Tuning-parameter-free optimal propensity score matching approach for causal inference

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Abstract

Propensity score matching (PSM) is a pseudo-experimental method that uses statistical techniques to construct an artificial control group by matching each treated unit with one or more untreated units of similar characteristics. To date, the problem of determining the optimal number of matches per unit, which plays an important role in PSM, has not been adequately addressed. We propose a tuning-parameter-free PSM method based on the nonparametric maximum-likelihood estimation of the propensity score under the monotonicity constraint. The estimated propensity score is piecewise constant, and therefore automatically groups data. Hence, our proposal is free of tuning parameters. The proposed estimator is asymptotically semiparametric efficient for the univariate case, and achieves this level of efficiency in the multivariate case when the outcome and the propensity score depend on the covariate in the same direction. We conclude that matching methods based on the propensity score alone cannot, in general, be efficient.

Keywords: Average treatment effect on the treated, pool adjacent violated algorithm, propensity score matching estimators, semiparametric efficiency, shape-restricted maximum likelihood estimator, simple score estimator, unconfoundedness

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1 Introduction

To assess the treatment effect in medical studies, randomized and controlled clinical trials are the gold standard because the baseline covariates are balanced in the treatment and control arms by the randomization. To evaluate the effectiveness of an economic program or policy in econometrics or political science, however, randomization is difficult or impossible to implement for various reasons. In observational studies, the available covariate information from people who participated in the program or not may be unbalanced. The simple two-sample $t$-test is likely to produce biased results. It is desirable to replicate a randomized experiment as closely as possible by obtaining treated and control groups with similar covariate distributions. Due to the simplicity and intuitiveness of adjusting the distribution of covariates among samples from different populations, matching methods are widely used in applied statistics, econometrics, and epidemiology. Many examples can be found in a comprehensive review paper by Stuart (2010).

A common feature of matching methods is the outcome-independence of matching, i.e., outcome values are not used in the matching process even if they are available at the time of matching. This precludes the selection of a matched sample that leads to a desired or undesired result. Commonly used matching methods are all based on covariate values. They use the “distance” between treated and untreated individuals, which is a measure of the similarity between two individuals. A well-known example is the Mahalanobis distance. Another popular matching method is propensity matching, which was proposed by Rosenbaum and Rubin (1983). The propensity score is the conditional probability of assignment to a treatment given a vector of covariates. Suppose that adjusting for a set of covariates is sufficient to eliminate confounding. A key observation made by Rosenbaum and Rubin (1983) is that adjusting for the propensity score is also sufficient to eliminate confounding. In contrast to covariate-based distance matching methods, propensity score matching (PSM) has the advantage of reducing the dimensionality of matching to a single dimension, making the matching process much easier.

Although various matching methods have been used, the theoretical results have only recently been studied by Abadie and Imbens (2006, 2012, 2016). This series of papers showed that matching estimators based on the covariate distance involve a biased term that is only negligible under certain regularity conditions. Moreover, the matching estimators are not necessarily root-$n$-consistent, and some strong conditions are needed to guarantee the root-$n$-consistency. Furthermore, they demonstrated that, even in settings where matching estimators are root-$n$-consistent, simple matching estimators with a fixed number of matches do not attain the semiparametric efficiency bound. Furthermore, they found that matching
estimators based on the estimated propensity score have smaller variances than those based on the true PSM. To make the matching methods accessible to practitioners, Imbens (2015) used three examples to demonstrate practical implementations from the theoretical literature, and provided detailed recommendations on how the procedures should be performed. In her review paper in Statistical Science, Stuart (2010) lists some of the major software packages that implement matching procedures. A regularly updated version is also available at [http://www.biostat.jhsph.edu/~stuart/propensityscoresoftware.html](http://www.biostat.jhsph.edu/~stuart/propensityscoresoftware.html).

In the PSM approach, the most commonly used strategy is to divide the interval [0, 1] into K subintervals \([a_i, a_{i+1}], i = 1, 2, ..., K\), where \(a_1 = 0\) and \(a_{K+1} = 1\). Then, one may compare the treatments and controls for propensity scores that fall into the same subinterval. The performance of this approach is always influenced by the choice of K, which is generally artificial, and the numbers of individuals falling into each subinterval, which is hard to control. Too many subintervals may lead to inflated variances, whereas too few subintervals may lead to biased results. Existing matching methods (Abadie and Imbens, 2006, 2012, 2016) require the matched number of controls for each treatment case to be fixed (not divergent to infinity). A natural question is “Are there any optimal methods for choosing K and the minimum number of observations in each matched interval?” To the best of our knowledge, no research has yet been conducted to address these issues.

In this paper, we present a tuning-parameter-free optimal matching method to solve the two thorny issues outlined above, where “optimal” means the resulting matching estimator achieves the asymptotic semiparametric efficiency lower bound. Rather than the commonly used parametric logistic model, we assume a nonparametric and monotone nondecreasing function for the propensity score in the univariate case. In the multivariate case, we assume a single-index propensity score model with a nonparametric and monotone nondecreasing link function. Our method is based on the semiparametric maximum-likelihood estimation of the propensity score function, which can be implemented numerically by the well-known pool adjacent violated algorithm (Ayer et al., 1955, PAVA). As the semiparametric maximum-likelihood estimator (MLE) of the propensity score is a piecewise step function, individuals in the treatment arm can be exactly matched by individuals in the control arm based on their estimated propensity scores. This matching method is purely data-driven and involves no artificial interference. We show that the proposed tuning-free matching estimator is not only asymptotically unbiased, but also achieves the semiparametric efficiency lower bound in the univariate case. For the multivariate case, the proposed estimator also achieves the semiparametric efficiency lower bound if the outcome and propensity score depend on the covariate in the same direction. Otherwise, the proposed estimator remains consistent, but is not efficient. In this situation, other PSM methods are relatively inefficient. Our theoretical
results depend critically on the shape-restricted inference and empirical process theory. Our numerical simulation results show that the proposed method outperforms existing commonly used PSM methods in terms of the mean square error. A real econometric dataset is analyzed for illustration. All technical proofs are given in the supplementary material for clarity.

2 Efficient estimation under shape constraints

2.1 Setup

We adopt the potential outcome framework (Neyman 1923/1990; Rubin 1974) with a binary treatment. Let $Y(1)$ and $Y(0)$ be the potential outcomes of a treatment and a control, respectively, which cannot be observed simultaneously. Let $X$ be the baseline covariate, and $D$ be the treatment indicator with $D = 1$ denoting a treatment and $D = 0$ denoting a control. The outcome is $Y(1)$ if $D = 1$ and $Y(0)$ otherwise, which can be written as $Y = Y(D) = DY(1) + (1 - D)Y(0)$. Let $(Y_i, X_i, D_i), i = 1, 2, ..., n$, be $n$ independent and identically distributed observations from $(Y, X, D)$. We focus on the estimation of the average treatment effect on the treated (ATT)

$$\tau = \mathbb{E}\{Y(1) - Y(0)|D = 1\};$$

the average treatment effect $\mathbb{E}\{Y(1) - Y(0)\}$ can be estimated similarly. For the identifiability of treatment effects, we make the commonly used unconfoundedness assumption (Rubin 1978; Rosenbaum and Rubin 1983), i.e., conditional on the observed covariates, the treatment indicator is independent of the potential outcomes.

**Assumption 1** (Unconfounded Treatment Assignment). $D \perp (Y(0), Y(1))|X$.

Denote the propensity score as $\pi(x) = \text{pr}(D = 1|X = x)$. Under Assumption Rosenbaum and Rubin (1983) showed that $D$ and $(Y(0), Y(1))$ are conditionally independent when $X$ is replaced by $\pi(X)$ in the condition, namely

$$D \perp (Y(0), Y(1)|\pi(X)).$$

The most commonly used model for the propensity score is the logistic regression model; however, misspecification of parametric models may lead to inconsistent or misleading treatment effect estimators. To alleviate the risk, we relax the parametric model assumption to a completely nonparametric model in the univariate case, or a semiparametric index model in the multivariate case.
Assumption 2. The covariate $X$ has an absolutely continuous density and $\text{Var}(X)$ is positive in the univariate case and positive-definite in the multivariate case. In addition, the functions $\mu_0(X) = \mathbb{E}\{Y(0) | X\}$, $\mu_1(X) = \mathbb{E}\{Y(1) | X\}$, $\sigma_0^2(X) = \text{Var}(Y(0) | X)$, and $\sigma_1^2(X) = \text{Var}(Y(1) | X)$ are all well-defined for $P_X$-almost surely, and the quantities $\mathbb{E}\{Y(1)^2\}$, $\mathbb{E}\{Y(0)^2\}$, $\mathbb{E}\{\mu_2^1(X)\}$, and $\mathbb{E}\{\mu_2^0(X)\}$ are all finite.

Assumption 2, which requires the covariate to be nondegenerate and the outcome and covariate variables to have finite variances, is trivial. Below, we consider the estimation problem of $\mu_1$ and $\tau$ in the univariate and multivariate cases separately.

2.2 Estimation in the univariate case

We do not make a parametric assumption on the propensity score, but instead assume that $\pi(x)$ is a nonparametric and monotone nondecreasing function. Without loss of generality, we assume $X_1 \leq X_2 \leq \ldots \leq X_n$. Based on $\{(X_i, D_i) : 1 \leq i \leq n\}$, the likelihood of $\pi$ is a binomial likelihood of the form

$$L_B(\pi) = \prod_{i=1}^{n} \pi(X_i)^{D_i} \{1 - \pi(X_i)\}^{1-D_i}, \quad \text{s.t.} \quad \pi(X_1) \leq \pi(X_2) \ldots \leq \pi(X_n).$$

By Theorem 2.12 of Barlow et al. (1972), maximizing this likelihood with respect to $\pi$ is equivalent to minimizing

$$\sum_{i=1}^{n} (D_i - \pi(X_i))^2$$

under the same monotonicity constraint. The solution or the MLE $\hat{\pi}$ is a step function and is the left derivative of the greatest convex minorant of the cumulative sum diagram (Barlow et al., 1972, Theorem 1.1).

Write $\hat{\pi}_i = \hat{\pi}(X_i)$, and let $0 = i_0 < i_1 < \ldots < i_k = n$ be the locations of the inflection points of the greatest convex minorant of the cumulative sum diagram. Then,

$$\hat{\pi}_i = \hat{\pi}(X_i) = \hat{\pi}_{ij}, \quad i_{j-1} < i \leq i_j, \quad j = 1, \ldots, k. \quad (1)$$

According to the lemma on page 34 of Barlow et al. (1972),

$$\hat{\pi}_{ij} = \frac{\sum_{l=i_{j-1}+1}^{i_j} D_l}{i_j - i_{j-1}}, \quad 1 \leq j \leq k. \quad (2)$$

We propose to estimate $\mu_1 = \mathbb{E}\{Y(1)\}$ by

$$\hat{\mu}_1 = \frac{1}{n} \sum_{i=1}^{n} \frac{D_i Y_i}{\pi(X_i)} = \frac{1}{n} \sum_{j=1}^{k} \frac{1}{\hat{\pi}_{ij}} \sum_{l=i_{j-1}+1}^{i_j} D_l Y_l = \sum_{j=1}^{k} \rho_j \hat{\mu}_{1ij}, \quad (3)$$

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where \( \rho_j = (i_j - i_{j-1})/n \) is the proportion of observations falling in the \( j \)-th interval \((x_{i_{j-1}}, x_{i_j}]\), and \( \mu_{ij} = \sum_{i=i_{j-1}+1}^{i_j} D_i Y_i / \sum_{i=i_{j-1}+1}^{i_j} D_i \) is the group mean. If \( \hat{\pi}(X_i) = 0 \), the accompanying \( D_i \) must also be zero, and we define \( D_i / \hat{\pi}(X_i) = 0/0 \) as 0. Essentially, \( \hat{\mu}_1 \) is a weighted average of subgroup means, where the subgroups are formed by the steps of the shape-restricted nonparametric MLE \( \hat{\pi} \). Note that this grouping method is automatically data-driven and is free from any tuning parameter.

**Assumption 3.** (i) There exists \( c_0 > 0 \) such that \( c_0 \leq \pi(t) \leq 1 - c_0 \) for all \( t \in X \). (ii) \( \pi(x) \) has a continuous derivative \( \pi'(x) \) and there exists \( c_1 > 0 \) such that \( 1/c_1 \leq \pi'(x) \leq c_1 \).

**Assumption 4.** There exists \( L > 0 \) such that \( |\mu_1(x_1) - \mu_1(x_2)| \leq L|x_1 - x_2| \).

Assumption 3(i) is the commonly used overlap assumption in the literature of causal inference. Under Assumption 3(ii), both \( \pi(x) \) and its inverse are Lipschitz-continuous. Assumption 3(ii) and Assumption 4 imply that the function \( \mu_1(\pi^{-1}(t)) \) is Lipschitz-continuous, which plays an important role in governing random fluctuations in our proof. Under these assumptions, we show that the proposed estimator \( \hat{\mu}_1 \) is asymptotically unbiased, normal, and achieves the semiparametric efficiency lower bound.

**Theorem 1.** Suppose that Assumptions 3 and 4 are all satisfied. The proposed estimator \( \hat{\mu}_1 \) is asymptotically normal, i.e., \( \sqrt{n}(\hat{\mu}_1 - \mu_1) \xrightarrow{d} N(0, \sigma^2_{\mu}) \) as \( n \to \infty \), where \( \xrightarrow{d} \) denotes “converges in distribution to” and \( \sigma^2_{\mu} = \mathbb{E}\{\sigma^2(X)/\pi(X)\} + \text{Var}\{\mu_1(X)\} \), and the asymptotic variance attains the semiparametric efficiency lower bound.

By PSM, we propose to estimate \( \tau \), the ATT, by

\[
\hat{\tau} = \frac{1}{n_1} \sum_{i=1}^{n} \left\{ Y_i - \frac{\sum_{j=1}^{n} (1 - D_j) Y_j I(\hat{\pi}(X_j) = \hat{\pi}(X_i))}{\sum_{j=1}^{n} (1 - D_j) I(\hat{\pi}(X_j) = \hat{\pi}(X_i))} \right\},
\]

where \( n_1 = \sum_{i=1}^{n} D_i \). A more concise form of \( \hat{\tau} \) is provided in Lemma 1.

**Lemma 1.** The proposed PSM estimator \( \hat{\tau} \) can be equivalently expressed as

\[
\hat{\tau} = \frac{1}{n_1} \sum_{j=1}^{n} \left\{ D_j Y_j - (1 - D_j) Y_j \frac{\hat{\pi}_j}{1 - \hat{\pi}_j} \right\},
\]

which is an inverse probability weighting estimator.

With the estimated propensity scores \( \hat{\pi}_i \), the estimator of \( \tau \) developed by Hirano, Imbens, and Ridder (2003) is

\[
\hat{\tau} = \frac{1}{\sum_{j=1}^{n} \hat{\pi}_j} \sum_{i=1}^{n} \left\{ D_i Y_i - (1 - D_i) Y_i \frac{\hat{\pi}_i}{1 - \hat{\pi}_i} \right\}.
\]
By Theorem 1.7 of [Barlow et al. (1972)], the shape-restricted MLEs $\hat{\pi}_i$ satisfy $\sum_{i=1}^n (\hat{\pi}_i - D_i) = 0$ or, equivalently, $\sum_{i=1}^n \hat{\pi}_i = \sum_{i=1}^n D_i = n_1$. We find that $\hat{\tau} = \tilde{\tau}$, i.e., the proposed PSM estimator is equal to that of [Hirano, Imbens, and Ridder (2003)] in the form for the ATT.

Assumption 5. There exists $L > 0$ such that $|\mu_0(x_1) - \mu_0(x_2)| \leq L |x_1 - x_2|$.

Assumption 5 and Assumption 3 (ii) imply that the function $\mu_0(\tau^{-1}(t))$ is Lipschitz-continuous, which is used to govern random fluctuations in our proof of the asymptotic normality of $\hat{\tau}$.

Theorem 2. Suppose that Assumptions 1–3 and 5 are all satisfied. Let $\eta = \Pr(D = 1)$ and $\tau(X) = \mu_1(X) - \mu_0(X)$. The proposed PSM estimator for the ATT is asymptotically normal, i.e., $\sqrt{n}(\hat{\tau} - \tau) \xrightarrow{d} N(0, \sigma^2_\tau)$ as $n \to \infty$, where

$$\sigma^2_\tau = \frac{1}{\eta^2} \mathbb{E} \left[ \pi(X) (\tau(X) - \tau)^2 + \pi(X) \sigma^2_1(X) + \frac{\pi^2(X)}{1 - \pi(X)} \sigma^2_0(X) \right],$$

and the asymptotic variance attains the semiparametric efficiency lower bound.

[Hahn (1998)] derived the semiparametric efficiency lower bound for the estimation of $\tau$ when the propensity score is unknown (his Theorem 1) and when it is known (his Theorem 2). Our asymptotic variance $\sigma^2_\tau$ is exactly equal to the asymptotic semiparametric efficiency lower bound when the propensity score is unknown. Therefore, it attains the semiparametric efficiency lower bound.

3 Estimation in the multivariate covariate case

When the covariate is a $d$-variate ($d > 1$), we assume that the propensity score is

$$\Pr(D = 1|X = x) = \pi(x^\top \beta),$$

where $\pi$ is a monotone nondecreasing function and $\beta$ is an unknown true $d$-variate parameter. We assume that $\|\beta\| = 1$ for identifiability. Suppose that a consistent estimator $\hat{\beta}$ of $\beta$ is available. We shall consider two estimation methods for $\beta$ in subsections 3.1 and 3.2. Let $Z_i(\hat{\beta}) = X_i^\top \hat{\beta}$ for $i = 1, 2, \ldots, n$. Without loss of generality, we assume that $Z_1(\hat{\beta}) \leq Z_2(\hat{\beta}) \leq \cdots \leq Z_n(\hat{\beta})$. The log-likelihood of $\pi$ becomes

$$\sum_{i=1}^n \left[ D_i \log \pi(Z_i(\hat{\beta})) + (1 - D_i) \log \{1 - \pi(Z_i(\hat{\beta}))\} \right].$$
The MLE of $\pi$ is a step function determined by $\pi(Z_1(\hat{\beta})), \pi(Z_2(\hat{\beta})), \ldots, \pi(Z_n(\hat{\beta}))$, which satisfy the monotonicity restriction $\pi(Z_1(\hat{\beta})) \leq \pi(Z_2(\hat{\beta})) \cdots \leq \pi(Z_n(\hat{\beta}))$. Denote the shape-restricted MLE of $\pi$ as $\hat{\pi}(\cdot)$. Our proposed PSM estimators for $\mu_1$ and $\tau$ are

$$
\hat{\mu}_1 = \frac{1}{n} \sum_{i=1}^{n} \frac{D_i Y_i}{\hat{\pi}(Z_i(\hat{\beta}))} = \frac{1}{n} \sum_{i=1}^{n} \frac{D_i Y_i}{\hat{\pi}(X_i\hat{\beta})},
$$

$$
\hat{\tau} = \frac{1}{n_1} \sum_{j=1}^{n} \left\{ D_j Y_j - (1 - D_j) Y_j \frac{\hat{\pi}(X_j\hat{\beta})}{1 - \hat{\pi}(X_j\hat{\beta})} \right\},
$$

respectively, where we have used a multivariate version of Lemma\[1\]

**Assumption 6.** The ranges of $X$ and $\beta$, $\mathcal{X}$ and $\mathcal{B}$, are convex and compact. Let $t_{low} = \inf\{X^\top \gamma : X \in \mathcal{X}, \gamma \in \mathcal{B}\} - \varepsilon_0$ and $t_{up} = \sup\{X^\top \gamma : X \in \mathcal{X}, \gamma \in \mathcal{B}\} + \varepsilon_0$ for some $\varepsilon_0 > 0$.

**Assumption 7.** There exists $c_0 \in (0, 1)$ such that $c_0 \leq \pi(t) \leq 1 - c_0$ and $\pi$ has a continuous second derivative on $[t_{low}, t_{up}]$, where $t_{low}$ and $t_{up}$ are defined in Assumption\[6\]

Under Assumption\[7\] $\pi'(t)$ is also continuous on the closed interval $[t_{low}, t_{up}]$. Therefore, it must be Lipschitz-continuous, i.e., there exists $c_1 > 0$ such that $|\pi'(t) - \pi'(s)| \leq c_1 |s - t|$ for any $t_{low} \leq s, t \leq t_{up}$.

**Assumption 8.** There exists a constant $M > 0$ such that the density function $f_{X^\top \gamma}(u)$ of $X^\top \gamma$ satisfies $f_{X^\top \gamma}(u) \leq M$ for all $x \in \mathcal{X}$ and $\gamma \in \mathcal{B}$.

Define $\mu_1^*(u; \gamma) = \mathbb{E}\{Y(1)|X^\top \gamma = u\} = \mathbb{E}\{\mu_1(X)|X^\top \gamma = u\}$, and $\mu_0^*(u; \gamma) = \mathbb{E}\{Y(0)|X^\top \gamma = u\}$ = $\mathbb{E}\{\mu_0(X)|X^\top \gamma = u\}$.

**Assumption 9.** The function $\mu_1^*(u; \gamma)$ is continuous in both $u$ and $\gamma$.

**Assumption 10.** The function $\mu_0^*(u; \gamma)$ is continuous in both $u$ and $\gamma$.

Because $\mathcal{X}$ and $\mathcal{B}$ are both compact, Assumptions\[8\] and \[9\] imply that the function $\mu_1^*(X^\top \gamma_1; \gamma_2)$ is Lipschitz-continuous with respect to $(\gamma_1, \gamma_2)$, i.e., there exists a constant $L$ such that

$$
|\mu_1^*(X^\top \gamma_1; \gamma_2) - \mu_1^*(X^\top \gamma_3; \gamma_4)| \leq L(\|\gamma_1 - \gamma_3\| + \|\gamma_2 - \gamma_4\|), \; \gamma_1, \gamma_2, \gamma_3, \gamma_4 \in \mathcal{B}.
$$

The function $\mu_0^*$ has the same property under Assumptions\[8\] and \[10\]. In general, if $\hat{\beta}$ is $\sqrt{n}$-consistent and asymptotically normal, the proposed estimators for $\mu_1$ and $\tau$ both follow asymptotically normal distributions, and both are asymptotically semiparametric efficient under certain additional conditions. Let $\mathbb{P}_n$ denote the empirical measure based on data $\{(X_i, D_i, Y_i) : 1 \leq i \leq n\}$.
Theorem 3. Suppose that model (4) is true, and that Assumptions (1)–(2) and (6)–(8) are satisfied. Define

\[ B_1 = \mathbb{E} \left[ \frac{\pi'(X^\top \beta)}{\pi(X^\top \beta)} \{\mu_1(X) - \mu_0^*(X^\top \beta; \beta)\} X^\top \right]. \]

If \( \hat{\beta} - \beta = O_p(n^{-1/2}) \), then the following results hold as \( n \to \infty \).

1. A linear approximation for \( \hat{\mu}_1 \) is

\[
\begin{align*}
\hat{\mu}_1 - \mu_1 &= \mathbb{P}_n \left[ \frac{D - \pi(X^\top \beta)}{\pi(X^\top \beta)} \{\mu_1(X) - \mu_0^*(X^\top \beta; \beta)\} \\
&\quad + \frac{D(Y - \mu_1(X))}{\pi(X^\top \beta)} + \mu_1(X) - \mu_1 \right] + B_1(\hat{\beta} - \beta) + o_p(n^{-1/2}). \tag{7}
\end{align*}
\]

2. If \( \mu_1(X) = \bar{\mu}_1(X^\top \beta) \) for some function \( \bar{\mu}_1(\cdot) \), then \( \mu_0^*(X^\top \beta; \beta) = \bar{\mu}_1(X^\top \beta) \) and

\[
\sqrt{n}(\hat{\mu}_1 - \mu_1) = \sqrt{n}\mathbb{E}_n \left\{ \frac{D(Y - \bar{\mu}_1(X^\top \beta))}{\pi(X^\top \beta)} + \bar{\mu}_1(X^\top \beta) - \mu_1 \right\} + o_p(1) \\
\xrightarrow{d} N(0, \sigma^2_{\mu,m}).
\]

where \( \sigma^2_{\mu,m} = \text{Var}(\bar{\mu}_1(X^\top \beta)) + \mathbb{E}\{\sigma_1(X)(1 - \pi(X^\top \beta))/\pi(X^\top \beta)\} \) is the asymptotic semiparametric efficiency lower bound. Namely, if both the propensity score and regression function depend on the covariate \( X \) in the same direction, then \( \bar{\mu}_1 \) achieves the asymptotic semiparametric efficiency lower bound, which holds for any \( n^{1/3} \)-consistent estimator \( \hat{\beta} \).

Theorem 4. Suppose that model (4) is true, and that Assumptions (1)–(2) and (6)–(8) and (10) are satisfied. Define

\[ B_2 = \mathbb{E} \left[ \frac{\pi'(X^\top \beta)}{1 - \pi(X^\top \beta)} \{\mu_0(X) - \mu_0^*(X^\top \beta; \beta)\} X^\top \right]. \tag{8} \]

If \( \hat{\beta} - \beta = O_p(n^{-1/2}) \), then the following results hold as \( n \to \infty \).

1. A linear approximation for \( \hat{\tau} \) is

\[
\begin{align*}
\hat{\tau} - \tau &= \frac{1}{\eta} \mathbb{P}_n \left\{ \frac{D(\tau(X) - \tau)}{\eta} + \frac{D(Y(1) - \mu_1(X))}{\eta} \right\} \\
&\quad - \frac{1}{\eta} \mathbb{P}_n \left[ (1 - D) \{Y(0) - \mu_0(X)\} \frac{\pi(X^\top \beta)}{1 - \pi(X^\top \beta)} \right] \\
&\quad + \frac{1}{\eta} \mathbb{P}_n \left[ \frac{D - \pi(X^\top \beta)}{1 - \pi(X^\top \beta)} \{\mu_0(X) - \mu_0^*(X^\top \beta; \beta)\} \right] \\
&\quad - \frac{1}{\eta} B_2(\hat{\beta} - \beta) + o_p(n^{-1/2}). \tag{9}
\end{align*}
\]
(2) If \( \mu_0(X) = \tilde{\mu}_0(X^\top \beta) \) for some function \( \tilde{\mu}_0(\cdot) \), then \( \mu_0(X) = \mu_0^*(X^\top \beta; \beta) = \tilde{\mu}_0(X^\top \beta) \) and

\[
\sqrt{n}(\hat{\tau} - \tau) = \frac{1}{\eta} \sqrt{n} \mathbb{P}_n \left[ D(\tau(X) - \tau) + D(Y(1) - \mu_1(X)) - (1 - D)\{Y(0) - \mu_0(X)\} \frac{\pi(X^\top \beta)}{1 - \pi(X^\top \beta)} \right] + o_p(1)
\]

\[\xrightarrow{d} N(0, \sigma^2_{\tau, \text{m}}),\]

where

\[
\sigma^2_{\tau, \text{m}} = \frac{1}{\eta^2} \left[ \mathbb{E}\{\pi(X)(\tau(X) - \tau)^2\} + \mathbb{E}(\pi(X^\top \beta)\sigma^2_{\tau}(X)) + \mathbb{E}(\sigma^2_0(X) \left\{ \frac{\pi(X^\top \beta)}{1 - \pi(X^\top \beta)} \right\}^2) \right]
\]

is the asymptotic semiparametric efficiency lower bound (Theorem 1 of Hahn, 1998). Namely if both the propensity score and regression function depend on covariate \( X \) in the same direction, then \( \hat{\tau} \) achieves the asymptotic semiparametric efficiency lower bound, which holds for any \( n^{1/3} \)-consistent estimator \( \hat{\beta} \).

Besides the asymptotic normality and efficiency results, Theorems 3 and 4 also indicate that if the propensity score and regression functions depend on the covariate \( X \) in different directions, or the regression functions do not obey single-index models, then neither \( \hat{\mu}_1 \) nor \( \hat{\tau} \) is asymptotically semiparametric efficient.

**Remark 1.** Imai and Ratkovic (2014) introduced a covariate balancing propensity score methodology that models treatment assignment while optimizing the covariate balance. Suppose that \( \pi(X^\top \beta) \) is a correctly specified model for the propensity score. Observing the fact that, for any function \( h(X) \),

\[
\mathbb{E} \left\{ \frac{D}{\pi(X^\top \beta)} h(X) - \frac{1 - D}{1 - \pi(X^\top \beta)} h(X) \right\} = 0,
\]

instead of estimating \( \beta \) by the maximum-likelihood method, Imai and Ratkovic (2014) proposed to estimate \( \beta \) by solving

\[
\mathbb{P}_n \left[ \frac{D - \pi(X^\top \beta)}{\pi(X^\top \beta)\{1 - \pi(X^\top \beta)\}} h(X) \right] = 0
\]

for some function \( h(x) \). For example, \( h(X) = X, \pi'_\beta(X\beta)X, \) or the vector consisting of all the linear and quadratic terms of \( X \). They argue that if the propensity score model is misspecified, the MLE of the propensity score might not balance the covariates, while their proposed approach can balance the first and second moments between the two arms. If the dimension of \( h(X) \) is greater than that of \( \beta \), this is a well-known over-identified
estimation problem. They estimate \( \beta \) using the generalized method of moments (Hansen, 1982) and the empirical likelihood method (Qin and Lawless, 1994). The idea of matching with empirical likelihood was also considered by Qin and Zhang (2007) for handling missing data problems. In general, a higher dimension of \( h \) produces more efficient estimators, but creates a heavier computational burden. In practical applications, one has to make a trade-off between computational cost and estimation efficiency.

Let \( \hat{\pi}(\cdot) \) be the MLE of \( \pi(\cdot) \) under the monotonicity constraint based on observations \( \{X_i^\top \hat{\beta} : 1 \leq i \leq n\} \) for any given \( \hat{\beta} \). By the characterization of such a shape-restricted MLE (Barlow et al., 1972), we have

\[
P_n\{D - \hat{\pi}(X^\top \hat{\beta})\} h(\hat{\pi}(X^\top \hat{\beta})) = 0
\]

for any function \( h \). Moreover, we can show that

\[
P_n\{D - \hat{\pi}(X^\top \hat{\beta})\} h(X^\top \hat{\beta}) = o_p(n^{-1/2})
\]

if \( h \) and \( \pi \) are sufficiently smooth (see the proof of Lemma 9 in the supplementary material). In other words, our proposal can balance any covariate function of the form \( h(X^\top \hat{\beta}) \) up to a higher than root-\( n \) asymptotic order \( o_p(n^{-1/2}) \).

### 3.1 When \( \pi(\cdot) \) is known

We first consider a simple case in which the function \( \pi \) is known. For such cases, we could pretend that \( \pi \) is unknown and monotone increasing, and apply the proposed estimation procedure. It is then natural to estimate \( \beta \) by its MLE \( \hat{\beta} = \arg \max \ell_B(\beta) \), where

\[
\ell_B(\beta) = \prod_{i=1}^n [D_i \log \{\pi(X_i^\top \beta)\} + (1 - D_i) \log \{1 - \pi(X_i^\top \beta)\}].
\]

**Assumption 11.** (1) The true parameter value \( \beta \) is an interior point of \( B \) and the unique solution to

\[
E \left[ \frac{D - \pi(X^\top \hat{\beta})}{\pi(X^\top \hat{\beta}) \{1 - \pi(X^\top \hat{\beta})\}}\pi'(X^\top \hat{\beta})X \right] = 0
\]

with respect to \( \hat{\beta} \).

(2) The matrix \( B_3 \) is nonsingular, where

\[
B_3 = E \left[ \frac{\{\pi'(X^\top \beta)\}^2}{\pi(X^\top \beta) \{1 - \pi(X^\top \beta)\}} XX^\top \right].
\]
If Assumptions 6, 7, and 11 are all satisfied, then \( \hat{\beta} \) is \( \sqrt{n} \)-consistent to \( \beta \) and admits a linear approximation (see Lemma 11 in the supplementary material).

**Theorem 5.** Suppose that model (4) is true, \( \pi \) is a known and monotone nondecreasing function, and that Assumptions 6-11 are satisfied. Then, the following results hold as \( n \to \infty \).

1. A linear approximation for \( \hat{\mu}_1 \) is

\[
\sqrt{n}(\hat{\mu}_1 - \mu_1) = \sqrt{n} \mathbb{P}_n \left[ \frac{D - \pi(X^\top \beta)}{\pi(X^\top \beta)} \left\{ \mu_1(X) - \mu_1^*(X^\top \beta; \beta) + \frac{B_1B_3^{-1}\pi'(X^\top \beta)X}{1 - \pi(X^\top \beta)} \right\} + \frac{D(Y(1) - \mu_1(X))}{\pi(X^\top \beta)} + \mu_1(X) - \mu_1 \right] + o_p(n^{-1/2}) \xrightarrow{d} N(0, \sigma_{\mu, kn}^2),
\]

where

\[
\sigma_{\mu, kn}^2 = \text{Var}(\mu_1(X)) + \mathbb{E} \left\{ \frac{1 - \pi(X^\top \beta)}{\pi(X^\top \beta)} \sigma_1(X) \right\} + \mathbb{E} \left[ \frac{1 - \pi(X^\top \beta)}{\pi(X^\top \beta)} \left\{ \mu_1(X) - \mu_1^*(X^\top \beta; \beta) + \frac{B_1B_3^{-1}\pi'(X^\top \beta)X}{1 - \pi(X^\top \beta)} \right\}^2 \right].
\]

2. A linear approximation for \( \hat{\tau} \) is

\[
\sqrt{n}(\hat{\tau} - \tau) = \sqrt{n} \frac{1}{n} \mathbb{P}_n \left[ D(\tau(X) - \tau) + D(Y(1) - \mu_1(X)) - (1 - D)\{Y(0) - \mu_0(X)\} \frac{\pi(X^\top \beta)}{1 - \pi(X^\top \beta)} \right.
\]

\[
+ \frac{D - \pi(X^\top \beta)}{1 - \pi(X^\top \beta)} \left\{ \mu_0(X) - \mu_0^*(X^\top \beta; \beta) - \frac{\pi'(X^\top \beta)}{\pi(X^\top \beta)} B_2B_3^{-1}X \right\} \right] + o_p(n^{-1/2}) \xrightarrow{d} N(0, \sigma_{\tau, kn}^2),
\]

where

\[
\sigma_{\tau, kn}^2 = \frac{1}{n^2} \mathbb{E} \left[ \pi(X^\top \beta)(\tau(X) - \tau)^2 + \pi(X^\top \beta)\sigma_1^2(X) + \sigma_0^2(X) \left\{ \frac{\pi(X^\top \beta)}{1 - \pi(X^\top \beta)} \right\}^2 \right.
\]

\[
+ \frac{\pi(X^\top \beta)}{1 - \pi(X^\top \beta)} \left\{ \mu_0(X) - \mu_0^*(X^\top \beta; \beta) - \frac{\pi'(X^\top \beta)}{\pi(X^\top \beta)} B_2B_3^{-1}X \right\}^2 \left. + 2 \left\{ \pi(X^\top \beta)(\mu_0(X) - \mu_0^*(X^\top \beta; \beta)) - \pi'(X^\top \beta)B_2B_3^{-1}X \right\} \cdot (\tau(X) - \tau) \right].
\]
Because the link function \( \pi \) is known, we may replace \( \hat{\pi}(\cdot) \) in (5) and (6) by \( \pi(\cdot) \) and consider the following two estimators:

\[
\hat{\mu}_1 = \frac{1}{n} \sum_{i=1}^{n} \frac{D_i Y_i}{\pi(X_i \beta)}, \quad \hat{\tau} = \frac{1}{n} \sum_{j=1}^{n} \left( D_j Y_j - (1 - D_j)Y_j \frac{\pi(X_j \hat{\beta})}{1 - \pi(X_j \hat{\beta})} \right).
\]

(10)

**Proposition 1.** Under the conditions of Theorem 5, as \( n \to \infty \), \( \sqrt{n}(\hat{\mu}_1 - \mu) \to^d N(0, \sigma^2_{\mu, kn}) \), where

\[
\sigma^2_{\mu, kn} = \text{Var}(\mu_1(X)) + \mathbb{E} \left\{ \frac{1 - \pi(X^\top \beta)}{\pi(X^\top \beta)} \sigma_1(X) \right\} + \mathbb{E} \left[ \frac{1 - \pi(X^\top \beta)}{\pi(X^\top \beta)} \left\{ \mu_1(X) + \frac{B_2 B_3^{-1} \pi'(X^\top \beta) X}{1 - \pi(X^\top \beta)} \right\}^2 \right]
\]

and

\[
B_4 = \mathbb{E} \left\{ \frac{\mu_1(X)}{\pi(X^\top \beta)} \pi'(X^\top \beta) X \right\},
\]

(11)

and \( \sqrt{n}(\hat{\tau} - \tau) \to^d N(0, \sigma^2_{\tau, kn}) \), where

\[
\sigma^2_{\tau, kn} = \frac{1}{\eta^2} \mathbb{E} \left[ \pi(X^\top \beta)(\tau(X) - \tau)^2 + \pi(X^\top \beta)\sigma_1^2(X) + \frac{\pi^2(X^\top \beta)}{1 - \pi(X^\top \beta)} \sigma_2^2(X) \right]
\]

\[
+ \left\{ \frac{\pi(X^\top \beta)}{1 - \pi(X^\top \beta)} \left\{ \mu_0(X) - \frac{\pi'(X^\top \beta)}{\pi(X^\top \beta)} B_4 B_3^{-1} X \right\}^2 \right\}
\]

\[
+ 2(\tau(X) - \tau) \cdot \left\{ \mu_0(X) \pi(X^\top \beta) - \pi'(X^\top \beta) B_4 B_3^{-1} X \right\} \right] \]
3.2 When $\pi(\cdot)$ is unknown

The known link function assumption may appear to be too strong, as it is rarely known in practice. In this subsection, we assume that the link function $\pi(\cdot)$ in \cite{Balabdaoui2019} is unknown and monotone nondecreasing. We propose to estimate $\beta$ via the simple score estimator (SSE) $\hat{\beta}$ of Balabdaoui et al. (2019). Once $\hat{\beta}$ has been obtained, we estimate $\pi(\cdot)$ by PAVA based on the observations $(D_i, X_i^\top \hat{\beta})$ $(1 \leq i \leq n)$.

We briefly review the SSE of Balabdaoui et al. (2019). We again use $\beta$ to denote the true index. To identify $\beta$, we assume that $\|\beta\| = 1$ and that its first nonzero component is positive. Given $\gamma$, let $Z_i(\gamma) = X_i^\top \gamma$ and assume that $Z_1(\gamma) \leq Z_2(\gamma) \leq \ldots \leq Z_n(\gamma)$. Let $\pi_i(\cdot)$ denote the PAVA estimator of $\pi(\cdot)$ that minimizes $\sum_{i=1}^n (D_i - \pi(Z_i(\gamma)))^2$. Define a $d - 1$-dimensional sphere as $S_{d-1} = \{ \gamma : \gamma \in \mathbb{R}^d, \|\gamma\| = 1 \}$, a one-to-one map $S : [0, \pi]^{(d-2)} \times [0, 2\pi] \mapsto S_{d-1}$ as

$$(\zeta(1), \zeta(2), \ldots, \zeta(d-1)) \mapsto (\cos(\zeta(1)), \sin(\zeta(1)) \cos(\zeta(2)), \sin(\zeta(1)) \sin(\zeta(2)) \cos(\zeta(3)), \ldots, \sin(\zeta(1)) \ldots \sin(\zeta(d-2)) \cos(\zeta(d-1)), \sin(\zeta(1)) \ldots \sin(\zeta(d-2)) \sin(\zeta(d-1))),$$

(12)

and a $d \times (d-1)$ matrix as $J(\zeta) = \partial S^\top(\zeta) / \partial \zeta$. Let $\zeta_0$ satisfy $\beta = S(\zeta_0)$ and $\hat{\zeta}$ be a zero-crossing of the function

$$\phi_n(\zeta) = \mathbb{P}_n[J^\top(\zeta) X \{ D - \pi_{S(\zeta)}(X^\top S(\zeta)) \}]$$

(13)

(see page 521 of Balabdaoui et al. (2019) for the definition of zero-crossing). Accordingly, we estimate $\beta$ by $\hat{\beta} = S(\hat{\zeta})$, and estimate the propensity score function by $\hat{\pi}_{\hat{\beta}}(\cdot)$. The resulting PSM estimators for $\mu_1$ and $\tau$ are

$$\hat{\mu}_1 = \frac{1}{n} \sum_{i=1}^n \frac{D_i Y_i}{\hat{\pi}_{\hat{\beta}}(X_i^\top \hat{\beta})} \quad \text{and} \quad \hat{\tau} = \frac{1}{n} \sum_{j=1}^n \left\{ D_j Y_j - (1 - D_j) Y_j \frac{\hat{\pi}_{\hat{\beta}}(X_j^\top \hat{\beta})}{1 - \hat{\pi}_{\hat{\beta}}(X_j^\top \hat{\beta})} \right\},$$

respectively. To study the large-sample properties of the two estimators, we assume the following conditions, which correspond to Assumptions A3, A5, A7, and A9, respectively, of Balabdaoui et al. (2019).

**Assumption 12.** There exists $\delta_0 > 0$ such that the function $\pi_{\gamma}(u) = \mathbb{E}\{ \pi(X^\top \beta) | X^\top \gamma = u \}$ is monotone increasing on $I_{\gamma} = \{ X^\top \gamma : X \in X \}$ for all $\gamma \in B(\beta, \delta_0) = \{ \gamma : \|\gamma - \beta\| \leq \delta_0 \}$.

**Assumption 13.** The distribution of $X$ admits a density $g$ that is differentiable on $X$. In addition, there exist positive constants $c_1, c_2, c_3, c_4 > 0$ such that $c_1 \leq g \leq c_2$ and $c_3 \leq \partial g / \partial x_j \leq c_4$ on $X$ for all $1 \leq j \leq d$. 
Assumption 14. For all $\gamma \neq \beta$ such that $S(\gamma) \in \mathcal{B}(\beta, \delta_0)$, the random variable
\[
\text{Cov}[(\zeta_0 - \zeta)^\top J(\zeta)X, \pi(X^\top(\zeta_0))]X^\top(\zeta)]
\]
is almost surely not equal to zero.

Assumption 15. $J(\zeta_0)\mathbb{E}\{\pi'(X^\top\beta)\text{Cov}(X|X^\top\beta)\}J(\beta)$ is nonsingular.

If Assumptions 6, 11(2), and 12–15 are satisfied, then Theorem 3 of Balabdaoui et al. (2019) implies that the estimator $\hat{\beta} = S(\hat{\zeta})$ is consistent and asymptotically normal (see Lemma 12 in the supplementary material).

Theorem 6. Suppose that model (4) is true, $\pi$ is an unknown and monotone nondecreasing function, and that Assumptions 7, 2, 10, and 12–15 are satisfied. Define
\[
B_5 = J(\zeta_0)\{J(\zeta_0)\mathbb{E}\{\pi'(X^\top\beta)\text{Var}(X|X^\top\beta)\}J(\zeta_0)\}^{-1}J(\zeta_0).
\]
Then, the following results hold as $n \to \infty$.

(1) $\sqrt{n}(\hat{\mu}_1 - \mu_1) \xrightarrow{d} N(0, \sigma_{\mu,\text{un}}^2)$, where
\[
\sigma_{\mu,\text{un}}^2 = \mathbb{E}\left[\left(1 - \frac{\pi(X^\top\beta)}{\pi(X^\top\beta)}\right)\left\{\mu_1(X) - \mu_1^*(X^\top\beta) + B_1B_5(X - \mathbb{E}(X|X^\top\beta))\pi(X^\top\beta)\right\}^2\right]
+ \mathbb{E}\left\{\frac{\sigma_0^2(X)}{\pi(X^\top\beta)}\right\} + \mathbb{E}\{\mu_1(X) - \mu_1\}^2.
\]

(2) $\sqrt{n}(\hat{\tau} - \tau) \xrightarrow{d} N(0, \sigma_{\tau,\text{un}}^2)$, where
\[
\sigma_{\tau,\text{un}}^2 = \frac{1}{\eta^2}\mathbb{E}\left[\pi(X^\top\beta)\sigma_0^2(X)\right] + \frac{1}{\eta^2}\mathbb{E}\left[\sigma_0^2(X)\left\{\frac{\pi(X^\top\beta)}{1 - \pi(X^\top\beta)}\right\}^2\right]
+ \frac{1}{\eta^2}\mathbb{E}\left\{\pi(X^\top\beta)(\tau(X) - \tau)^2\right\} + \frac{1}{\eta^2}\mathbb{E}\left[\pi(X^\top\beta)\{1 - \pi(X^\top\beta)\}\right]
\left\{\frac{\mu_0(X) - \mu_0^*(X^\top\beta)}{1 - \pi(X^\top\beta)} - B_2B_5(X - \mathbb{E}(X|X^\top\beta))\right\}^2\right]
+ \frac{2}{\eta^2}\mathbb{E}\left[\tau(X) - \tau)^2\pi(X^\top\beta)\{1 - \pi(X^\top\beta)\}\right]\left\{\frac{\mu_0(X) - \mu_0^*(X^\top\beta)}{1 - \pi(X^\top\beta)}\right\}^2\right]
+ \mathbb{E}\{\mu_1(X) - \mu_1\}^2.
\]

Theorem 6 indicates that, in general, if the link function $\pi(\cdot)$ is unknown and estimated by PAVA, the proposed estimators $\hat{\mu}_1$ and $\tau$ are still consistent and asymptotically normal. However, by Theorems 3 and 4, they are not asymptotically semiparametric efficient if $Y(1)$ or $Y(0)$ does not depend on the covariate in the same direction as the treatment indicator does.
4 Simulations

To evaluate the finite-sample performance of the proposed estimators, we conduct simulations to compare the following estimation methods:

- **PAVA-MLE**: the proposed PSM method with $\beta$ estimated by the MLE under the logistic propensity score model and $\pi$ estimated by PAVA;
- **PAVA-SSE**: the proposed PSM method with $\beta$ estimated by SSE and $\pi$ estimated by PAVA;
- **PARA**: the proposed PSM estimator (6) with $\hat{\pi}$ replaced by the logistic function and $\hat{\beta}$ being the MLE under the logistic propensity score model;
- **PSM-M**: the PSM method with the propensity score estimated by the logistic regression model and each case matched with $M$ controls. Four choices of $M$ are considered: 3, 5, 10, and 15.

To generate data, we consider the bivariate $X = (X_1, X_2)$, a linear logistic propensity score model

$$\Pr(D = 1|x_1, x_2) = \pi(2 + x_1 + x_2),$$

and the following regression models:

$$Y(1) = -(X_1 + X_2)^a + \epsilon, \quad Y(0) = 3h(X_1, X_2) - (X_1 + bX_2)^a + \epsilon,$$

where $\epsilon, X_1,$ and $X_2$ are independent and identically distributed as $N(0, 1)$. We choose $\pi(t) = e^t/(1 + e^t)$ or the standard normal distribution function, $h(X_1, X_2) = \cos(X_1 + bX_2)$ (Model 1), $X_1$ (Model 2), $a = 1, 2,$ and $b = 1, 0, -1$. From each case, we generate 1000 samples with a sample size of $n = 500$ and calculate the seven estimators for the ATT $\tau$.

We first examine the results in Table 1, which presents the biases and root mean square errors (RMSEs) of the seven estimators when $\pi(t) = e^t/(1 + e^t)$. The overall rate of nonmissing data is about $\Pr(D = 1) = 81.6\%$. As $\pi(t)$ is the logistic function, the seven estimators under comparison all have correctly specified propensity score models. The propensity score satisfies model (4) with $\beta = (1/\sqrt{2}, 1/\sqrt{2})^\top$. In all cases, although having negligible biases, the PARA estimator (which uses the true logistic propensity score function) always has the largest RMSE, meaning that it is always the most unreliable among the seven estimators under comparison. This coincides with the finding of Hirano et al. (2003) that “weighting by the inverse of a nonparametric estimate of the propensity score, rather than the true propensity score, leads to an efficient estimate of the average treatment effect.”
Under Model 1, the regression function in the control group is a single-index model

$$\mu_0(X) = \cos(\sqrt{1 + b^2} \cdot X^\top \theta) - (\sqrt{1 + b^2} \cdot X^\top \theta)^a$$

with \( \theta = (1, b) / \sqrt{1 + b^2} \). When \( b = 1 \), \( \theta = \beta \). By Theorem 4, the proposed estimator \( \hat{\tau} \) in (6) is asymptotically semiparametric efficient, regardless of whether \( \beta \) is estimated by the MLE or SSE. We see from Table 1 that PAVA-SSE has very similar performance to PAVA-MLE, and both of them perform uniformly better than the five competitors in terms of bias and RMSE. The performance of the PSM estimator is dramatically influenced by the number of matches, \( M \), per unit; the PSM estimator has increasing biases and RMSEs as \( M \) increases from 3 to 15, and PSM-15 with \( M = 15 \) has twice the biases and RMSEs as PSM-3 with \( M = 3 \).

When \( b \neq 1 \), we have \( \theta \neq \beta \). The proposed estimator \( \hat{\tau} \) loses its semiparametric optimality. Even so, when \( b = 0 \) (the angle between \( \theta \) and \( \beta \) is 45 degrees), the proposed estimators PAVA-SSE and PAVA-MLE still achieve better performances than the other estimators, but the relative advantage is smaller. When \( b = -1 \), \( \theta \) is perpendicular to \( \beta \), and the relative advantage of our estimators decreases further until PSM becomes comparable or even better. Surprisingly, we find that, in this case, the PSM estimator has decreasing biases and RMSEs as \( M \) increases from 3 to 15, which is contrary to the case where \( \theta = \beta \). These findings indicate that the optimal choice of \( M \) for the PSM method critically depends on the true regression function \( \mu_0(X) \), and without any information on \( \mu_0(X) \), it is impossible to correctly specify the optimal \( M \). Additionally, the performance of the proposed estimator may be improved by making use of information on \( \mu_0(X) \).

Under model 2, \( \mu_0(X) \) does not follow a single-index model, and it cannot be written as \( \tilde{\mu}_0(X^\top \theta) \) for some function \( \tilde{\mu}_0 \). By Theorem 4, the proposed estimator \( \hat{\tau} \) is no longer semiparametric efficient, but is still asymptotically normal. The results in Table 1 corresponding to Model 2 suggest that, compared with the PSM estimators, the proposed estimators are at least comparable and perform uniformly better in some cases.

Table 2 presents the results when \( \pi(t) \) is chosen to be the standard normal distribution function. In this situation, the overall rate of nonmissing data is about \( \text{pr}(D = 1) = 87.5\% \) and only the proposed PAVA-SSE has a correctly specified propensity score model. Compared with the four PSM estimators, the proposed PAVA-MLE and PAVA-SSE estimators have uniformly smaller RMSEs and generally smaller biases. Again, the two proposed estimators exhibit rather similar performance, although the index coefficient in the PAVA-MLE method is estimated by the MLE under the logistic propensity score model. As \( M \) increases from 3 to 15, the PSM method may perform worse in some cases and better in other cases. When the true propensity score model changes from a logistic model to a probit model, the RMSEs of the PAVA-MLE and PAVA-SSE estimators increase by no more than 26% in eight out of the twelve cases. In contrast, the RMSE of PSM-3 increases by at least 60% in all
cases, and can be as large as 200% (e.g., the case with Model 2, a = 1, and b = −1). This suggests that the PSM estimators are more sensitive than the proposed estimator to the misspecification of the propensity score model.

To obtain further insights into the performance of the proposed estimators and the PSM estimators, Figures 1 and 2 display their boxplots in the case of a = 1; those of the PARA estimates are excluded as they spread too widely. As we can see from the boxplots, PAVA-MLE and PAVA-SSE have smaller biases and better overall performance in most cases compared with the four PSM estimators. As the number of matches M increases from 3 to 15, the PSM estimators exhibit decreasing variances, but increasing biases except in the case of Model 1, a = 1, and b = −1. The advantage of the proposed estimators over the PSM estimators is clarified in Figure 2, where π(t) is chosen to be the standard normal distribution function.

Overall, the proposed PAVA-based estimation method is more reliable than the PSM method: it usually has smaller RMSEs and biases, and is not influenced by the tuning parameters. The performance of the PSM method is strongly influenced by the number of matches per unit; however, determining the optimal value of M is quite challenging and no research has been done on this issue. The direction in which the control response depends on the covariate does not influence the consistency, but does affect the estimation efficiency of the proposed method: if it coincides with the direction in which the treatment status depends on the covariate, the proposed method achieves optimal performance both numerically and theoretically.

5 An application

For illustration, we apply the proposed PAVA-based estimation method to data from the National Supported Work (NSW) Demonstration, which have previously been analyzed by LaLonde (1986), Dehejia and Wahba (2002), and Smith and Todd (2005). The primary parameters of interest in these papers concern the average treatment effect of a job training program. We focus on the estimation of the average treatment effect on the treated, τ. The data consist of 297 treated and 425 untreated observations. We take earnings in 1978 as the outcome variable of interest (Y) and take age and education as the basic covariates X1 and X2, respectively. To examine the sensitivity of the proposed method to the model specifications, we model the propensity score using a linear logistic model and a quadratic logistic model.

We calculate the point estimates of the seven estimation methods considered in the previous section. We also conduct bootstrap sampling with 1000 bootstrap replications from the LaLonde data to obtain the 2.5% and 97.5% sample quantiles, the mean, and the
Figure 1: Boxplots of the seven estimators when $\pi(\cdot)$ is correctly specified, $a = 1$, and $n = 500$. As $b$ varies between 1, 0, and -1, the angle between $\hat{\beta}$ and $\hat{\beta}$ increases from 0 degrees to 90 degrees. Model 1: $h(X_1, X_2) = \cos(X_1 + aX_2)$; Model 2: $h(X_1, X_2) = X_1$. 
Figure 2: Boxplots of the seven estimators when \( \pi(\cdot) \) is chosen to be the standard normal distribution function, \( a = 1 \), and \( n = 500 \). As \( b \) varies between 1, 0, and -1, the angle between \( \beta \) and \( \beta' \) increases from 0 degrees to 90 degrees. Model 1: \( h(X_1, X_2) = \cos(X_1 + aX_2) \); Model 2: \( h(X_1, X_2) = X_1 \).
standard deviation of the resulting point estimates for each method. Each pair of 2.5% and 97.5% sample quantiles constitutes a 95% confidence interval of the percentile method. The analysis results are presented in Table 3.

Under either the linear or quadratic logistic model, the point estimates of the PAVA-MLE and PAVA-SSE methods are all around 915 with bootstrap standard deviations of around 500. This implies that the proposed estimation methods are rather robust to different model specifications. As PAVA-SSE makes the weakest model assumption, we believe that the results of PAVA-SSE should be the most trustable among the seven methods considered here. The bootstrap means of all methods are around 950 and the point estimates of PSM-15 are about 900 in both cases, which seemingly provide evidence for the rationality of the PAVA-MLE and PAVA-SSE point estimates. Although PARA also has bootstrap standard deviations of around 500, it produces very different point estimates (875.37 and 809.43) in the linear and quadratic logistic propensity score models. The PSM method is rather sensitive to the number of matches per unit. Its point estimate changes from 514.42 to nearly 900 with the linear logistic model, and varies even more dramatically with the quadratic logistic model.

Figure 3 displays the fitted propensity scores (versus the estimated index $X^\top \hat{\beta}$) using a parametrically logistic model and the estimations of the semiparametric PAVA method after $\beta$ is replaced by its MLE under the logistic model. The parametric propensity score estimates for both the linear and quadratic logistic models apparently form straight lines; unlike the semiparametric PAVA-based propensity score estimates, they may not capture local changes in the propensity score. As the semiparametric method requires fewer model assumptions and is more flexible, we believe that the semiparametric PAVA-based propensity score estimates and the corresponding PAVA-MLE estimates are more reliable than those based on the parametric propensity score estimates, including PARA and the four PSM methods. This may explain why the proposed PAVA-based method is superior to PARA and the four PSM methods.

6 Discussion

Among many others, Abadie and Imbens (2006, 2011, 2012, 2016) have established different matching methods for causal inference. Moreover, motivated by the empirical likelihood method in the presence of auxiliary information and choice-based sampling, Hirano, Imbens, and Ridder (2003) proposed an efficient inverse weighting method using the fully nonparametric estimated propensity score. Even though their theoretical results are elegant, the finite-sample performance of their method is unclear. In practical applications, the dimen-
Figure 3: Fitted propensity scores versus the estimated index $X^\top \hat{\beta}$ under a linear (left) and quadratic (right) logistic propensity score model based on the Lalonde data. Here, $\hat{\beta}$ is the MLE of $\beta$ under the corresponding linear logistic model. Solid line: link function estimated by PAVA; dashed line: link function set to the logistic function.

sion of the explanatory variable is high, and the fully nonparametric estimation of the regression function may suffer from the curse of dimensionality. Compared with other efficient estimates, Hirano, Imbens, and Ridder (2003) stated that “Which estimators have more attractive finite sample properties, and which have more attractive computational properties, remain open questions.” The connection between their matching methods and the probabilistic inverse weighting method, however, is unclear. In contrast to Hirano, Imbens, and Ridder (2003), this paper has proposed an inverse weighting method that uses the maximum shape-restricted semiparametric likelihood estimation of the monotone index propensity score. Our method is very easy to implement using existing statistical software in R, such as the Iso and Isotone packages. Remarkably, our inverse weighting method is seamlessly related to the tuning-parameter-free propensity matching method. Theoretical results show that our estimates can achieve the semiparametric efficiency lower bound for the average treatment effect and the average treatment effect for the treated if the explanatory variable is univariate or the regression function and propensity score depend on the explanatory variables in the same direction. Our results underline the important role played by the propensity score and the regression function in estimating average causal effects. In general, the propensity score matching method or the regression function matching method alone cannot be efficient. An efficient estimation method should take both of them into consideration.
Henmi and Eguchi (1982) observed a paradox associated with parameter estimation in the presence of nuisance parameters. In particular, they found that the inverse probability weighting estimator with an estimated proposed score has a smaller asymptotic variance than that derived from the true propensity score. This paradox was also observed by Abadie and Imbens (2016), i.e., matching estimators based on estimated propensity scores have smaller asymptotic variances than those based on the true PSM. Our results further echo this message that matching estimators based on the shape-restricted nonparametric MLE of the propensity score have smaller asymptotic variances than their counterparts based on the parametric MLE of the propensity score.

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Table 1: Simulated biases and RMSEs based on 1000 samples of size $n = 500$ when $\pi(\cdot)$ is correctly specified. Model=1: $h = \cos(X_1 + aX_2)$; Model=2: $h = X_1$.

| Model | $a$ | $b$ | Bias   | RMSE   | Bias   | RMSE   | Bias   | RMSE   | Bias   | RMSE   | Bias   | RMSE   | Bias   | RMSE   | Bias   | RMSE   | Bias   | RMSE   |
|-------|-----|-----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 1     | 1   | 1   | Bias   | -0.167 | -0.158 | -0.023 | -0.482 | -0.646 | -0.933 | -1.117 |
| 1     | 1   | 1   | RMSE   | 0.458  | 0.468  | 1.063  | 0.614  | 0.744  | 0.992  | 1.156  |
| 1     | 1   | 0   | Bias   | 0.125  | 0.128  | 0.012  | -0.200 | -0.251 | -0.357 | -0.424 |
| 1     | 1   | 0   | RMSE   | 0.407  | 0.414  | 0.552  | 0.463  | 0.446  | 0.478  | 0.507  |
| 1     | 1   | -1  | Bias   | 0.128  | 0.129  | -0.038 | -0.025 | -0.020 | -0.017 | -0.017 |
| 1     | 1   | -1  | RMSE   | 0.448  | 0.473  | 0.584  | 0.521  | 0.484  | 0.429  | 0.399  |
| 1     | 2   | 1   | Bias   | -0.599 | -0.604 | -0.148 | -0.901 | -1.124 | -1.467 | -1.639 |
| 1     | 2   | 1   | RMSE   | 0.936  | 0.955  | 1.959  | 1.039  | 1.222  | 1.522  | 1.677  |
| 1     | 2   | 0   | Bias   | -0.024 | -0.024 | -0.010 | -0.257 | -0.311 | -0.399 | -0.441 |
| 1     | 2   | 0   | RMSE   | 0.506  | 0.515  | 0.878  | 0.575  | 0.556  | 0.571  | 0.585  |
| 1     | 2   | -1  | Bias   | -0.122 | -0.141 | -0.007 | -0.031 | -0.043 | -0.039 | -0.024 |
| 1     | 2   | -1  | RMSE   | 0.865  | 0.895  | 1.146  | 0.986  | 0.906  | 0.827  | 0.788  |
| 2     | 1   | 1   | Bias   | 0.071  | 0.080  | 0.008  | 0.062  | 0.086  | 0.145  | 0.191  |
| 2     | 1   | 1   | RMSE   | 0.380  | 0.444  | 0.572  | 0.447  | 0.403  | 0.372  | 0.383  |
| 2     | 1   | 0   | Bias   | 0.159  | 0.164  | 0.036  | 0.138  | 0.189  | 0.291  | 0.381  |
| 2     | 1   | 0   | RMSE   | 0.380  | 0.411  | 0.602  | 0.391  | 0.396  | 0.427  | 0.478  |
| 2     | 1   | -1  | Bias   | 0.243  | 0.241  | 0.017  | 0.230  | 0.298  | 0.452  | 0.581  |
| 2     | 1   | -1  | RMSE   | 0.449  | 0.461  | 0.812  | 0.387  | 0.418  | 0.531  | 0.644  |
| 2     | 2   | 1   | Bias   | -0.319 | -0.338 | -0.009 | -0.308 | -0.343 | -0.341 | -0.299 |
| 2     | 2   | 1   | RMSE   | 0.553  | 0.615  | 1.222  | 0.561  | 0.552  | 0.520  | 0.479  |
| 2     | 2   | 0   | Bias   | 0.034  | 0.030  | 0.002  | 0.095  | 0.147  | 0.262  | 0.374  |
| 2     | 2   | 0   | RMSE   | 0.360  | 0.416  | 0.566  | 0.440  | 0.437  | 0.459  | 0.532  |
| 2     | 2   | -1  | Bias   | -0.080 | -0.103 | -0.035 | 0.172  | 0.239  | 0.390  | 0.533  |
| 2     | 2   | -1  | RMSE   | 0.622  | 0.662  | 0.936  | 0.770  | 0.739  | 0.751  | 0.802  |
Table 2: Simulated biases and RMSEs based on 1000 samples of size $n = 500$ when $\pi(\cdot)$ is chosen to be the standard normal distribution function. Model=1: $h = \cos(X_1 + aX_2)$; Model=2: $h = X_1$.

| Model | $a$ | $b$ | PAVA-MLE | PAVA-SSE | PARA | PSM-3 | PSM-5 | PSM-10 | PSM-15 |
|-------|-----|-----|----------|----------|------|-------|-------|--------|-------|
| 1     | 1   | 1   | Bias     | -0.114   | -0.109 | -0.471 | -1.624 | -1.667 | -1.605 | -1.474 |
| 1     | 1   | 1   | RMSE     | 0.309    | 0.318  | 0.636  | 1.686  | 1.709  | 1.634  | 1.501  |
| 1     | 0   | 0   | Bias     | 0.608    | 0.612  | 0.278  | -0.631 | -0.656 | -0.693 | -0.712 |
| 1     | 0   | 0   | RMSE     | 0.714    | 0.724  | 0.722  | 0.850  | 0.812  | 0.784  | 0.778  |
| 1     | -1  | 1   | Bias     | 0.541    | 0.535  | 0.384  | -0.068 | -0.019 | -0.022 | -0.019 |
| 1     | -1  | 1   | RMSE     | 0.696    | 0.708  | 0.912  | 0.983  | 0.847  | 0.660  | 0.557  |
| 1     | 2   | 1   | Bias     | -0.747   | -0.747 | -0.930 | -1.977 | -1.846 | -1.414 | -0.918 |
| 1     | 2   | 1   | RMSE     | 0.815    | 0.821  | 1.069  | 2.034  | 1.900  | 1.495  | 1.068  |
| 1     | 0   | 0   | Bias     | 0.333    | 0.333  | 0.151  | -0.512 | -0.500 | -0.410 | -0.302 |
| 1     | 0   | 0   | RMSE     | 0.552    | 0.560  | 1.118  | 0.934  | 0.837  | 0.695  | 0.591  |
| 1     | -1  | 1   | Bias     | -0.521   | -0.555 | -0.426 | -0.177 | -0.148 | -0.126 | -0.135 |
| 1     | -1  | 1   | RMSE     | 0.971    | 0.994  | 1.222  | 1.880  | 1.592  | 1.268  | 1.115  |
| 2     | 1   | 1   | Bias     | 0.266    | 0.269  | 0.268  | 0.312  | 0.405  | 0.503  | 0.582  |
| 2     | 1   | 1   | RMSE     | 0.459    | 0.494  | 0.667  | 0.955  | 0.843  | 0.739  | 0.741  |
| 2     | 0   | 0   | Bias     | 0.529    | 0.532  | 0.554  | 0.652  | 0.785  | 0.974  | 1.127  |
| 2     | 0   | 0   | RMSE     | 0.608    | 0.626  | 0.829  | 0.935  | 0.970  | 1.069  | 1.188  |
| 2     | -1  | 1   | Bias     | 0.808    | 0.804  | 0.812  | 1.054  | 1.207  | 1.485  | 1.690  |
| 2     | -1  | 1   | RMSE     | 0.855    | 0.853  | 1.305  | 1.197  | 1.300  | 1.538  | 1.727  |
| 2     | 2   | 1   | Bias     | -0.361   | -0.370 | -0.199 | 0.005  | 0.178  | 0.660  | 1.103  |
| 2     | 2   | 1   | RMSE     | 0.528    | 0.563  | 0.640  | 0.918  | 0.841  | 0.939  | 1.271  |
| 2     | 2   | 0   | Bias     | 0.275    | 0.291  | 0.433  | 0.816  | 0.986  | 1.289  | 1.549  |
| 2     | 2   | 0   | RMSE     | 0.452    | 0.520  | 0.685  | 1.284  | 1.307  | 1.467  | 1.665  |
| 2     | 2   | -1  | Bias     | -0.280   | -0.294 | 0.052  | 0.941  | 1.138  | 1.419  | 1.629  |
| 2     | 2   | -1  | RMSE     | 0.650    | 0.726  | 0.975  | 1.708  | 1.650  | 1.697  | 1.816  |
Table 3: Estimation results for ATT based on the Lalonde data. 2.5% and 97.5% quantiles, Bootstrap mean, and Standard Deviation denote the corresponding characteristics of the point estimates based on 1000 bootstrap samples from the Lalonde data.

| Methods | PAVA-MLE | PAVA-SSE | PARA | PSM-3 | PSM-5 | PSM-10 | PSM-15 |
|---------|----------|----------|------|-------|-------|--------|--------|
| Case (a): $X_1$ and $X_2$ are covariates |          |          |      |       |       |        |        |
| Point estimate | 917.33 | 911.47 | 875.37 | 514.42 | 714.39 | 802.88 | 898.99 |
| 2.5% quantile | -41.13 | -43.71 | -74.50 | -156.27 | -50.18 | -20.66 | -12.11 |
| 97.5% quantile | 1857.84 | 1914.45 | 1815.51 | 2202.33 | 2086.06 | 2009.02 | 1966.01 |
| Bootstrap mean | 894.19 | 906.39 | 861.61 | 1071.51 | 1033.38 | 993.00 | 985.47 |
| Standard deviation | 496.56 | 495.75 | 487.74 | 603.06 | 558.29 | 523.40 | 510.66 |
| Case (b): $X_1$, $X_2$, $X_1X_2$, $X_1^2$ and $X_2^2$ are covariates |          |          |      |       |       |        |        |
| Point estimate | 913.10 | 918.46 | 809.43 | 88.21 | 337.75 | 947.25 | 903.67 |
| 2.5% quantile | -9.21 | -27.03 | -119.09 | -204.43 | -93.13 | -40.47 | -23.02 |
| 97.5% quantile | 1925.33 | 1964.92 | 1849.40 | 2257.50 | 2116.52 | 2065.41 | 2015.76 |
| Bootstrap mean | 936.21 | 950.03 | 835.23 | 997.70 | 997.80 | 1019.41 | 1028.54 |
| Standard deviation | 507.33 | 508.74 | 503.50 | 645.31 | 592.54 | 532.30 | 515.47 |