \sum_{i=1}^n D_{di} \{ Y_i - g(X_i) \}^2.$$ 

Then the outcome regression (OR) estimator of $\beta^*_d$ is defined to be
$$\hat{\beta}_d^{OR} = \frac{1}{n} \sum_{i=1}^n \hat{g}_d(X_i).$$

#### Theorem 5.
Under Assumptions 1-8, for any $d \in \{0, 1, \ldots, J\}$, we have that
$$\sqrt{n}(\hat{\beta}_d^{OR} - \beta^*_d) = \frac{1}{\sqrt{n}} \sum_{i=1}^n \left[ \frac{D_{di}}{\pi^*_d(X_i)} Y_i - \left( \frac{D_{di} - \pi^*_d(X_i)}{\pi^*_d(X_i)} \right) g^*_d(X_i) - \mathbb{E}[g^*_d(X_i)] \right] + o_P(1).$$

Hence the estimator $\hat{\beta}^{OR}$ attains the semiparametric efficiency bound of $\beta^*$ derived by Ai, Linton, Motegi, and Zhang (2018).

The proof of Theorem 5 is presented in Supplement ??.
8. Related extensions

8.1. Treatment effect on the treated

We consider another causal parameters defined on the treated subgroup. Let

$$\beta_{d'} := \arg\min_{\beta} \sum_{d=0}^{J} \mathbb{E} [L (Y^\ast (d) - \beta_d)|D = d'],$$

(15)

for some fixed $d' \in \{0, 1, ..., J\}$, where $\beta = (\beta_0, \beta_1, ..., \beta_J)$ and $\beta^* = (\beta^*_0, d', \beta^*_1, d', ..., \beta^*_J, d').$

The formulation (15) includes the following important cases discussed in Lee (2018):

- $L(v) = v^2$, then $\beta^*_{d', d'} = \mathbb{E}[Y^\ast (d)|D = d']$ is the average treatment effects on the treated.
- $L(v) = v\{\tau - I(v \leq 0)\}$, then $\beta^*_{d,d'} = F_{Y^\ast (d)}^{-1}(\tau|d')$ is the $\tau$th quantile of $Y^\ast (d)$ conditioned on the treated group $\{D = d'\}$.

Under Assumption 1, using the property of conditional expectation, the parameter of interest $\beta^*_{d'}$ is identified by

$$\hat{\beta}^*_{d'} := \arg\min_{\beta} \sum_{d=0}^{J} \frac{1}{p_{d'}} \mathbb{E} [I(D = d')L (Y^\ast (d) - \beta_d)]$$

$$= \arg\min_{\beta} \sum_{d=0}^{J} \frac{1}{p_{d'}} \mathbb{E} [\pi^\ast_{d'}(X) \cdot \mathbb{E}[L (Y^\ast (d) - \beta_d) | X]]$$

$$= \arg\min_{\beta} \sum_{d=0}^{J} \frac{1}{p_{d'}} \mathbb{E} \left[ \pi^\ast_{d'}(X) \cdot \mathbb{E}[L (Y^\ast (d) - \beta_d) | X] \cdot \mathbb{E} \left[ \frac{I(D = d)}{\pi^\ast_{d'}(X)} | X \right] \right]$$

$$= \arg\min_{\beta} \sum_{d=0}^{J} \frac{1}{p_{d'}} \mathbb{E} \left[ I(D = d) \cdot \frac{\pi^\ast_{d'}(X)}{\pi^\ast_{d'}(X)} \cdot L (Y - \beta_d) \right].$$

Therefore, we define the estimator of $\beta^*_{d'}$ by minimizing the empirical analogue of the above equation:

$$\hat{\beta}_{d'} = \arg\min_{\beta} \sum_{d=0}^{J} \frac{\sum_{i=1}^{n} D_{d,i} \tilde{\pi}_{d'}(X_i) L (Y_i - \beta_d) / \tilde{\pi}_{d'}(X_i)}{\sum_{i=1}^{n} D_{d,i}},$$

where $\tilde{\pi}_{d'}(X)$ is the ANN estimator of $\pi^\ast_{d'}(X)$. Similar to Theorem 4, we can establish the following result of efficient estimation of $\beta^*_{d'}$.

**Theorem 6.** Under Assumptions 1-8, for any $d \in \{0, 1, ..., J\}$, we have that

$$\sqrt{n}(\hat{\beta}_{d,d'} - \beta^*_{d,d'}) = H_{d,d'}^{-1} \cdot \frac{1}{\sqrt{n}} \sum_{i=1}^{n} S_{d,d'}(X_i, D_{d,i}, Y_i) + o_P(1),$$
where $H_{d,d'} = \partial_{\beta_d} \mathbb{E}[L'(Y^*_d(d) - \beta^*_d)|D_{d,i} = 1]$ and

$$S_{d,d'}(X_i, D_{d,i}, Y_i) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left\{ \frac{\pi^{*}_{d}(X_i)}{p_{d'}} \cdot \frac{D_{d,i}}{\pi^{*}_{d}(X_i)} L'(Y_i - \beta^*_{d,d'}) \right. - \left. \frac{\pi^{*}_{d}(X_i)}{p_{d'}} \cdot \frac{D_{d,i} - \pi^{*}_{d}(X_i)}{\pi^{*}_{d}(X_i)} \cdot \mathbb{E} \left[ L'(Y^*_d(d) - \beta^*_{d,d'})|X_i \right] \right\}.$$  

Hence the estimator $\hat{\beta}_d$ attains the semiparametric efficiency bound of $\beta^*_d$ derived by Ai, Linton, Motegi, and Zhang (2018).

### 8.2. Deep neural networks

The proposed method can be extended to networks with multiple hidden layers. To motivate the idea, we consider the following ReLU feed-forward network function space indexed by the number of parameter $W$,

$$\mathcal{G}_W = \{ h_{L+1,1}(x) \},$$

where $h_{u,j}(x)$ is the output of the $j^{th}$ node of the layer $u$ in the network with input $x$, $u = 0$ or $u = L + 1$ correspond to the input and output layers, respectively, and $1 \leq u \leq L$ correspond to the $u^{th}$ hidden layer. We also have $j \in \{1, 2, ..., H_u\}$, where $H_u$ is the number of nodes (width) in the $u^{th}$ layer, $H_0 = p$, and $H_{L+1} = 1$. For $1 \leq u \leq L$, the formula for $h_{u,j}(x)$ is

$$h_{u,j}(x) = \text{ReLU} \left( \sum_{k=1}^{H_{u-1}} \gamma_{u,j,k} \cdot h_{u-1,k}(x) + \gamma_{u,j,0} \right),$$

where $h_{0,j}(x) = x_k$, the $k^{th}$ element of $x$.

We use the upper bound

$$\max_{1 \leq j \leq H_u} \sum_{k=0}^{H_{u-1}} |\gamma_{u,j,k}| \leq M_u, \text{ for all } 1 \leq u \leq L + 1,$$

where $M_u > 1$, $M_u$ can depend on $u$, and $M_0 = 1$. Let $W$ be the number of parameters $\gamma_{u,j,k}$ in the network, with $W = \sum_{u=0}^{L}(H_u + 1)H_{u+1}$. Replacing $\mathcal{G}_n$ in (8) by $\mathcal{G}_W$, the estimator of the propensity score, denoted by $\hat{\pi}_d(x)$, can be constructed. Then the estimator of $\beta^*_d$, denoted by $\hat{\beta}_d$, can be obtained through (9).

Suppose $\pi^*_d(x)$ is $s$-times differentiable, by Yarotsky (2018, Proposition 1), there exists $\text{Proj}_{\mathcal{G}_W} \pi^*_d \in \mathcal{G}_W$ s.t.

$$\|\text{Proj}_{\mathcal{G}_W} \pi^*_d - \pi^*_d\|_\infty = O \left( W^{-\frac{s}{s+1}} \right).$$

Unfortunately, unlike Proposition 1 where a “dimension free” approximation rate can be obtained by using ANNs with one hidden layers, (16) indicates
that the approximation rate decreases as the dimension of \( X \) grows, when the propensity score function is estimated by ANNs with multiple hidden layers in which neurons between two adjacent layers are fully-connected. Hence, the curse of dimensionality problem still exists. We treat \( p \) as a fixed integer in this subsection.

Let

\[
M^*_{L+1} = \prod_{i=1}^{L+1} M_u, \quad M^{\text{all}}_{L+1} = \max_{1 \leq u \leq L+1} M_u, \quad \text{and} \quad C^*_{L+1, W} = W \cdot \log \left( p \cdot M^*_{L+1} \cdot W \cdot (M^{\text{all}}_{L+1})^L \right).
\]

By (??) in the supplement, the convergence rate of estimated \( \pi^*_d(X) \), denoted by \( \hat{\pi}_d(X) \), is

\[
\|\hat{\pi}_d(X) - \pi^*_d(X)\|_{L^2} = O_P \left( \max \{ \delta_n, \| \pi^*_d(X) - \text{Proj}_{G^W} \pi^*_d(X) \| \} \right),
\]

where

\[
\delta_n = \inf \left\{ \delta > 0 : \delta^{-2} \int_{2^{-1}w}^{\delta} [H(w, G^W)]^{1/2} dw \leq \text{const} \times n^{1/2} \right\}. \tag{17}
\]

By van der Vaart (1998), the bracketing number \( H(w, G^W) \) has the following upper bound:

\[
H(w, G^W) = \log N\left( \frac{1}{2} w, G^W, \| \cdot \|_\infty \right) \leq \log N \left( \frac{1}{2} w, G^W, \| \cdot \|_\infty \right),
\]

where \( N \left( \frac{1}{2} w, G^W, \| \cdot \|_\infty \right) \) denotes the covering number of \( G^W \) by balls with radius \( 2^{-1}w \) under \( \| \cdot \|_\infty \)-metric. By Anthony and Bartlett (2009, Theorem 14.5), the covering number has the following upper bound:

\[
N \left( \frac{1}{2} w, G^W, \| \cdot \|_\infty \right) \leq \left( \frac{8 \cdot e \cdot p \cdot M^*_{L+1} \cdot W \cdot (M^{\text{all}}_{L+1})^L}{w \cdot (M^{\text{all}}_{L+1} - 1)} \right)^W.
\]

Then

\[
H(w, G^W) \leq W \cdot \log \left( \frac{8 \cdot e \cdot p \cdot M^*_{L+1} \cdot W \cdot (M^{\text{all}}_{L+1})^L}{w \cdot (M^{\text{all}}_{L+1} - 1)} \right).
\]

We choose

\[
\delta_n = \text{const} \times \{ W \cdot \log W \}^{1/2} \cdot n^{-1/2},
\]

such that (17) is satisfied. Setting \( \delta_n = \| \pi^*_d(X) - \text{Proj}_{G^W} \pi^*_d(X) \|_{L^2} \) yields:

\[
W^{1+\frac{p}{2}} \log W = O(n).
\]
Assume that the width of the $u$th layer satisfies $H_u = H$ for all $1 \leq u \leq L$. Then $W = \{p+1\} \cdot H + \sum_{u=1}^{L-1} \{H + 1\} H + \{H + 1\} = (L-1)H^2 + (L+p+1)H + 1$. The above condition implies that $L$ and $H$ need to satisfy $L^{1+2s} H^{2(1+2s)} \log(LH^2) = O(n)$.

We see that if using a deep ANNs with $L \to \infty$, the width of each hidden layer $H$ can be much smaller than the width of the single hidden layer ANNs $r_n$ that needs to satisfy Assumption 4 (ii).

As a consequence,

$$\|\widehat{\pi}_d - \pi^*_d\|_{L^2} = O_P \left( \left[ \frac{n}{\log n} \right]^{s/2s^2} \right).$$

If $p < 2s$, then we can obtain

$$\|\widehat{\pi}_d - \pi^*_d\|_{L^2} = o_P(n^{-1/4}).$$

With these results, the arguments in Lemma 3 and Theorem 4 are still valid. Therefore, the proposed estimator $\hat{\beta}_d$ constructed by using the deep ReLU networks still achieves the semiparametric efficiency bound.

9. Simulation studies

9.1. Background and methods used

In this section, we illustrate the finite sample performance of our proposed methods via simulations in which we generate data from models in Section 9.2. Our proposed IPW estimator can be applied to various types of treatment effects. We use ATE, ATT (average treatment effects on the treated), QTE and QTT (quantile treatment effects on the treated) for illustration of the performance of the IPW estimator. For QTE and QTT, we consider the 25th (Q1), 50th (Q2) and 75th (Q3) quantiles. We also illustrate the performance of the OR estimator for ATE and ATT. For these estimators, we estimate the PS and OR functions by using our proposed feed-forward artificial neural networks (ANN) method. We also compare the TE estimator from the ANN method with that obtained by estimating the PS and OR functions from five other popular methods, including the generalized linear models (GLM), the generalized additive models (GAM), the kernel regression models (KN), the random forests (RF) and the gradient boosted machines (GBM). Moreover, we compare these estimators to the oracle estimators. The oracle estimators are constructed based on the efficient influence function with the true PS and OR functions plugged in, see Hahn (1998). The oracle estimators are infeasible in practice, but they are expected to perform the best, and they can provide good references to compare the performance of other estimators with.

For the ANN method, we use the Rectified Linear Unit (ReLU) as the activation function and one hidden layer. For the GAM method, we use a cubic
regression spline basis. For the methods involving hyper parameter selection: the number of neurons, batch size, number of epochs and the learning rate in the NN method, the bandwidth in the KN method, the number of trees and max depths in the RF and GBM methods, we apply grid search with 5-fold cross-validation, and select the hyper parameters which minimize cross entropy for the PS functions and mean squared error for the OR functions. All the other hyper parameters are set to be the default values from the software packages. All the simulations are implemented in Python 3.6. The ANN method is implemented using package tensorflow, the GLM and KN methods are implemented using package statsmodel, the GAM method is implemented using package pyGAM, and the RF and GBM methods are implemented using package h2o.

9.2. Data generating process

For illustration of different methods, we generate data from the following nonlinear PS and OR models:

\[
\begin{align*}
\text{logit}\{\mathbb{E}(D_i | X_i)\} &= X_{i1}X_{i2} - X_{i3}X_{i4}X_{i5} \\
\mathbb{E}(Y_i(1)|X_i) &= X_{i1}^2 + X_{i2}^2 + 2X_{i1}X_{i2} - 2\sin(X_{i3} + X_{i4}X_{i5}) + 1 \\
\mathbb{E}(Y_i(0)|X_i) &= X_{i1}^2 + X_{i2}^2 + 2X_{i1}X_{i2} + \sin(X_{i3} + X_{i4}X_{i5}) - 1,
\end{align*}
\]

where \(Y_i(d) = \mathbb{E}(Y_i \mid D_i = d, X_i) + \epsilon_i\) for \(d = \{0, 1\}\), \(X_i\) are independently generated from \(\mathcal{U}([-1, 1]^p)\), and \(\epsilon_i\) are independently generated from the standard normal distribution for \(1 \leq i \leq n\). We consider \(p = 5, 10, 15, 20\) and \(n = 2000, 5000\). All simulation results are based on 200 realizations.

9.3. Simulation results

Tables 1 - 8 report the empirical coverage rates (rate) of the 95% confidence intervals, the average of the absolute values of biases (bias), the average values of the estimated standard deviations (est\_sd), and the empirical standard deviations (emp\_sd) of the estimators for ATE, ATT, QTE and QTT for \(p = 5, 10, 15, 20\), respectively, based on 200 simulation realizations. The estimated standard deviations of treatment effect estimators are calculated as in Section 6.

We observe that the ANN estimates and the oracle estimates have similar bias and est\_sd values in all simulation settings. The proposed ANN method has superior performance comparing to other five methods. The OR estimates for ATE and ATT have slightly smaller bias and est\_sd values than the IPW estimates. In contrast, the GLM and GAM estimates have very small coverage rates but yield large biases and est\_sd. This implies that when the PS and OR models are nonlinear, the estimates from GLM and GAM can be very biased and inefficient due to the model misspecification. The KN estimates perform relatively better compared to the parametric models when \(p = 5\), but the performance deteriorate severely when \(p\) increases since the KN method suffers from curse of
Table 1
The empirical coverage rates (rate), the average of the absolute values of biases (bias), the empirical standard deviation (emp_sd) and the average of the estimated standard deviations (est_sd) of the estimated ATE and ATT for p=5

| n=2000 | n=5000 |
|--------|--------|
| ANN | GLM | GAM | KN | RF | GBM | Oracle | ANN | GLM | GAM | KN | RF | GBM | Oracle |
| ATE rate | 0.935 | 0.150 | 0.150 | 0.870 | 0.640 | 0.855 | 0.950 | 0.935 | 0.000 | 0.005 | 0.875 | 0.745 | 0.910 | 0.955 |
| IPW bias | 0.050 | 0.211 | 0.212 | 0.059 | 0.083 | 0.054 | 0.047 | 0.011 | 0.213 | 0.213 | 0.038 | 0.039 | 0.032 | 0.028 |
| emp_sd | 0.062 | 0.072 | 0.072 | 0.064 | 0.071 | 0.061 | 0.059 | 0.039 | 0.043 | 0.042 | 0.036 | 0.046 | 0.041 | 0.036 |
| OR rate | 0.965 | 0.170 | 0.145 | 0.670 | 0.305 | 0.830 | 0.950 | 0.945 | 0.010 | 0.015 | 0.560 | 0.125 | 0.905 | 0.955 |
| OR bias | 0.045 | 0.211 | 0.212 | 0.085 | 0.125 | 0.080 | 0.067 | 0.041 | 0.213 | 0.213 | 0.065 | 0.104 | 0.036 | 0.028 |
| emp_sd | 0.055 | 0.072 | 0.071 | 0.066 | 0.073 | 0.061 | 0.059 | 0.036 | 0.043 | 0.042 | 0.036 | 0.046 | 0.041 | 0.036 |
| ATT rate | 0.940 | 0.180 | 0.205 | 0.665 | 0.345 | 0.590 | 0.950 | 0.945 | 0.010 | 0.015 | 0.540 | 0.320 | 0.470 | 0.965 |
| ATT bias | 0.057 | 0.214 | 0.217 | 0.104 | 0.147 | 0.123 | 0.053 | 0.035 | 0.212 | 0.213 | 0.115 | 0.095 | 0.087 | 0.033 |
| emp_sd | 0.074 | 0.079 | 0.082 | 0.073 | 0.077 | 0.071 | 0.053 | 0.044 | 0.046 | 0.044 | 0.044 | 0.045 | 0.043 | 0.033 |
| est_sd | 0.072 | 0.076 | 0.064 | 0.058 | 0.065 | 0.061 | 0.059 | 0.042 | 0.047 | 0.047 | 0.047 | 0.047 | 0.046 | 0.046 |

Table 2
The empirical coverage rates (rate), and the average of the absolute values of biases (bias), the empirical standard deviation (emp_sd) and the average of the estimated standard deviations (est_sd) of the estimated ATE and ATT for p=10

| n=2000 | n=5000 |
|--------|--------|
| ANN | GLM | GAM | KN | RF | GBM | Oracle | ANN | GLM | GAM | KN | RF | GBM | Oracle |
| ATE rate | 0.925 | 0.100 | 0.110 | 0.645 | 0.495 | 0.895 | 0.960 | 0.945 | 0.005 | 0.005 | 0.770 | 0.770 | 0.830 | 0.950 |
| IPW bias | 0.051 | 0.216 | 0.216 | 0.080 | 0.097 | 0.050 | 0.043 | 0.036 | 0.209 | 0.208 | 0.035 | 0.038 | 0.038 | 0.031 |
| emp_sd | 0.059 | 0.063 | 0.065 | 0.060 | 0.061 | 0.057 | 0.055 | 0.047 | 0.047 | 0.047 | 0.047 | 0.047 | 0.047 | 0.047 |
| OR rate | 0.970 | 0.105 | 0.100 | 0.270 | 0.235 | 0.690 | 0.960 | 0.970 | 0.005 | 0.005 | 0.095 | 0.150 | 0.710 | 0.950 |
| OR bias | 0.041 | 0.216 | 0.214 | 0.135 | 0.135 | 0.080 | 0.043 | 0.031 | 0.209 | 0.209 | 0.112 | 0.051 | 0.051 | 0.033 |
| emp_sd | 0.053 | 0.063 | 0.066 | 0.061 | 0.059 | 0.055 | 0.047 | 0.047 | 0.047 | 0.047 | 0.047 | 0.047 | 0.047 | 0.047 |
| est_sd | 0.059 | 0.068 | 0.066 | 0.064 | 0.064 | 0.061 | 0.059 | 0.047 | 0.047 | 0.047 | 0.047 | 0.047 | 0.047 | 0.047 |
| ATT rate | 0.945 | 0.170 | 0.220 | 0.265 | 0.220 | 0.525 | 0.955 | 0.935 | 0.005 | 0.005 | 0.175 | 0.170 | 0.340 | 0.975 |
| ATT bias | 0.059 | 0.215 | 0.212 | 0.148 | 0.148 | 0.124 | 0.053 | 0.041 | 0.209 | 0.209 | 0.123 | 0.036 | 0.036 | 0.036 |
| emp_sd | 0.074 | 0.078 | 0.076 | 0.070 | 0.071 | 0.065 | 0.058 | 0.044 | 0.044 | 0.044 | 0.044 | 0.044 | 0.044 | 0.044 |
| est_sd | 0.072 | 0.076 | 0.078 | 0.066 | 0.067 | 0.062 | 0.061 | 0.048 | 0.048 | 0.048 | 0.048 | 0.048 | 0.048 | 0.048 |

Overall, the GBM method has the second best performance. It performs similar to the KN method when p is small, but it is better than KN when p is large. The RF estimates are relatively inferior compared to the KN estimates for small p but are more stable when p increases. We show that the proposed ANN method performs well in estimating ATE, ATT, QTE and QTT when the true model structure is not known a priori. The method can also be applied to estimate the asymmetric least square TE and other types of TEs by setting the loss function as \( L(v) = v^2 \cdot |\tau - I(v \leq 0)| \) and so forth, and has similar patterns of the numerical results. The results were not presented here due to space limitations.

10. Application
In this section, we apply the proposed methods to the data from the National Health and Nutrition Examination Survey (NHANES) to investigate the causal effect of smoking on body mass index (BMI). The collected data consist of 6647 subjects, including 3359 smokers and 3288 nonsmokers. The confounding variables include four continuous variables: age, family poverty income ratio (Family PIR), systolic blood pressure (SBP), and diastolic blood pressure (DBP);
The empirical coverage rates (rate), and the average of the absolute values of biases (bias), the empirical standard deviation (emp \text{std}) and the average of the estimated standard deviations (est \text{std}) of the estimated ATE and ATT for p=15

| n=2000 | n=5000 |
|--------|--------|
| IPW    |        |        |
| base   | 0.051  | 0.021  |
| emplge | 0.062  | 0.065  |
| ATT    | 0.050  | 0.061  |
| base   | 0.062  | 0.065  |
| emplge | 0.066  | 0.068  |

The empirical coverage rates (rate), and the average of the absolute values of biases (bias), the empirical standard deviation (emp \text{std}) and the average of the estimated standard deviations (est \text{std}) of the estimated ATE and ATT for p=20

| n=2000 | n=5000 |
|--------|--------|
| IPW    |        |        |
| base   | 0.060  | 0.068  |
| emplge | 0.065  | 0.067  |
| ATT    | 0.050  | 0.061  |
| base   | 0.062  | 0.065  |
| emplge | 0.066  | 0.068  |

The empirical coverage rates (rate), and the average of the absolute values of biases (bias), the empirical standard deviation (emp \text{std}) and the average of the estimated standard deviations (est \text{std}) of the estimated QTE and QTT for p=5

| n=2000 | n=5000 |
|--------|--------|
| QTE    |        |        |
| base   | 0.080  | 0.089  |
| emplge | 0.086  | 0.092  |
| QTT    | 0.085  | 0.095  |
| base   | 0.080  | 0.089  |
| emplge | 0.086  | 0.092  |

The empirical coverage rates (rate), and the average of the absolute values of biases (bias), the empirical standard deviation (emp \text{std}) and the average of the estimated standard deviations (est \text{std}) of the estimated QTE and QTT for p=10

| n=2000 | n=5000 |
|--------|--------|
| QTE    |        |        |
| base   | 0.080  | 0.089  |
| emplge | 0.086  | 0.092  |
| QTT    | 0.085  | 0.095  |
| base   | 0.080  | 0.089  |
| emplge | 0.086  | 0.092  |
Table 6

The empirical coverage rates (rate), and the average of the absolute values of biases (bias), the empirical standard deviation (emp_sd) and the average of the estimated standard deviations (est_sd) of the estimated QTE and QTT for p=10

|        | ANN | GLM | GAM | KN | RF | GBM | Oracle |
|--------|-----|-----|-----|----|----|-----|---------|
| rate   |     |     |     |    |    |     |         |
| Q1     | 0.945 | 0.430 | 0.400 | 0.540 | 0.420 | 0.400 | 0.940 |
|        |     |     |     |    |    |     |         |
| rate   |     |     |     |    |    |     |         |
| Q2     | 0.945 | 0.340 | 0.400 | 0.540 | 0.420 | 0.400 | 0.940 |
|        |     |     |     |    |    |     |         |
| rate   |     |     |     |    |    |     |         |
| Q3     | 0.945 | 0.240 | 0.270 | 0.305 | 0.250 | 0.305 | 0.930 |
|        |     |     |     |    |    |     |         |
| rate   |     |     |     |    |    |     |         |
| Q4     | 0.945 | 0.120 | 0.140 | 0.170 | 0.130 | 0.170 | 0.930 |
|        |     |     |     |    |    |     |         |
| rate   |     |     |     |    |    |     |         |
| Q5     | 0.945 | 0.060 | 0.070 | 0.090 | 0.060 | 0.090 | 0.920 |
|        |     |     |     |    |    |     |         |
| rate   |     |     |     |    |    |     |         |

Table 7

The empirical coverage rates (rate), and the average of the absolute values of biases (bias), the empirical standard deviation (emp_sd) and the average of the estimated standard deviations (est_sd) of the estimated QTE and QTT for p=15

|        | ANN | GLM | GAM | KN | RF | GBM | Oracle |
|--------|-----|-----|-----|----|----|-----|---------|
| rate   |     |     |     |    |    |     |         |
| Q1     | 0.945 | 0.430 | 0.400 | 0.540 | 0.420 | 0.400 | 0.940 |
|        |     |     |     |    |    |     |         |
| rate   |     |     |     |    |    |     |         |
| Q2     | 0.945 | 0.340 | 0.400 | 0.540 | 0.420 | 0.400 | 0.940 |
|        |     |     |     |    |    |     |         |
| rate   |     |     |     |    |    |     |         |
| Q3     | 0.945 | 0.240 | 0.270 | 0.305 | 0.250 | 0.305 | 0.930 |
|        |     |     |     |    |    |     |         |
| rate   |     |     |     |    |    |     |         |
| Q4     | 0.945 | 0.120 | 0.140 | 0.170 | 0.130 | 0.170 | 0.930 |
|        |     |     |     |    |    |     |         |
| rate   |     |     |     |    |    |     |         |
| Q5     | 0.945 | 0.060 | 0.070 | 0.090 | 0.060 | 0.090 | 0.920 |
|        |     |     |     |    |    |     |         |
| rate   |     |     |     |    |    |     |         |


Table 8

The empirical coverage rates (rate), and the average of the absolute values of biases (bias), the empirical standard deviation (emp sd) and the average of the estimated standard deviations (est sd) of the estimated QTE and QTT for p=20

| p   | N=2000 | N=5000 |
|-----|--------|--------|
|     | ANN    | GLM    | GAM    | KN     | RF     | GBM    | Oracle | ANN    | GLM    | GAM    | KN     | RF     | GBM    | Oracle |
| QTE  |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| rate | 0.945  | 0.560  | 0.695  | 0.605  | 0.610  | 0.615  | 0.950  | 0.950  | 0.130  | 0.175  | 0.175  | 0.180  | 0.280  | 0.950  |
| Q1   | 0.078  | 0.174  | 0.169  | 0.166  | 0.161  | 0.164  | 0.140  | 0.145  | 0.005  | 0.005  | 0.005  | 0.005  | 0.005  | 0.005  |
| bias | 0.080  | 0.081  | 0.094  | 0.091  | 0.095  | 0.092  | 0.055  | 0.055  | 0.005  | 0.005  | 0.005  | 0.005  | 0.005  | 0.005  |
| emp sd | 0.097  | 0.096  | 0.109  | 0.095  | 0.095  | 0.094  | 0.059  | 0.059  | 0.005  | 0.005  | 0.005  | 0.005  | 0.005  | 0.005  |
| est sd |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| QTE  |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| rate | 0.970  | 0.185  | 0.410  | 0.220  | 0.185  | 0.280  | 0.950  | 0.950  | 0.055  | 0.115  | 0.050  | 0.070  | 0.175  | 0.965  |
| Q1   | 0.087  | 0.087  | 0.108  | 0.082  | 0.084  | 0.089  | 0.057  | 0.057  | 0.005  | 0.005  | 0.005  | 0.005  | 0.005  | 0.005  |
| bias | 0.090  | 0.094  | 0.112  | 0.097  | 0.097  | 0.096  | 0.060  | 0.060  | 0.005  | 0.005  | 0.005  | 0.005  | 0.005  | 0.005  |
| emp sd | 0.098  | 0.099  | 0.115  | 0.099  | 0.100  | 0.099  | 0.064  | 0.064  | 0.005  | 0.005  | 0.005  | 0.005  | 0.005  | 0.005  |
| est sd |        |        |        |        |        |        |        |        |        |        |        |        |        |        |

Table 9

Group comparisons

| Covariate | Non-smoker (Nns=3288) | Smoker (Ns=3359) | Std. Dif. | p-value |
|-----------|------------------------|-----------------|-----------|---------|
| Gender    | 1 = Male 1404 (41.8%)  | 2019 (61.41%)   | -15.99    | <0.001  |
| 0 = Female| 1955 (58.2%)          | 1269 (38.59%)   |           |         |
| Age       | Mean(SD) 48.97 (19)   | 51.73 (17.57)   | -6.14     | <0.001  |
| Marital   | 1 = Yes 1989 (59.21%)  | 1867 (56.78%)   | 2.01      | 0.0446  |
| 0 = No    | 1370 (40.79%)         | 1421 (43.22%)   |           |         |
| Education | 1 = College or above 1626 (48.41%) | 1297 (39.45%) | 7.36     | <0.001  |
| 0 = Less than college | 2257 (67.19%) | 2380 (72.38%) |           |         |
| Family PIR| Mean(SD) 2.79 (1.63)  | 2.57 (1.41)     | 5.62      | <0.001  |
| Alcohol   | 1 = Yes 1907 (56.48%)  | 2708 (82.36%)   | -22.87    | <0.001  |
| 0 = No    | 1462 (43.52%)         | 580 (17.64%)    |           |         |
| PHSVIG    | 1 = Yes 1102 (32.81%)  | 908 (27.62%)    | 4.61      | <0.001  |
| 0 = No    | 2257 (67.19%)         | 2380 (72.38%)   |           |         |
| PHSMOD    | 1 = Yes 1491 (44.39%)  | 1376 (41.85%)   | 4.61      | <0.001  |
| 0 = No    | 1868 (55.61%)         | 1912 (58.15%)   |           |         |
| SBP       | Mean(SD) 126.42 (21.04) | 126.63 (19.98) | -0.43     | 0.6604  |
| DBP       | Mean(SD) 72.1 (13.56)  | 71.41 (14.41)   | 1.44      | 0.15    |

six binary variables: gender, marital status, education, alcohol use, vigorous activity over past 30 days (PHSVIG), and moderate activity over past 30 days (PHSMOD). Table 9 presents the group comparisons of all confounding variables in the full dataset. Mean and standard deviation (SD) are presented for continuous variables, while the count and percentage (%) of observations for each group are presented for categorical variables. Standardized difference (Std. Dif.) is calculated as \( (\bar{x}_{ns} - \bar{x}_s) / \sqrt{\frac{s^2_{ns}}{n_{ns}} + \frac{s^2}{n_s}} \) for continuous variables, and \( (p_{ns} - p_s) / \sqrt{\frac{pq}{n_{ns} + n_s}} \) for categorical variables, where \( \bar{x}, s^2 \) and \( p \) denote sample mean, sample variance and sample proportion, and the subscripts \( ns \) and \( s \) refer to nonsmokers and smokers respectively, and \( p, q \) are the overall proportions. The last column shows the p-value of group comparison for each covariate. We notice that smoking group and nonsmoking group differ greatly in their group characteristics. A naive comparison of the sample mean between smoking and nonsmoking groups will lead to a biased estimation of the smoking effects on BMI.
We apply our proposed ANN methods to estimate the PS and OR functions, respectively. Hyper parameters for neural network including number of hidden units, learning rates, batches and number of epochs are selected using grid search with 5-fold cross-validation, and all the other hyper parameters are set to be the default values in the Python package tensorflow. Table 10 reports the estimates, estimated standard deviations (est sd), z-values and p-values for ATE and QTE. The negative values of the estimates indicate that smoking has adverse effects on BMI. We can see that the p-values of ATE are 0.065 and 0.112 by the IPW and OR methods respectively. We also notice that the p-value for the 25th QTE is smaller than 0.05, but the p-values for the 50th quantile and 75th quantile are 0.087 and 0.672 respectively. This indicates that smoking has more prominent effect on the population with smaller BMI, and its effect diminishes as BMI increases.

We also examine the relationship between BMI and two continuous confounding variables, age and family poverty income ratio (Family PIR). Figure 1 depicts the estimated conditional mean functions (OR functions) $\tau_1(\cdot)$ and $\tau_0(\cdot)$ versus the two continuous variables for the smoking and nonsmoking groups, and for males and females, respectively. For each comparison, all the other confounding variables are fixed as constants: the continuous variables take the values of their means while the categorical variables are kept as married, college or above, drinks alcohol, no vigorous activity and no moderate activity. It is interesting to notice that for the same age or Family PIR, the estimated conditional mean in the smoking group is smaller than that in the nonsmoking group for both male and female, and the estimated conditional mean in the male group is also smaller than that in the female group for both smoker and nonsmoker. We can clearly see nonlinear relationships between age and BMI as well as between Family PIR and BMI. Age is positively associated with BMI when it is less than 50, and the association between age and BMI becomes more negative as people get older. We also see that the smoking effects on BMI are very different between the male group and female group. Smoking has more significant effect on BMI for male than for female at the same age. In the male group, the BMI decreases as family income increases until it reaches the poverty threshold, and then the BMI increases with family income for smokers. For nonsmokers, it shows a relatively flatter trend. In the female group, the BMI keeps decreasing as family income increases for both smokers and nonsmokers.

|                | ATE   | QTE   |
|----------------|-------|-------|
|                | IPW   | OR    | Q1   | Q2   | Q3   |
| estimate       | -0.256| -0.221| -0.410| -0.289| -0.100|
| est sd         | 0.139 | 0.139 | 0.162 | 0.169 | 0.236 |
| z-value        | -1.842| -1.590| -2.531| -1.710| -0.423|
| p-value        | 0.065 | 0.112 | 0.011 | 0.087 | 0.672 |
Fig 1. The plots of $\tau_1(\cdot)$ and $\tau_0(\cdot)$ versus two continuous variables for the smoking and nonsmoking groups, and for males and females, respectively, where the blue solid curves represent nonsmoking group and red dashed line represent smoking group.
11. Conclusions

In this paper, we provide a unified framework for efficient estimation of various types of TEs in observational data with a diverging number of covariates. The framework can be applied to the settings with binary or multi-valued treatment variables, and it includes the average, quantile and asymmetric least squares TEs as special cases. We propose to estimate the TEs through a generalized optimization. The resulting TE estimator only involves the estimate of one nuisance function, which is approximated by ANNs with one hidden layer. In contrast, for other existing related works that use machine learning, they construct the TE estimator based on its efficient influence function, so that the estimator can have desirable theoretical properties for conducting causal inference. However, this method loses generalizations as one has to work out the influence function first for each type of TE. Other than ATE, estimation of the influence function for different types of TEs can be a difficult undertaking. Theoretically, we show that the number of confounders is allowed to increase with the sample size, and further investigate how fast it can grow with the sample size to ensure root-n consistency of the resulting TE estimator, when the nuisance function is approximated by ANNs with one hidden layer. Moreover, we establish asymptotic normality and semiparametric efficiency of the TE estimator. These statistical properties are essential for inferring causations. Practically, we illustrate the proposed method through simulation studies and a real data example. The numerical studies support our theoretical findings.

We also discuss the extension of our proposed method for TE estimation when the nuisance function is approximated by fully-connected ANNs with multiple hidden layers, and investigate its statistical properties. We show that the fully-connected deep ANNs requires that the number of covariates be fixed to ensure the desirable statistical properties of the resulting TE estimator, whereas it enjoys narrower width than the single hidden layer ANNs when its depth grows with the sample size. As a future work, we will consider sparse deep ANNs to overcome the dimensionality issue of the fully-connected ones, and will investigate the statistical properties in this framework. These interesting yet challenging technical problems deserve further studies. Moreover, the proposed method can be extended to causal analysis with continuous treatment variables and with longitudinal data designs. Thorough investigations are needed to develop the computational algorithms and establish the theoretical properties of the resulting estimators in these settings.

Supplementary Material

Supplement to “Efficient Estimation of General Treatment Effects using Neural Networks with A Diverging Number of Confounders” (). The supplement contains the technical proofs of Lemma 3, Proposition 2 and Theorems 4 and 5.
References

Abadi, M., A. Agarwal, P. Barham, and et al. (2016): “TensorFlow: Large-scale machine learning on heterogeneous systems,” http://arxiv.org/abs/1603.04467.

Ai, C., O. Linton, K. Motegei, and Z. Zhang (2018): “A Unified Framework for Efficient Estimation of General Treatment Models,” arXiv preprint arXiv:1808.04936.

Andrews, D. W. (1994): “Empirical process methods in econometrics,” Handbook of Econometrics, 4, 2247–2294.

Anthony, M., and P. L. Bartlett (2009): Neural network learning: Theoretical foundations. Cambridge University Press.

Athey, S., J. Tibshirani, and S. Wager (2019): “Generalized random forests,” Annals of Statistics, 47(523), 1148–1178.

Bang, H., and J. M. Robins (2005): “Doubly robust estimation in missing data and causal inference models,” Biometrics, 61, 962–973.

Bauker, B., and M. Kohler (2019): “On deep learning as a remedy for the curse of dimensionality in nonparametric regression,” The Annals of Statistics, 47(4), 22612285.

Bellman, R. (1961): Curse of dimensionality. Adaptive control processes: a guided tour. Princeton, NJ.

Cao, W., A. A. Tsiatis, and M. Davidian (2009): “Improving efficiency and robustness of the doubly robust estimator for a population mean with incomplete data,” Biometrika, 96, 723–734.

Cattaneo, M. D. (2010): “Efficient semiparametric estimation of multi-valued treatment effects under ignorability,” Journal of Econometrics, 155(2), 138–154.

Chan, K. C. G., and S. C. P. Yam (2014): “Oracle, multiple robust and multipurpose calibration in a missing response problem,” Statistical Science, 29, 380–396.

Chan, K. C. G., S. C. P. Yam, and Z. Zhang (2016): “Globally efficient non-parametric inference of average treatment effects by empirical balancing calibration weighting,” Journal of the Royal Statistical Society: Series B (Statistical Methodology), 78(3), 673–700.

Chen, X. (2007): “Large sample sieve estimation of semi-nonparametric models,” Handbook of Econometrics, 6(B), 5549–5632.

Chen, X., H. Hong, A. Tarozzi, et al. (2008): “Semiparametric efficiency in GMM models with auxiliary data,” The Annals of Statistics, 36(2), 808–843.

Chen, X., and X. Shen (1998): “Sieve extremum estimates for weakly dependent data,” Econometrica, pp. 289–314.

Chen, X., and H. White (1999): “Improved rates and asymptotic normality for nonparametric neural network estimators,” IEEE Transactions on Information Theory, 45(2), 682–691.

Ding, P., and F. Li (2018): “Causal inference: a missing data perspective,” Statistical Science, 33, 214–237.

Farrell, M. H. (2015): “Robust inference on average treatment effects with
possibly more covariates than observations,” *Journal of Econometrics*, 189(1), 1–23.

Farrell, M. H., T. Liang, and S. Misra (2019): “Deep Neural Networks for Estimation and Inference,” *arXiv preprint arXiv:1809.09953*.

Firpo, S. (2007): “Efficient Semiparametric Estimation of Quantile Treatment Effects,” *Econometrica*, 75(1), 259–276.

Freedman, D. A., and R. A. Berk (2008): “Weighting regression by propensity scores,” *Evaluation Review*, 32, 392–409.

Hahn, J. (1998): “On the role of the propensity score in efficient semiparametric estimation of average treatment effects,” *Econometrica*, 66(2), 315–331.

Han, P. (2018): “A General Framework for Quantile Estimation with Incomplete Data,” *Statistica Sinica*, 28, 1307–1332.

Han, P., L. Kong, and J. Zhao (2019): “A General Framework for Quantile Estimation with Incomplete Data,” *Journal of the Royal Statistical Society, Series B*, 81, 305333.

Heckman, J. J., H. Ichimura, and P. Todd (1998): “Matching as an econometric evaluation estimator,” *The Review of Economic Studies*, 65(2), 261–294.

Hirano, K., G. W. Imbens, and G. Ridder (2003): “Efficient Estimation of Average Treatment Effects Using the Estimated Propensity Score,” *Econometrica*, 71(4), 1161–1189.

Hornik, K., M. Stinchcombe, H. White, and P. Auer (1994): “Degree of approximation results for feedforward networks approximating unknown mappings and their derivatives,” *Neural Computation*, 6(6), 1262–1275.

Huang, M.-Y., and K. C. G. Chan (2017): “Joint sufficient dimension reduction and estimation of conditional and average treatment effects,” *Biometrika*, 104(3), 583–596.

Kang, J. D., and J. L. Schafer (2007): “Demystifying double robustness: a comparison of alternative strategies for estimating a population mean from incomplete data,” *Statistical Science*, 22, 523–539.

Kennedy, E., Z. Ma, M. McHugh, and D. Small (2017): “Nonparametric methods for doubly robust estimation of continuous treatment effects,” *Journal of the Royal Statistical Society: Series B*, 79, 1229–1245.

Kingma, D. P., and J. Ba (2014): “Adam: A method for stochastic optimization,” *arXiv preprint arXiv:1412.6980*.

Lee, Y.-Y. (2018): “Efficient propensity score regression estimators of multivalued treatment effects for the treated,” *Journal of Econometrics*, 204(2), 207–222.

Li, Q., and J. S. Racine (2007): *Nonparametric econometrics: theory and practice*. Princeton University Press.

Luo, W., Y. Zhu, and D. Ghosh (2017): “On estimating regression-based causal effects using sufficient dimension reduction,” *Biometrika*, 104, 51–65.

Ma, S., L. Zhu, Z. Zhang, C.-L. Tsai, and R. J. Carroll (2019): “A robust and efficient approach to causal inference based on sparse sufficient dimension reduction,” *Annals of statistics*, 47(3), 1505.

Newey, W. K., and D. McFadden (1994): “Large sample estimation and
hypothesis testing,” *Handbook of econometrics*, 4, 2111–2245.
NING, Y., S. PENG, AND K. IMAI (2020): “Robust estimation of causal effects via a high-dimensional covariate balancing propensity score,” *Biometrika*, 107(3), 533–554.
PAKES, A., AND D. POLLARD (1989): “Simulation and the asymptotics of optimization estimators,” *Econometrica: Journal of the Econometric Society*, pp. 1027–1057.
ROSENBAUM, P. R., AND D. B. RUBIN (1983): “The central role of the propensity score in observational studies for causal effects,” *Biometrika*, 70(1), 41–55.
ROTNITZKY, A., Q. LEI, M. SUED, AND J. M. ROBINS (2012): “Improved double-robust estimation in missing data and causal inference models,” *Biometrika*, 99, 439–456.
SCHMIDT-HIEBER, J. (2020): “Nonparametric regression using deep neural networks with ReLU activation function,” *Annals of Statistics*, 48, 1875–1897.
TAN, Z. (2010): “Bounded, efficient and doubly robust estimation with inverse weighting,” *Biometrika*, 97, 661–682.
——— (2020): “Model-assisted inference for treatment effects using regularized calibrated estimation with high-dimensional data,” *Annals of Statistics*, 48, 811837.
VAN DER LAAN, M. J., AND J. M. ROBINS (2003): *Unified Methods for Censored Longitudinal Data and Causality*. Springer, New York.
VAN DER LAAN, M. J., AND S. ROSE (2011): *Targeted Learning: Causal Inference for Observational and Experimental Data*. Springer, New York.
VAN DER VAART, A. W. (1998): *Asymptotic statistics*. Cambridge University Press.
WAGER, S., AND S. ATHEY (2018): “Estimation and Inference of Heterogeneous Treatment Effects using Random Forests,” *Journal of the American Statistical Association*, 113(523), 1228–1242.
WHITE, H. (1992): *Artificial neural networks: approximation and learning theory*. Blackwell Publishers, Inc.
YAO, Q., AND H. TONG (1996): “Asymmetric least squares regression estimation: A nonparametric approach,” *Journal of Nonparametric Statistics*, 6, 2–3.
YAROTSKY, D. (2018): “Optimal approximation of continuous functions by very deep ReLU networks,” *arXiv preprint arXiv:1802.03620*. 