Robust inference of conditional average
treatment effects using dimension reduction

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Abstract: It is important to make robust inference of the conditional average treatment effect from observational data, but this becomes challenging when the confounder is multivariate or high-dimensional. In this article, we propose a double dimension reduction method, which reduces the curse of dimensionality as much as possible while keeping the nonparametric merit. We identify the central mean subspace of the conditional average treatment effect using dimension reduction. A nonparametric regression with prior dimension reduction is also used to impute counterfactual outcomes. This step helps improve the stability of the imputation and leads to a better estimator than existing methods. We then propose an effective bootstrapping procedure without bootstrapping the estimated central mean subspace to make valid inference.

Key words: augmented inverse probability weighting; matching; kernel smoothing; U-statistic; weighted bootstrap.

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1 Introduction

In recent biomedical and public health research, there has been growing interest in developing valid and robust inference methods for the conditional average treatment effect, which is also known as the treatment contrast or heterogeneity of treatment effect. In particular, the sign of conditional average treatment effects can be used to determine the optimal individualized treatment regime (Qian and Murphy; 2011). In the era of big data, large observational data with multivariate or high-dimensional confounders are becoming increasingly available for research purposes, such as electronic health records, claims, and disease registries. It becomes challenging to make robust inference of the conditional average treatment effect due to the curse of dimensionality, calling for new techniques such as dimension reduction.

A large body of literature focuses on modeling the prognostic scores, defined as the outcome mean functions under the treated and control conditions. Parametric approaches include likelihood-based methods (Thall et al., 2000; 2002; 2007) and parametric Q-learning (Chakraborty et al., 2010). Machine learning-based methods include Bayesian additive regression trees (Chipman et al., 2010), causal multivariate adaptive regression splines (Powers et al., 2018), random forest, causal boosting trees, and reinforcement learning (Zhao et al., 2011). Although the conditional average treatment effect is simply the difference between the treated and the control prognostic scores, they may have different model features. Thus, in some applications, direct modeling on the conditional average treatment effect may provide a more accurate characterization of treatment effects, avoiding redundancy of non-useful features. Another body of literature focuses on modeling and approximating the conditional average treatment effect both parametrically (Murphy, 2003; Robins, 2004) and using machine learning methods (Zhao et al., 2012; Zhang et al., 2012; Rzepakowski and Jaroszewicz, 2012; Athey and Imbens, 2016; Athey et al., 2019). However, parametric methods are susceptible to model misspecification. Although machine learning is flexible, it often produces results that are too complicated to be interpretable. Most importantly, it is a daunting task to draw valid inference based on machine learning methods. Semiparametric methods offer compromises between fully parametric and machine learning approaches. Song et al. (2017) and Liang and Yu (2020) considered single index and multiple index models for the treatment contrast function, respectively. See also Luo et al. (2019).
In this article, we propose a nonparametric framework to make robust inference of the conditional average treatment effect. To mitigate the possible curse of dimensionality, we consider the central mean subspace of the conditional average treatment effect, which is the smallest linear subspace spanned by a set of linear index that can sufficiently characterize the estimand of interest (Cook and Li 2002). Precisely speaking, a series of nested multiple index models are considered and the most saturated model is the fully nonparametric regression. Any conditional average treatment effect must belong to this series with a particular number of linear indices, which is called the structural dimension. The primary goal is to estimate this structural dimension and the corresponding index coefficients. Under this framework, we specify the conditional average treatment effect nonparametrically and use a model selection procedure to determine a sufficient structural dimension.

To estimate the central mean subspace, we propose imputing counterfactual outcomes by kernel regression with a prior dimension reduction. The prior dimension reduction helps to improve the stability of the imputation and the subsequent estimation of the conditional average treatment effect. It is worth comparing our imputation approach to alternative methods. For example, nearest neighbor imputation can be used to impute the missing potential outcome by pairing each unit with the nearest neighbor in the opposite treatment group. However, matching is generally not effective in the presence of many covariates. Abrevaya et al. (2015) considered an inverse probability weighted adjusted outcome for the conditional average treatment effect. It is well known that weighted by the inverse probabilities is highly unstable (Kang and Schafer 2007). To overcome this instability, Zhao et al. (2012) further considered combining weighting and outcome regression as an augmented inverse probability adjusted outcome. In our simulation study, regression imputation and augmented inverse probability weighting have comparable performances. Because the inverse weighting methods require additional propensity score estimation, we suggest regression imputation to save more computational time in practice.

Theoretically, we derive the consistency and asymptotic normality of the proposed estimator of the conditional average treatment effect. The main challenge is that the imputed counterfactual outcomes are not independent. To overcome this challenge, we calculate the difference between imputed and conditional counterfactual outcomes, which can be expressed as a weighted empirical average of the influence functions of the kernel regression estimator. Thus, we can show that the
influence function of the proposed estimator can be approximated by a U-statistic. Invoking the properties of degenerate U-processes discussed in Nolan and Pollard (1987), we can derive the asymptotic distribution of the estimated conditional average treatment effect and show that the imputation step plays a non-negligible role. To make valid inference, we propose a under-smooth strategy such that the asymptotic bias is dominated by the asymptotic variance. We can estimate the asymptotic variances by applying weighted bootstrap techniques and construct Wald confidence intervals. Interestingly, the fact that the central mean subspace is estimated does not affect the asymptotic distribution of the proposed estimator of the conditional average treatment effect. Thus, in our bootstrap procedure, we can safely skip the step of bootstrapping the estimated central mean subspace, which saves a lot of computation time in practice.

2 Methodology

2.1 Preliminaries

We use potential outcomes to define causal effects. Suppose that the binary treatment is $A \in \{0, 1\}$, with 0 and 1 being the labels for the control and active treatment, respectively. Each level of treatment $a$ corresponds to a potential outcome $Y(a)$, representing the outcome had the subject, possibly contrary to the fact, been given treatment $a$. The individual causal effect is $D = Y(1) - Y(0)$. Let $X \in \mathbb{R}^p$ be a $p$-vector of pre-treatment covariates. The covariate-specific average treatment effect is $\tau(x) = E\{Y(1) - Y(0) \mid X = x\} = E(D \mid X = x)$. The observed outcome is $Y = Y(A) = AY(1) + (1 - A)Y(0)$. The main goal of this article is to estimate $\tau(x)$ based on observational data $\{(A_i, Y_i, X_i) : i = 1, \ldots, n\}$, which independently and identically follows $f(A, Y, X)$.

To identify the treatment effects, we assume the following assumptions, which are standard in causal inference with observational studies (Rosenbaum and Rubin 1983):

**Assumption 1.** $\{Y(0), Y(1)\} \perp A \mid X$.

**Assumption 2.** There exist constants $c_1$ and $c_2$ such that $0 < c_1 \leq \pi(X) \leq c_2 < 1$ almost surely, where $\pi(x) = \text{pr}(A = 1 \mid X = x)$ is the propensity score.

Let $\mu_a(x) = E\{Y(a) \mid X = x\}$ ($a = 0, 1$). Under Assumptions 1, 2, $\mu_a(x) = E(Y \mid A = a, X = x)$.
and $\tau(x) = \mu_1(x) - \mu_0(x)$ are identifiable from $f(A, Y, X)$. This identification formula motivates a common strategy of estimating $\tau(x)$ by approximating $\mu_a(X)$ separately for $a = 0, 1$. Alternatively, we propose robust inference of $\tau(x)$ directly using dimension reduction, which requires no parametric model assumptions and can detect accurate and parsimonious structures of $\tau(x)$.

### 2.2 Dimension reduction on conditional average treatment effect

The main idea is to search for the fewest linear indices $B_T^T x$ such that

$$ \tau(x) = g(B_T^T x), $$

(1)

where $B_T$ is a $p \times d_T$ matrix consisting of index coefficients, and $g$ is an unknown $d_T$-variate function. Since $\tau(x) = E(D | X = x)$, the column space of $B_T$ is called the central mean subspace of $D$ given $X$, denoted by $S_{E(D/X)}$ [Cook and Li, 2002].

The central mean subspace $S_{E(D/X)}$ is nonparametric. In other words, for any multivariate function $\tau(x)$, without particular parametric or semiparametric modeling, there always exists a unique central mean subspace. To illustrate, consider the single-index model $g(x^T \beta)$ which leads to a one-dimensional central mean subspace spanned by $\beta$. Unlike the single-index model that prefixes the dimension of the central mean subspace, we leave both $d_T$ and $B_T$ unspecified, and the primary goal of dimension reduction is to estimate $d_T$ and $B_T$. In addition, the curse of dimensionality can be avoided if $d_T$ is much smaller than $p$.

**Remark 1.** Recall that $\tau(x) = \mu_1(x) - \mu_0(x)$. An alternative way to employ dimension reduction is to search for two sets of linear indices $B_0^T x$ and $B_1^T x$ such that

$$ \mu_0(x) = g_0(B_0^T x), \quad \mu_1(x) = g_1(B_1^T x), $$

(2)

where $g_0$ and $g_1$ are unknown functions. That is, we can also estimate $S_{E(Y(0)/X)} = \text{span}(B_0)$ and $S_{E(Y(1)/X)} = \text{span}(B_1)$, and then recover $\tau(x)$ by $g_1(B_1^T x) - g_0(B_0^T x)$. In fact, we can show that $S_{E(D/X)} \subseteq S_{E(Y(0)/X)} + S_{E(Y(1)/X)}$, where the sum of two linear subspaces is $U + V = \{u + v : u \in U, v \in V\}$. In some cases $S_{E(D/X)}$ may have a strictly smaller dimension than $S_{E(Y(0)/X)}$ and $S_{E(Y(1)/X)}$ as demonstrated by the following example. Thus, using model (1) may detect more
parsimonious structures of $\tau(x)$ than using model (2).

Example 1. Let $Y(0) = \alpha^T X + (\beta^T X)^2$ and $Y(1) = \alpha^T X + (\beta^T X)^3$, where $\alpha, \beta \in \mathbb{R}^p$, and $\alpha$ and $\beta$ are not linearly dependent. Then, $\dim(\mathcal{S}_{E\{Y(0)|X\}}) = \dim(\mathcal{S}_{E\{Y(1)|X\}}) = \dim(\text{span}(\alpha, \beta)) = 2$, while $\dim(\mathcal{S}_{E(D|X)}) = \dim(\text{span}(\beta)) = 1$.

Remark 2. As discussed in Ma and Zhu (2013), the parameter $B$ is not identifiable without further restrictions. To see this, suppose that $Q$ is an invertible $d \times d$ matrix and consider $g^*(u) = g\{(Q^T)^{-1}u\}$. Then we can derive another equivalent representation of $\tau(x)$ as

$$\tau(x) = g(B^T x) = g\{(Q^T)^{-1}Q^T B^T x\} = g^\ast\{(BQ)^T x\}.$$

Thus, the two sets of parameters $(B, g)$ and $(BQ, g^*)$ correspond to the same conditional average treatment effect. As a result, the central subspace was introduced to make the column space invariant to these invertible linear transformations. We use a particular parametrization of the central mean subspace as used in Ma and Zhu (2013). Without loss of generality, we set the upper $d \times d$ block of $B$ to be the identity matrix $I_{d \times d}$ and write $X = (X_u^T, X_l^T)^T$, where $X_u \in \mathbb{R}^d$ and $X_l \in \mathbb{R}^{p-d}$. Hence, the free parameters are the lower $(p-d) \times d$ entries of $B$, corresponding to the coefficients of $X_l$. For generic matrix $B$, we now denote $\text{vecl}(B)$ as the vector formed by the lower $(p-d) \times d$ entries of $B$.

2.3 Imputation and Estimation

If $D$ were known, existing methods can be directly applied to estimate $\mathcal{S}_{E(D|X)}$. However, the fundamental problem in causal inference is that the two potential outcomes can never be jointly observed for each unit, one is factual $Y(A)$ and the other one is counterfactual $Y(1-A)$. To overcome this challenge, we propose an imputation step to impute the counterfactual outcomes. A natural choice to impute $Y(1-A)$ is using its conditional mean given $X$, $\mu_{1-A}(X)$. As mentioned in §2.1 $\mu_a(x)$ can be estimated by matching or other nonparametric smoothing techniques. To further reduce the possible curse of dimensionality, we propose a prior dimension reduction procedure to estimate $\mu_a(x)$.

The proposed imputation and estimation procedure proceeds as follows.
**Step 1.** Estimate the central mean subspace \( S_{E(Y(a)|X)} \) \((a = 0, 1)\). Let \( \mu_a(u; B) = E(Y \mid A = a, B^TX = u) \), where \( B \) is a \( p \times d \) parameter matrix. Given \( B \), the kernel smoothing estimator of \( \mu_a(u; B) \) is

\[
\hat{\mu}_a(u; B) = \frac{\sum_{j=1}^{n} Y_j 1(A_j = a)K_{q,h}(B^TX_j - u)}{\sum_{j=1}^{n} 1(A_j = a)K_{q,h}(B^TX_j - u)},
\]

where \( 1(\cdot) \) is the indicator function, \( K_{q,h}(u) = \prod_{k=1}^d K_q(u_k/h)/h \) with \( u = (u_1, \ldots, u_d) \), \( K_q \) is a \( q \)th ordered and twice continuously differentiable kernel function with bounded support, and \( h \) is a positive bandwidth. The basis matrix of \( S_{E(Y(a)|X)} \) can be estimated by \( \hat{B}_a \), where \((\hat{d}_a, \hat{B}_a, \hat{h}_a)\) is the minimizer of the cross-validation criterion

\[
CV_a(d, B, h) = \sum_{i=1}^{n} \left\{ Y_i - \hat{\mu}_a^{-i}(B^TX_i; B) \right\}^2 1(A_i = a),
\]

where the superscript \(-i\) indicates the estimator \( \hat{\mu}_a \) based on data without the \( i \)th subject. This criterion \( CV \) is a mean regression version of Huang and Chiang (2017). In the optimization, the order of the kernel function \( q > \max(d/2 + 1, 2) \) is specified for each working dimension \( d \).

**Step 2.** Impute the individual treatment effect by

\[
\hat{D}_i = A_i\{Y_i - \hat{\mu}_0(\hat{B}_0^TX_i; \hat{B}_0)\} + (1 - A_i)\{\hat{\mu}_1(\hat{B}_1^TX_i; \hat{B}_1) - Y_i\} \quad (i = 1, \ldots, n)
\]

with specified orders \((q_0, q_1)\) of kernel functions and bandwidths \((h_0, h_1)\) in \( \hat{\mu}_0(\hat{B}_0^TX_i; \hat{B}_0) \) and \( \hat{\mu}_1(\hat{B}_1^TX_i; \hat{B}_1) \). The choices of \( q_0 \) and \( q_1 \) will be discussed in §2.4. The bandwidths can be chosen as estimated optimal bandwidths by nonparametric smoothing methods, such that \( h_a = O_p\{n^{-1/(2q_a+d_a)}\} \), where \( d_a = \dim(S_{E(Y(a)|X)}) \) \((a = 0, 1)\).

**Step 3.** Estimate the central mean subspace \( S_{E(D|X)} \) based on \( \{(\hat{D}_i, X_i) : i = 1, \ldots, n\} \). Let \( \tau(u; B) = E\{Y(1) - Y(0) \mid B^TX = u\} \). Given \( B \), the kernel smoothing estimator of \( \tau(u; B) \) is

\[
\hat{\tau}(u; B) = \frac{\sum_{j=1}^{n} \hat{D}_jK_{q,h}(B^TX_j - u)}{\sum_{j=1}^{n} K_{q,h}(B^TX_j - u)}. \tag{5}
\]

We then estimate \((d_\tau, B_\tau)\) and a suitable bandwidth for \( \hat{\tau}(u; B) \) by the minimizer \((\hat{d}, \hat{B}, \hat{h})\) of the
following criterion:

$$cv(d, B, h) = n^{-1} \sum_{i=1}^{n} \{ \hat{D}_i - \tilde{\tau}^{-i}(B^T X_i; B) \}^2,$$

where the superscript $-i$ indicates the estimator based on data without the $i$th subject. Here, $q > \max(d/2 + 1, 2)$ is also specified for each working dimension $d$.

**Step 4.** Estimate $\tau(x)$ by $\tilde{\tau}(\hat{B}^T x; \hat{B})$ with some suitable choice of $(q, h_{\tau})$, which will be further discussed in §2.4.

**Remark 3.** In Step 2, we estimate the structural dimension and the basis matrix simultaneously. On the other hand, Liang and Yu (2020) considered the multiple index model with a fixed dimension of the index and proposed the semiparametric efficient score of $B_{\tau}$. As we will show in Theorem 1, the asymptotic distribution of $\hat{B}$ does not affect the asymptotic distribution of the estimated conditional average treatment effect as long as $\hat{B}$ is root-$n$ consistent. Therefore, it is not necessary to pursue the semiparametric efficiency estimation of the central mean subspace in our context.

**Remark 4.** An alternative method of imputing the counterfactual outcomes is matching. To fix ideas, we consider matching without replacement and with the number of matches fixed at one. Then the matching procedure becomes nearest neighbor imputation (Little and Rubin 2002). Without loss of generality, we use the Euclidean distance to determine neighbors; the discussion applies to other distances (Abadie and Imbens 2006). Let $J_i$ be the index set for the matched subject of $i$th subject. Define the imputed missing outcome as $\tilde{Y}_i(A_i) = Y_i$ and $\tilde{Y}_i(1 - A_i) = \sum_{j \in J_i} Y_j$. Then the individual causal effect can be estimated by $\hat{D}_{\text{MAT},i} = \tilde{Y}_i(1) - \tilde{Y}_i(0)$. Matching uses the full vector of confounders to determine the distance and corresponding neighbors. When the number of confounders gets larger, this distance may be too conservative to determine proper neighbors due to the curse of dimensionality. In the simulation studies, we find that the estimation of $S_{E(D|X)}$ based on $\hat{D}_{\text{MAT},i}$ has a poor performance.

**Remark 5.** Instead of imputing the counterfactual outcomes, weighting can also be used to estimate $D_i$ directly. Several authors have considered an adjusted outcome $\hat{D}_{\text{IPW},i} = \{A_i - \pi(X_i)\} Y_i / [\pi(X_i)\{1 - \pi(X_i)\}]$ by inverse propensity score weighting. The adjusted outcome is unbi-
ased of \( \tau(X_i) \) due to

\[
E(\hat{D}_{\text{IPW},i} \mid X_i) = E \left\{ \frac{A_i Y_i}{\pi(X_i)} - \frac{(1 - A_i)Y_i}{1 - \pi(X_i)} \mid X_i \right\} = E\{Y_i(1) - Y_i(0) \mid X_i\} = \tau(X_i).
\]

This approach is attractive in clinical trials, where \( \pi(X_i) \) is known by trial design. In observational studies, \( \pi(X_i) \) is usually unknown and needs to be estimated. \[\text{Abrevaya et al. (2015)}\]

considered kernel regression to estimate \( \pi(X_i) \). To avoid possible curse of dimensionality and keep the nonparametric merit, we can perform a prior dimension reduction to find \( B_\pi \) such that

\[
\pi(\hat{B}^T_\pi X_i; \hat{\tau}) = \frac{\sum_{j=1}^{n_j} A_j K_{q,h}(\hat{B}^T_\pi X_j - \hat{B}^T_\pi X_i)}{\sum_{j=1}^{n_j} K_{q,h}(\hat{B}^T_\pi X_j - \hat{B}^T_\pi X_i)},
\]

where \( \hat{B}_\pi \) can be obtained similarly following Step 1 in \[\text{2.3}\] by changing the outcome to \( A \). However, the estimator \( \hat{D}_{\text{IPW},i} = \{A_i - \hat{\pi}(\hat{B}^T_\pi X_i; \hat{B}_\pi)\}Y_i / [\hat{\pi}(\hat{B}^T_\pi X_i; \hat{B}_\pi)\{1 - \hat{\pi}(\hat{B}^T_\pi X_i; \hat{B}_\pi)\}] \) still suffers from the instability due to the inverse weighting, especially when \( \hat{\pi}(\hat{B}^T_\pi X_i; \hat{B}_\pi) \) is close to zero or one.

It is well known that the augmented inverse propensity weighted estimator reduces this instability by combining inverse propensity weighting and outcome regressions. Specifically, the corresponding estimator of \( D_i \) is

\[
\hat{D}_{\text{AIPW},i} = \frac{Y_i - \{1 - \hat{\pi}(\hat{B}^T_\pi X_i; \hat{B}_\pi)\} \hat{\mu}_1(\hat{B}^T_\pi X_i; \hat{\tau}) - \hat{\pi}(\hat{B}^T_\pi X_i; \hat{B}_\pi) \hat{\mu}_0(\hat{B}^T_0 X_i; \hat{\tau}_0)}{\hat{\pi}(\hat{B}^T_\pi X_i; \hat{B}_\pi)\{1 - \hat{\pi}(\hat{B}^T_\pi X_i; \hat{B}_\pi)\}}.
\]

One can easily show that \( E(\hat{D}_{\text{AIPW},i} \mid X_i) \) is asymptotically unbiased of \( \tau(X_i) \). The estimator \( \hat{D}_{\text{AIPW},i} \) is a refined version of \[\text{Lee et al. (2017)}\], in which the propensity scores are estimated without a prior dimension reduction. Our simulation shows that the estimated central mean subspace and conditional average treatment effect based on \( \hat{D}_i \) and \( \hat{D}_{\text{AIPW},i} \) are comparable and both outperform those based on \( \hat{D}_{\text{MAT},i} \) and \( \hat{D}_{\text{IPW},i} \). Since \( \hat{D}_{\text{AIPW},i} \) requires an extra dimension reduction on \( \pi(x) \) and, hence, more computational time, our proposed \( \hat{D}_i \) is more computationally efficient in practice.
2.4 Inference

In this subsection, we derive the large sample properties of \( \hat{B} \) and \( \hat{\tau}(\hat{B}^T x; \hat{B}) \). Based on the notation and regularity conditions in the Supplementary Material, we first establish the following theorem for the prior sufficient dimension reduction for \( \mu_a(x) \) \((a = 0, 1)\).

**Theorem 1.** Suppose that Assumption 1 and Conditions A1–A5 are satisfied. Then \( \text{pr}(\hat{d}_a = d_a) \to 1, \hat{h}_a = O_P\{n^{-1/(2q + d_a)}\} \), and

\[
\frac{1}{n^{1/2}} \text{vec}(\hat{B}_a - B_a)1(\hat{d}_a = d_a) = n^{1/2} \sum_{i=1}^{n} \xi_{B_a,i} + o_P(1) \to N(0, \Sigma_{B_a})
\]

in distribution as \( n \to \infty \), where \( \xi_{B_a} = \{V_a(B_a)\}^{-1}S_a(B_a) \) and \( \Sigma_{B_a} = \{V_a(B_a)\}^{-1}E\{S_a \otimes 2 (B_a)\}\{V_a(B_a)\}^{-1} \) \((a = 0, 1)\).

Exact forms of \( V_a(B_a) \) and \( S_a(B_a) \) are presented in the Supplementary Material. Theorem 1 is a modification of results in Huang and Chiang (2017) and hence we omit the proof. Theorem 1 is a building block to derive the asymptotic distributions of the estimated central mean space and the proposed estimator for \( \tau(x) \), taking into account the fact that \( D_i \) is imputed.

**Theorem 2.** Suppose that Assumption 1 and Conditions A1–A8 are satisfied. Then \( \text{pr}(\hat{d} = d_\tau) \to 1, \hat{h} = O_P\{n^{-1/(2q + d_\tau)}\} \), and

\[
\frac{1}{n^{1/2}} \text{vec}(\hat{B} - B_\tau)1(\hat{d} = d_\tau) = n^{1/2} \sum_{i=1}^{n} \xi_{B_\tau,i} + o_P(1) \to N(0, \Sigma_{B_\tau})
\]

in distribution as \( n \to \infty \), where \( \xi_{B_\tau} = \{V(B_\tau)\}^{-1}S(B_\tau) \) and \( \Sigma_{B_\tau} = \{V(B_\tau)\}^{-1}E\{S \otimes 2 (B_\tau)\}\{V(B_\tau)\}^{-1} \).

Exact forms of \( V(B_\tau) \) and \( S(B_\tau) \) are presented in the Supplementary Material.

**Theorem 3.** Suppose that Assumption 1 and Conditions A1–A10 are satisfied. Then,

\[
(n h_\tau^{1/2})^{1/2} \{\hat{\tau}(\hat{B}^T x; \hat{B}) - \tau(x) - h_\tau^{q_\tau} \gamma(x)\} \to N(0, \sigma_\tau^2(x))
\]

in distribution as \( n \to \infty \), where

\[
\gamma(x) = \frac{\kappa \partial^{q_\tau} \{E(Z \mid B_{\tau}^TX = u) f_{B_{\tau}X}(u)\} - E(Z \mid B_{\tau}^TX = u) \partial^{q_\tau} f_{B_{\tau}X}(u)}{f_{B_{\tau}X}(u)} \Big|_{u = B_{\tau}^Tx},
\]
\[ \sigma^2_\tau(x) = \frac{\int K^2_{q_\tau}(s) ds}{\int B^*_\tau x(B^*_\tau x)} \text{var}[Z + \{1 - \pi(X)\} \varepsilon_1 - \pi(X)\varepsilon_0 \mid B^*_\tau X = B^*_\tau x], \]

\[ \kappa = \int s^{q_\tau} K_{q_\tau}(s) ds / q_\tau!, \quad Z = (2A - 1)\{Y - \mu_{1-A}(B^*_{1-A}X; B_{1-A})\}, \quad \varepsilon_n = \{Y - \mu_n(X)\}1(A = a) (a = 0, 1). \]

The proofs of Theorems 2–3 are given in the Supplementary Material. The proof of Theorem 2 is similar to that of Theorem 1. The main difference is that the outcome contributing to the asymptotic distribution is now \( Z \) instead of the counterfactual \( D \). The proof of Theorem 3 mainly focuses on approximating the influence function coupled with the difference between imputed and non-imputed counterfactual outcomes.

**Remark 6.** One should note that the asymptotic bias of \( \hat{\mu}_a(u; B) \) is not involved in the asymptotic distribution of \( \hat{\tau}(\hat{B}^*_\tau x; \hat{B}) \). This is an important result of Condition A6, which ensures that the convergence rate of \( \hat{\mu}_a(u; B) - \mu_a(u; B) \) is always faster than that of \( \hat{\tau}(u; B) - E(Z \mid B^* X = u) \).

**Remark 7.** The most important feature of Theorem 3 is that the asymptotic variance of \( \hat{B} \) is not involved in the asymptotic variance of \( \hat{\tau}(\hat{B}^*_\tau x; \hat{B}) \). More precisely speaking, \( \hat{\tau}(\hat{B}^*_\tau x; \hat{B}) \) has the same asymptotic variance as the one of \( \hat{\tau}(B^*_\tau x; B_\tau) \). The reason is that \( \| \hat{B} - B_\tau \| = O_p(n^{-1/2}) \), which is much faster than the convergence rate \( O_p[h^q_\tau + \{\log n/(nh^d_\tau)\}^{1/2}] \) of \( \hat{\tau}(B^*_\tau x; B_\tau) - \tau(x) \).

Based on Theorem 3, we can make inference of \( \tau(x) \) by estimating the asymptotic bias and variance. However, in practice, direct estimates of \( \gamma(x) \) and \( \sigma^2_\tau(x) \) are usually unstable, especially when the imputed counterfactual outcomes are involved. For a pre-specified \( q_\tau \) that satisfies Condition A10, we propose a under-smooth strategy such that the asymptotic bias is dominated by the asymptotic variance. We propose to choose an optimal bandwidth \( h_{\tau,\text{opt}} = O\{n^{-1/(2q_\tau+2d_\tau)}\} \) by using standard cross-validation criterion and use \( h_\tau = h_{\tau,\text{opt}} n^{-\delta\tau} \) for some small positive value \( \delta_\tau \) in the inference procedure. We then use a bootstrapping method to estimate the asymptotic distribution of \( \hat{\tau}(\hat{B}^*_\tau x; \hat{B}) - \tau(x) \).

Let \( \xi_i (i = 1, \ldots, n) \) be independent and identically distributed from a certain distribution with mean \( \mu_\xi \) and variance \( \sigma^2_\xi(x) \). Then \( w_i = \xi_i / \sum_{j=1}^n \xi_j \) (\( i = 1, \ldots, n \)) are exchangeable random weights.
The bootstrapped estimator $\hat{\tau}^*(x)$ is calculated as

$$\hat{\tau}^*(x) = \frac{\sum_{j=1}^{n} w_j \hat{D}^*_j K_{q,r} (\hat{B}^T x_j - \hat{B}^T x)}{\sum_{j=1}^{n} w_j K_{q,r} (\hat{B}^T x_j - \hat{B}^T x)},$$

where

$$\hat{D}^*_j = A_i \{Y_i - \hat{\mu}_0^i(\hat{B}_0^T X_i; \hat{B}_0)\} + (1 - A_i) \{\hat{\mu}_1^i(\hat{B}_1^T X_i; \hat{B}_1) - Y_i\},$$

$$\hat{\mu}_a(u; B) = \frac{\sum_{j=1}^{n} w_j Y_j 1(A_j = a) K_{q,a} (\hat{B}_a^T X_j - u)}{\sum_{j=1}^{n} w_j 1(A_j = a) K_{q,a} (\hat{B}_a^T X_j - u)} \quad (a = 0, 1).$$

According to Remark 7, $\hat{B}$, $\hat{B}_0^T$, and $\hat{B}_1^T$ require no bootstrapping in the inference, which highly reduces the computational burden in practice.

The asymptotic variance of $\hat{\tau}(\hat{B}^T x; \hat{B})$ is estimated by $[\text{se}\{\hat{\tau}^*(x)\}]^2 / \sigma_\xi$, where $\text{se}(\cdot)$ denote the standard error of $N$ bootstrapped estimators. The confidence region of $\tau(x)$ with $1 - \alpha$ confidence level can then be constructed as

$$\hat{\tau}(\hat{B}^T x; \hat{B}) \pm Z_{1-\alpha/2} \text{se}\{\hat{\tau}^*(x)\} \frac{\mu_\xi}{\sigma_\xi},$$

where $Z_p$ is the $p$th quantile of the standard normal distribution.

### 3 Simulation

#### 3.1 Data generating processes

In this section we present a Monte Carlo exercise aimed at evaluating the finite-sample accuracy of the asymptotic approximations given in the previous section. The covariates $X = (X_1, \ldots, X_{10})$ are generated from independent and identical $\text{Unif}(-3^{1/2}, 3^{1/2})$. The propensity score is $\text{logit}\{\pi(X)\} = 0.5(1 + X_1 + X_2 + X_3)$. The percentage of treated is about 60%. The potential outcomes are designed as following two settings:

**M1.** $Y(0) = X_1 - X_2 + \varepsilon(0)$ and $Y(1) = 2X_1 + X_3 + \varepsilon(1)$, where $\varepsilon(0)$ and $\varepsilon(1)$ independently follow $\mathcal{N}(0, 0.02^2)$. Hence, the conditional average treatment effect is $\tau(x) = x_1 + x_2 + x_3$, and the central mean subspace is $\text{span}\{(1, 1, 1, 0, \ldots, 0)^T\}$. 

M2. \( Y(0) = (X_1 + X_3)(X_2 - 1) + \varepsilon(0) \) and \( Y(1) = 2X_2(X_1 + X_3) + \varepsilon(1) \), where \( \varepsilon(0) \) and \( \varepsilon(1) \) independently follow \( N(0, 0.02^2) \). Hence, the conditional average treatment effect is \( \tau(x) = (x_1 + x_3)^2(x_2 + 1)^2 \), and the central mean subspace is \( \text{span}\{(1, 0, 1, 0, \ldots, 0)^T, (0, 1, 0, \ldots, 0)^T\} \).

The sample size ranges from \( n = 250 \) and \( n = 500 \). All the results are based on 1000 replications.

### 3.2 Competing estimators and simulation results

First, we compare the finite-sample performance of the estimated central mean subspaces using different imputed or adjusted outcomes. In addition to our proposed \( \hat{D}_i \), the nearest neighbor imputation \( \hat{D}_{\text{MAT},i} \), the inverse weighted outcome \( \hat{D}_{\text{IPW},i} \), as well as \( \hat{D}_{\text{AIPW},i} \), we also consider \( \hat{D}_{X,i} = (2A_i - 1)\{Y_i - \hat{\mu}_{1-A_i}(X_i; I_p)\} \), which is the imputed outcome without any dimension reduction. To compare the information loss for counterfactual outcomes and prior dimension reduction, we further perform the dimension reduction based on the true individual effect \( D_i \) and the imputed outcome \( \hat{D}_{\text{OR},i} = (2A_i - 1)\{Y_i - \hat{\mu}_{1-A_i}(X_i; B_{1-A_i})\} \) based on true oracle central mean subspaces of the prognostic scores. The proportions of estimated structural dimension and the mean squared errors

\[
\|\hat{B}(\hat{B}^T\hat{B})^{-1}\hat{B}^T - B_\tau(B_\tau^TB_\tau)^{-1}B_\tau^TB_\tau\|^2
\]

of the estimated central mean subspaces are displayed in Table 1. In general, all the proportions of selecting correct structural dimension tend to one and the mean squared errors tend to zero as sample size increases. Moreover, our proposed estimator outperforms the others and is comparable with respect to the simulated estimators based on \( \hat{D}_{\text{OR},i} \).

Second, we compare the finite-sample performance of the estimated conditional average treatment effects, which include our proposed estimator \( \hat{\tau}(\hat{B}^T x; \hat{B}) \), the estimator \( \hat{\tau}_X(x) \) based on imputed outcome \( \hat{D}_{X,i} \), the estimator \( \hat{\tau}_{\text{MAT}}(x) \) based on the imputed outcome \( \hat{D}_{\text{MAT},i} \), the estimator \( \hat{\tau}_{\text{IPW}}(x) \) based on the adjusted outcome \( \hat{D}_{\text{IPW},i} \), and the estimator \( \hat{\tau}_{\text{AIPW}}(x) \) based on the adjusted outcome \( \hat{D}_{\text{AIPW},i} \). In addition, we also estimate the conditional average treatment effect by using the difference of two estimated prognostic scores \( \hat{\tau}_{\text{prog}}(x) = \hat{\mu}_1(\hat{B}_1^T x; \hat{B}_1) - \hat{\mu}_0(\hat{B}_0^T x; \hat{B}_0) \). The smoothing estimator \( \hat{\tau}_0(x) \) based on \( D_i \) is also considered as a reference to demonstrate the information loss. The conditional average treatment effects are evaluated at \( x = (0, \ldots, 0)^T \). The means, standard deviations, and the mean squared errors are displayed in Table 2. In general, our proposed estimator and the \( \hat{\tau}_{\text{AIPW}} \) have comparable performance, and both of them outperform the others.

Finally, we construct confidence intervals and inference for the conditional average treatment
effects by using bootstrapping. Here naive bootstrapping is adopted. That is, \((w_1, \ldots, w_n)\) follows a multinomial distribution with number of trials being \(n\) and event probabilities \((1/n, \ldots, 1/n)\). Table 3 includes the standard deviations, bootstrapped standard errors and 95% quantile intervals of estimated conditional average treatment effects, as well as the normal-type 95% confidence intervals with corresponding coverage probabilities and quantile-type 95% confidence intervals with corresponding coverage probabilities for true conditional average treatment effect. As expected, the standard errors get close to the standard deviations, and the coverage probabilities tend to the nominal level when the sample size gets larger.

4 Empirical examples

4.1 The effect of maternal smoking on birth weight

We apply our proposed method to two existing datasets to estimate the effect of maternal smoking on birth weight conditional on different levels of confounders. In the literature, many studies documented that mother’s health, educational and labor market status have important effects on child birth weight \((\text{Currie and Almond } 2011)\). In particular, maternal smoking is considered as the most important preventable negative cause \((\text{Kramer } 1987)\). \text{Lee et al. } (2017) studied the conditional average treatment effect of smoking given mother’s age. In this work, our goal is to fully characterize the conditional average treatment effect of smoking on child birth weight given a vector of important confounding variables while maintaining the interpretability.

4.2 Pennsylvania data

The first dataset consists of observations collected in 2002 from mothers in Pennsylvania in the U.S.A. available from the STATA website (http://www.stata-press.com/data/r13/cattaneo2.dta). Following \text{Lee et al. } (2017), we focus on white and non-Hispanic mothers, leading to the sample size 3754. The outcome \(Y\) of interest is infant birth weight measured in grams. The treatment variable \(A\) is equal to 1 if the mother is a smoker and 0 otherwise. The set of covariates \(X\) includes the number of prenatal care visits, mother’s educational attainment, age, an indicator for the first baby, an indicator for alcohol consumption during pregnancy, an indicator for the first prenatal visit in the first trimester, and an indicator for whether there was a previous birth where the newborn died.
Table 1: The proportions of $\hat{d}$ and the mean squared errors (MSE) of $\hat{B}$ under different model settings, sample sizes ($n$), and imputation of $D_i$

| Model | $n$ | $\hat{D}_i$ | $\hat{D}_{X,i}$ | $\hat{D}_{MAT,i}$ | $\hat{D}_{IPW,i}$ | $\hat{D}_{AIPW,i}$ | $\hat{D}_{OR,i}$ | MSE |
|-------|-----|--------------|------------------|-------------------|-------------------|-------------------|--------------|-----|
| M1    | 250 | 0.000        | 0.976            | 0.024             | 0.000             | 0.000             | 0.0293       |
|       |     | 0.000        | 0.716            | 0.246             | 0.037             | 0.001             | 0.5840       |
|       |     | 0.000        | 0.833            | 0.148             | 0.018             | 0.001             | 0.2927       |
|       |     | 0.000        | 0.680            | 0.299             | 0.087             | 0.004             | 0.7143       |
|       |     | 0.000        | 0.955            | 0.045             | 0.000             | 0.000             | 0.0555       |
|       |     | 0.000        | 0.999            | 0.001             | 0.000             | 0.000             | 0.0013       |
|       | 500 | 0.000        | 0.985            | 0.015             | 0.000             | 0.000             | 0.0171       |
|       |     | 0.000        | 0.676            | 0.295             | 0.029             | 0.000             | 0.5392       |
|       |     | 0.000        | 0.897            | 0.097             | 0.006             | 0.000             | 0.1588       |
|       |     | 0.000        | 0.615            | 0.256             | 0.119             | 0.01              | 0.6744       |
|       |     | 0.000        | 0.980            | 0.020             | 0.000             | 0.000             | 0.0236       |
|       |     | 0.000        | 0.999            | 0.001             | 0.000             | 0.000             | 0.0012       |
|       |     | 0.000        | 0.985            | 0.015             | 0.000             | 0.000             | 0.0171       |
| M2    | 250 | 0.000        | 0.000            | 0.995             | 0.005             | 0.000             | 0.0237       |
|       |     | 0.000        | 0.062            | 0.883             | 0.053             | 0.002             | 0.3222       |
|       |     | 0.000        | 0.050            | 0.894             | 0.052             | 0.004             | 0.3608       |
|       |     | 0.000        | 0.269            | 0.610             | 0.110             | 0.011             | 0.9581       |
|       |     | 0.000        | 0.008            | 0.978             | 0.014             | 0.000             | 0.0616       |
|       |     | 0.000        | 0.000            | 0.995             | 0.005             | 0.000             | 0.0119       |
|       | 500 | 0.000        | 0.003            | 0.992             | 0.004             | 0.001             | 0.0243       |
|       |     | 0.000        | 0.000            | 0.997             | 0.003             | 0.000             | 0.0139       |
|       |     | 0.000        | 0.008            | 0.955             | 0.035             | 0.002             | 0.1858       |
|       |     | 0.000        | 0.013            | 0.963             | 0.021             | 0.003             | 0.2040       |
|       |     | 0.000        | 0.165            | 0.714             | 0.109             | 0.012             | 0.7532       |
|       |     | 0.000        | 0.001            | 0.995             | 0.004             | 0.000             | 0.0224       |
|       |     | 0.000        | 0.000            | 1.000             | 0.000             | 0.000             | 0.0090       |
|       |     | 0.000        | 0.000            | 1.000             | 0.000             | 0.000             | 0.0027       |
### Table 2: The mean squared errors of estimated conditional average treatment effects under different model settings and sample sizes ($n$)

| model | $n$ | $\hat{\tau}(\hat{B}^T x; \hat{B})$ | $\hat{\tau}_X(x)$ | $\hat{\tau}_{\text{MAT}}(x)$ | $\hat{\tau}_{\text{IPW}}(x)$ | $\hat{\tau}_{\text{AIPW}}(x)$ | $\hat{\tau}_{\text{prog}}(x)$ | $\hat{\tau}_0(x)$ |
|-------|-----|---------------------------------|-------------------|------------------|-------------------|------------------|------------------|------------------|
| M1    | 250 | mean                           | 0.003             | -0.025           | 0.094             | 0.008            | 0.002            | 0.003            | -0.000          |
|       |     | s.d.                           | 0.0493            | 0.2203           | 0.2325            | 0.5903           | 0.0532           | 0.0545           | 0.0258          |
|       |     | MSE                            | 0.0024            | 0.0492           | 0.0629            | 0.3485           | 0.0028           | 0.0030           | 0.0007          |
|       | 500 | mean                           | -0.000            | 0.006            | 0.065             | -0.005           | -0.000           | 0.003            | -0.000          |
|       |     | s.d.                           | 0.0300            | 0.1474           | 0.1417            | 0.3642           | 0.0311           | 0.0310           | 0.0159          |
|       |     | MSE                            | 0.0009            | 0.0218           | 0.0243            | 0.1327           | 0.0010           | 0.0010           | 0.0003          |
| M2    | 250 | mean                           | -0.029            | -0.091           | -0.180            | -0.035           | -0.007           | -0.048           | 0.001           |
|       |     | s.d.                           | 0.1006            | 0.2072           | 0.3103            | 0.3803           | 0.1074           | 0.1399           | 0.0639          |
|       |     | MSE                            | 0.0110            | 0.0512           | 0.1288            | 0.1459           | 0.0116           | 0.0219           | 0.0041          |
|       | 500 | mean                           | -0.015            | -0.104           | -0.157            | -0.010           | -0.002           | -0.024           | 0.001           |
|       |     | s.d.                           | 0.0651            | 0.1418           | 0.2024            | 0.2463           | 0.0566           | 0.0926           | 0.0410          |
|       |     | MSE                            | 0.0045            | 0.0309           | 0.0655            | 0.0607           | 0.0032           | 0.0092           | 0.0017          |

### Table 3: The standard deviations (s.d.), bootstrapped standard errors (s.e.), and 95% quantile intervals (Q.I.) of estimated conditional average treatment effects, and normal-type 95% confidence intervals (N.C.I.) with corresponding coverage probabilities (N.C.P.) and quantile-type 95% confidence intervals (Q.C.I.) with corresponding coverage probabilities (Q.C.P.) for true conditional treatment effect

| model | $n$ | s.d. | s.e. | Q.I.      | N.C.I.        | N.C.P.    | Q.C.I.     | Q.C.P.    |
|-------|-----|------|------|-----------|---------------|-----------|------------|-----------|
| M1    | 250 | 0.0493 | 0.0621 | (-0.095,0.107) | (-0.119,0.125) | 0.966   | (-0.119,0.124) | 0.975   |
|       | 500 | 0.0300 | 0.0365 | (-0.066,0.062) | (-0.072,0.071) | 0.965   | (-0.074,0.067) | 0.972   |
| M2    | 250 | 0.1006 | 0.0998 | (-0.226,0.159) | (-0.225,0.166) | 0.944   | (-0.224,0.167) | 0.921   |
|       | 500 | 0.0651 | 0.0645 | (-0.132,0.109) | (-0.142,0.111) | 0.951   | (-0.140,0.112) | 0.937   |
The continuous covariates are centralized and standardized.

The estimated central mean subspace has dimension one. The coefficients of estimated linear index and corresponding standard errors are displayed in Table 4. Figure 1 shows the estimated conditional average treatment effect at different levels of linear index values along with corresponding normal-type confidence intervals. In general, smoking has significant effects on low birth weights, as detected in the existing studies. In particular, this effect decreases when the linear index value increases. Interestingly, the larger number of prenatal care visits and the first baby lead to significantly smaller effects than other confounding variables. This result shows that more frequent prenatal care visits and whether it is a first pregnancy mitigate the effect of smoking on low birth weights.

### 4.3 North Carolina data

The second dataset is based on the records between 1988 and 2002 by the North Carolina Center Health Services. The dataset was analyzed by Abrevaya et al. (2015) and can be downloaded from Prof. Leili’s website. To make a comparison with the Pennsylvania data, we focus on white and first-time mothers and form a random sub-sample with sample size \( n = 3754 \) among the subjects collected in 2002. The outcome \( Y \) and the treatment variable \( A \) remain the same as for the Pennsylvania data. The set of covariates includes those used in the analysis of Pennsylvania data but the indicator for the first baby and the indicator for whether there was a previous birth where the newborn died. Besides, it includes indicators for gestational diabetes, hypertension, amniocentesis, and ultrasound exams.

The estimated central mean subspace has dimension one. The coefficients of estimated linear index and corresponding standard errors are also displayed in Table 4. Figure 1 shows the estimated conditional average treatment effect at different levels of linear index values along with corresponding normal-type confidence intervals. Similar to the results from the Pennsylvania data, smoking has significant effects on low birth weights. Differently, this effect decreases when the level of estimated linear index values decreases. In particular, lower values of mothers educational attainment, higher values of mothers age, the absence of hypertension, and the amniocentesis significantly lead to larger treatment effects. This result shows that mother’s education attainment, age, and health status are also important modifying factors of smoking on low birth weight.
Table 4: The estimated coefficients of linear indices and corresponding standard errors (s.e.) for the Pennsylvania and North Carolina data.

| covariate                      | Pennsylvania data | North Carolina data |
|-------------------------------|-------------------|---------------------|
|                               | coefficient      | s.e.                | coefficient      | s.e.                |
| $X_1$ prenatal visit number   | -0.668           | 0.0645              | 0.043            | 0.0719              |
| $X_2$ education               | -0.059           | 0.2101              | -0.271           | 0.0477              |
| $X_3$ age                     | -0.210           | 0.3076              | 0.243            | 0.0485              |
| $X_4$ first baby              | 1                |                     |                   |                     |
| $X_5$ alcohol                 | 0.142            | 0.6103              | -0.101           | 0.2122              |
| $X_6$ first prenatal visit    | 0.275            | 0.3224              | -0.104           | 0.1556              |
| $X_7$ previous newborn death  | 0.169            | 0.1257              |                   |                     |
| $X_8$ diabetes                | -0.129           | 0.1268              |                   |                     |
| $X_9$ hypertension            | -0.333           | 0.1084              |                   |                     |
| $X_{10}$ amniocentesis        | 1                |                     |                   |                     |
| $X_{11}$ ultrasound           | -0.006           | 0.1612              |                   |                     |

Figure 1: The estimated conditional average treatment effects at different levels of linear index values with corresponding confidence intervals.
5 Discussion

The proposed framework of robust inference of conditional average treatment effect can be generalized in the following directions. First, we use under-smoothing to avoid the asymptotic bias of the conditional average treatment effect estimator. Without under-smoothing, the asymptotic bias is not negligible but may be estimated empirically as in Cheng and Chen (2019). We will investigate the possibility of a bias-corrected estimator in the future. Second, we can extend to estimate the conditional average treatment effect with continuous treatment. In this case, the first-stage dimension reduction applies to the potential outcomes for a given treatment level and a reference treatment level, and the second-stage searches the central space for the contrast between the two prognostic scores under the two levels. Third, the first-stage dimension reduction is not confined to the central mean space but can be applied to a transformation of the outcome $g(Y(a))$ for any function $g(\cdot)$. This allows the estimation of the general type of conditional treatment effects such as conditional distribution or quantile treatment effects. Similar to the main paper, we can also derive robust estimators for these causal estimands.

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Supplementary material

Supplementary Material includes additional notation and the regularity conditions and the proofs of Theorems 2–3.

References

Abadie, A. and Imbens, G. W. (2006). Large sample properties of matching estimators for average treatment effects, *Econometrica* 74(1): 235–267.
Abrevaya, J., Hsu, Y.-C. and Lieli, R. P. (2015). Estimating conditional average treatment effects, *J. Bus. Econom. Statist.* **33**(4): 485–505. 1 5 4.3

Athey, S. and Imbens, G. (2016). Recursive partitioning for heterogeneous causal effects, *Proc. Natl. Acad. Sci. USA* **113**(27): 7353–7360. 1

Athey, S., Tibshirani, J. and Wager, S. (2019). Generalized random forests, *Ann. Statist.* **47**(2): 1148–1178. 1

Chakraborty, B., Murphy, S. and Strecher, V. (2010). Inference for non-regular parameters in optimal dynamic treatment regimes, *Stat. Methods Med. Res.* **19**(3): 317–343. 1

Chen, J. and Shao, J. (2000). Nearest neighbor imputation for survey data, *Journal of official statistics* **16**(2): 113.

Chen, J. and Shao, J. (2001). Jackknife variance estimation for nearest-neighbor imputation, *J. Amer. Statist. Assoc.* **96**(453): 260–269.

Cheng, G. and Chen, Y.-C. (2019). Nonparametric inference via bootstrapping the debiased estimator, *Electron. J. Stat.* **13**(1): 2194–2256. 5

Chipman, H. A., George, E. I. and McCulloch, R. E. (2010). BART: Bayesian additive regression trees, *Ann. Appl. Stat.* **4**(1): 266–298. 1

Cook, R. D. and Li, B. (2002). Dimension reduction for conditional mean in regression, *Ann. Statist.* **30**(2): 455–474. 1 2.2

Currie, J. and Almond, D. (2011). Human capital development before age five, *Handbook of labor economics*, Vol. 4, Elsevier, pp. 1315–1486. 4.1

Dawid, A. P. (1979). Conditional independence in statistical theory, *J. Roy. Statist. Soc. Ser. B* **41**(1): 1–31.

Huang, M.-Y. and Chiang, C.-T. (2017). An effective semiparametric estimation approach for the sufficient dimension reduction model, *J. Amer. Statist. Assoc.* **112**(519): 1296–1310. 1 2.4 S2 S3.1
Kang, J. D. Y. and Schafer, J. L. (2007). Rejoinder: Demystifying double robustness: a comparison of alternative strategies for estimating a population mean from incomplete data [mr2420458], Statist. Sci. 22(4): 574–580.

Kramer, M. S. (1987). Intrauterine growth and gestational duration determinants, Pediatrics 80(4): 502–511.

Lee, S., Okui, R. and Whang, Y.-J. (2017). Doubly robust uniform confidence band for the conditional average treatment effect function, Journal of Applied Econometrics 32(7): 1207–1225.

Liang, M. and Yu, M. (2020). A semiparametric approach to model effect modification, J. Amer. Statist. Assoc. 4.1, 4.2

Little, R. J. A. and Rubin, D. B. (2002). Statistical analysis with missing data, Wiley Series in Probability and Statistics, second edn, Wiley-Interscience [John Wiley & Sons], Hoboken, NJ.

Luo, W., Wu, W. and Zhu, Y. (2019). Learning heterogeneity in causal inference using sufficient dimension reduction, Journal of Causal Inference 7(1).

Ma, Y. and Zhu, L. (2013). Efficient estimation in sufficient dimension reduction, Ann. Statist. 41(1): 250–268.

Murphy, S. A. (2003). Optimal dynamic treatment regimes, J. R. Stat. Soc. Ser. B Stat. Methodol. 65(2): 331–366.

Nolan, D. and Pollard, D. (1987). U-processes: rates of convergence, Ann. Statist. 15(2): 780–799.

Powers, K. A., Poole, C., Pettifor, A. E. and Cohen, M. S. (2008). Rethinking the heterosexual infectivity of hiv-1: a systematic review and meta-analysis, The Lancet infectious diseases 8(9): 553–563.

Powers, S., Qian, J., Jung, K., Schuler, A., Shah, N. H., Hastie, T. and Tibshirani, R. (2018). Some methods for heterogeneous treatment effect estimation in high dimensions, Stat. Med. 37(11): 1767–1787.
Qian, M. and Murphy, S. A. (2011). Performance guarantees for individualized treatment rules, *Ann. Statist.* **39**(2): 1180–1210.

Robins, J. M. (2004). Optimal structural nested models for optimal sequential decisions, *Proceedings of the Second Seattle Symposium in Biostatistics*, Vol. 179 of *Lect. Notes Stat.*, Springer, New York, pp. 189–326.

Rosenbaum, P. R. and Rubin, D. B. (1983). The central role of the propensity score in observational studies for causal effects, *Biometrika* **70**(1): 41–55.

Rzepakowski, P. and Jaroszewicz, S. (2012). Decision trees for uplift modeling with single and multiple treatments, *Knowledge and Information Systems* **32**(2): 303–327.

Song, R., Luo, S., Zeng, D., Zhang, H. H., Lu, W. and Li, Z. (2017). Semiparametric single-index model for estimating optimal individualized treatment strategy, *Electron. J. Stat.* **11**(1): 364–384.

Thall, P. F., Millikan, R. E. and Sung, H.-G. (2000). Evaluating multiple treatment courses in clinical trials, *Stat. Med.* **19**(8): 1011–1028.

Thall, P. F., Sung, H.-G. and Estey, E. H. (2002). Selecting therapeutic strategies based on efficacy and death in multicourse clinical trials, *J. Amer. Statist. Assoc.* **97**(457): 29–39.

Thall, P. F., Wooten, L. H., Logothetis, C. J., Millikan, R. E. and Tannir, N. M. (2007). Bayesian and frequentist two-stage treatment strategies based on sequential failure times subject to interval censoring, *Stat. Med.* **26**(26): 4687–4702.

Zhang, B., Tsiatis, A. A., Davidian, M., Zhang, M. and Laber, E. (2012). Estimating optimal treatment regimes from a classification perspective, *Stat* **1**: 103–114.

Zhao, Y., Zeng, D., Rush, A. J. and Kosorok, M. R. (2012). Estimating individualized treatment rules using outcome weighted learning, *J. Amer. Statist. Assoc.* **107**(499): 1106–1118.

Zhao, Y., Zeng, D., Socinski, M. A. and Kosorok, M. R. (2011). Reinforcement learning strategies for clinical trials in nonsmall cell lung cancer, *Biometrics* **67**(4): 1422–1433.
S1 Additional Notation and Regularity Conditions

Let $(\cdot)^\otimes$ denote the Kronecker power of a vector and let $\| \cdot \|$ represent the Frobenius norm of a matrix. Denote $f_{B^T X}(u)$ as the marginal density of $B^T X$,

\[
\begin{align*}
 f^{[m]}(x, u; B) &= \partial^{m}_u [E\{(X_l - x_l)^{\otimes m} \mid B^T X = u\} f_{B^T X}(u)], \\
 E^{[m]}_a(x, u; B) &= \partial^{m}_u [\text{pr}(A = a \mid B^T X = u) E\{(X_l - x_l)^{\otimes m} \mid B^T X = u\} f_{B^T X}(u)], \\
 F^{[m]}_a(x, u; B) &= \partial^{m}_u [E\{Y_1(A = a) \mid B^T X = u\} E\{(X_l - x_l)^{\otimes m} \mid B^T X = u\} f_{B^T X}(u)], \\
 G^{[m]}(x; u; B) &= \partial^{m}_u [E(Z \mid B^T X = u) E\{(X_l - x_l)^{\otimes m} \mid B^T X = u\} f_{B^T X}(u)],
\end{align*}
\]

where $Z = (2A - 1)\{Y - \mu_{1-A}(B_{1-A} X; B_{1-A})\}$. We will show that

\[
\partial^{m}_{\text{vecl}(B)} \hat{\mu}_a(B^T x; B) \rightarrow \mu^{[m]}(x; B) = \sum_{\ell=0}^{m} \binom{m}{\ell} F^{[\ell]}_a(x, B^T x; B) E^{[m-\ell]}_{a, \text{inv}}(x, B^T x; B),
\]

and

\[
\partial^{m}_{\text{vecl}(B)} \hat{\tau}(B^T x; B) \rightarrow \tau^{[m]}(x; B) = \sum_{\ell=0}^{m} \binom{m}{\ell} G^{[\ell]}(x, B^T x; B) f^{[m-\ell]}_{\text{inv}}(x, B^T x; B),
\]

uniformly as $n \rightarrow \infty$, where

\[
\begin{align*}
 f^{[0]}_{\text{inv}}(x, u; B) &= 1/f_{B^T X}(u), & E^{[0]}_{a, \text{inv}}(x, u; B) &= 1/E^{[0]}_a(x, u; B), \\
 f^{[1]}_{\text{inv}}(x, u; B) &= -f^{[1]}(x, u; B)/f_{B^T X}^2(u), & f^{[2]}_{\text{inv}}(x, u; B) &= 2\{f^{[1]}(x, u; B)/f_{B^T X}(u)\}^2 f_{B^T X}(u) - f^{[2]}_{B^T X}(u),
\end{align*}
\]
According to the notation, we can define the corresponding score vectors and information matrices of $c_{V_a}(d, B, h)$ and $c_v(d, B, h)$:

\[
S_a(B) = -1(A = a)\{Y - \mu_a(B^TX; B)\}\mu^{[1]}(X; B),
\]

\[
V_a(B) = E(1(A = a)[\{\mu^{[1]}(X; B)\}^{\otimes 2} - \{Y - \mu_a(B^TX; B)\}\mu^{[2]}(X; B)]),
\]

\[
S(B) = -\{Z - E(Z \mid B^TX)\}\tau^{[1]}(X; B),
\]

\[
V(B) = E[\{\tau^{[1]}(X; B)\}^{\otimes 2} - \{Z - E(Z \mid B^TX)\}\tau^{[2]}(X; B)].
\]

In addition, let $B_{d,a}$ be the minimizer of $b_a^2(B) = E[\{\mu_a(B^TX; B) - \mu(X)\}^2]$ and let $B_{d,\tau}$ be the minimizer of $b_{\tau}^2(B) = E[\{E(Z \mid B^TX) - \tau(X)\}^2]$ over all $p \times d$ matrices $B$. Then, $b_a^2(B) \to b_a^2(B_{d,a})$ implies $B \to B_{d,a}$ for $\text{span}(B) \not\supset \text{span}(B_a)$, and $b_{\tau}^2(B) \to b_{\tau}^2(B_{d,\tau})$ implies $B \to B_{d,\tau}$ for $\text{span}(B) \not\supset \text{span}(B_{\tau})$. The following regularity conditions are imposed for our theorems:

A1 \quad $\partial_a^{\theta+m}E\{(X_i - x_i)^{\otimes m} \mid B^TX = u\} = \partial_a^{\theta+2}f_{B^TX}(u)$, $\partial_a^{\theta+2}\Pr(A = a \mid B^TX = u)$, $\partial_a^{\theta+2}E\{Y1A = a \mid B^TX = u\}$, and $\partial_a^{\theta+2}E(Z \mid B^TX = u)$ ($a = 0, 1, m = 1, 2$), are Lipschitz continuous in $u$ with the Lipschitz constants being independent of $(x, B)$.

A2 \quad $\inf_{(x,B)} f_{B^TX}(B^Tx) > 0$ and $\inf_{(x,B)} \Pr(A = a \mid B^TX = B^tx) > 0$ ($a = 0, 1$).

A3 \quad For each working dimension $d > 0$, $h$ falls in the interval $H_{d,n} = [h_in^{-\delta}, h_un^{-\delta}]$ for some positive constants $h_i$ and $h_u$ and $\delta \in (1/(4q), 1/\max\{2d + 2, d + 4\})$. In particular, this requires $q > \max(d/2 + 1, 2)$.

A4 \quad $\inf_{\{B:d<d_a\}} b_a^2(B) > 0$ and $b_a^2(B) = 0$ if and only if $B = B_a$ when $d = d_a$ ($a = 0, 1$).

A5 \quad $V_a(B_{d,a})$ is non-singular for $d \geq d_a$ ($a = 0, 1$).

A6 \quad For each working dimension $d$, $q_a > qd_a/d$ ($a = 0, 1$).

A7 \quad $\inf_{\{B:d<d_\tau\}} b_{\tau}^2(B) > 0$ and $b_{\tau}^2(B) = 0$ if and only if $B = B_{\tau}$ when $d = d_{\tau}$.

A8 \quad $V(B_{d,\tau})$ is non-singular for $d \geq d_{\tau}$.
A9 \( h_\tau \to 0 \) and \( nh_\tau^d \to \infty \).

A10 For each working dimension \( d, q_\tau > qd_\tau/d \).

Conditions A1–A2 are the smoothness and boundedness conditions for the population functions to ensure the uniform convergence of kernel estimators. Moreover, to remove the remainder terms in the approximation of \( \text{cv}(d, B, h) \) and \( \text{cv}(d, B, h) \) to their target functions, the constraints for the orders of kernel functions and the bandwidths are drawn in Conditions A3 and A6. Conditions A4–A5 and A7–A8 ensure the identifiability of \( B_a \) \((a = 0, 1)\) and \( B_\tau \), respectively. The requirements of \( h_\tau \) and \( q_\tau \) used in \( \hat{\tau}(\hat{B}^T x; \hat{B}) \) are given in Condition A9–A10.

S2 Preliminary Lemmas

The proofs of the main theorems rely on the following lemma:

**Lemma S1.** Suppose that Assumption 1 and Conditions A1–A6 are satisfied. Then,

\[
\hat{\tau}(u; B) - E(Z \mid B^T X = u) = \frac{1}{n} \sum_{i=1}^{n} \left( Z_i - E(Z \mid B^T X = u) \right) + \left\{ 1 - \pi(X_i) \right\} \varepsilon_{1,i} - \pi(X_i) \varepsilon_{0,i} \omega_{h,i}(u; B) + r_{n}(u; B),
\]

where \( \varepsilon_{a,i} = \{Y_i - \mu_a(X_i)\}1(A_i = a), \ (a = 0, 1) \), \( \omega_{h,i}(u; B) = K_{q,h}(B^T X_i - u) / \sum_{j=1}^{n} K_{q,h}(B^T X_j - u) \), and \( \sup_{(u, B)} |r_{n}(u, B)| = o_P[h^q + \{ \log n/(nh^d) \}^{1/2}] \).

**Proof.** First note that

\[
\hat{\tau}(u; B) - E(Z \mid B^T X = u) = \frac{1}{n} \{ \hat{D}_i - E(Z \mid B^T X = u) \} \omega_{h,i}(u; B)
\]

\[
= \frac{1}{n} \{ Z_i - E(Z \mid B^T X = u) \} \omega_{h,i}(u; B) + \frac{1}{n} \{ \hat{D}_i - Z_i \} \omega_{h,i}(u; B).
\]

Further,

\[
\frac{1}{n} (\hat{D}_i - Z_i) \omega_{h,i}(u; B)
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \left[ (1 - A_i) \{ \hat{\mu}_1(\hat{B}_1^T X_i; \hat{B}_1) - \mu_1(X_i) \} - A_i \{ \hat{\mu}_0(\hat{B}_0^T X_i; \hat{B}_0) - \mu_0(X_i) \} \right] \omega_{h,i}(u; B)
\]
Thus, by selecting the application of Theorem 6 in Nolan and Pollard (1987) ensures that

\[ E(\|u\|/\sum_{i=1}^{n}I_{n}J_{n}^{-1}(A_{n} - B_{n})\| = O_{p}(n^{-1/2}) \] by Theorem 1. Now let \( \kappa_{a,h,i}(u) = \mathcal{K}_{a,h}(B_{a}^{n}X_{i} - u) / \sum_{j=1}^{n}1(A_{j} = a)\mathcal{K}_{a,h}(B_{a}^{n}X_{j} - u) \). Then, we decompose \( I_{1} \)

\[
\frac{1}{n} \sum_{i=1}^{n}(1 - A_{i})\{\hat{\mu}_{1}(B_{1}^{T}X_{i}; B_{1}) - \mu_{1}(X_{i})\}\omega_{h,i}(u; B)
\]

\[
- \frac{1}{n} \sum_{i=1}^{n}A_{i}\{\hat{\mu}_{0}(B_{0}^{T}X_{i}; B_{0}) - \mu_{0}(X_{i})\}\omega_{h,i}(u; B) + O_{p}(n^{-1/2})
\]

\[ \triangleq I_{1} + I_{2} + O_{p}(n^{-1/2}), \] (S1)

because of \( \|\text{vec}(\hat{B}_{a} - B_{a})\| = O_{p}(n^{-1/2}) \) by Theorem 1. Now let \( \kappa_{a,h,i}(u) = \mathcal{K}_{a,h}(B_{a}^{n}X_{i} - u) / \sum_{j=1}^{n}1(A_{j} = a)\mathcal{K}_{a,h}(B_{a}^{n}X_{j} - u) \). Then, we decompose \( I_{1} \) into

\[
\frac{1}{n} \sum_{i=1}^{n}(1 - A_{i})\hat{\mu}_{1}(B_{1}^{T}X_{i}; B_{1}) - \mu_{1}(X_{i})\}\omega_{h,i}(u; B)
\]

\[
= \frac{1}{n} \sum_{i=1}^{n}\{1 - \pi(X_{i})\}\omega_{h,i}(u; B)\sum_{j=1}^{n}\{Y_{j} - \mu_{1}(X_{i})\}1(A_{j} = 1)\kappa_{1,h_{1},j}(B_{1}^{T}X_{i})
\]

\[
+ \frac{1}{n} \sum_{i=1}^{n}\{\pi(X_{i}) - A_{i}\}\omega_{h,i}(u; B)\sum_{j=1}^{n}\{Y_{j} - \mu_{1}(X_{i})\}1(A_{j} = 1)\kappa_{1,h_{1},j}(B_{1}^{T}X_{i})
\]

\[ = \frac{1}{n} \sum_{i=1}^{n}\{1 - \pi(X_{i})\}\varepsilon_{1,i}\omega_{h,i}(u; B)
\]

\[
+ \frac{1}{n} \sum_{i=1}^{n}\{1 - \pi(X_{i})\} \left( \sum_{j=1}^{n}\varepsilon_{1,j}\kappa_{1,h_{1},j}(B_{1}^{T}X_{i}) - \varepsilon_{1,i} \right)\omega_{h,i}(u; B)
\]

\[
+ \frac{1}{n} \sum_{i=1}^{n}\{\pi(X_{i}) - A_{i}\}\omega_{h,i}(u; B)\sum_{j=1}^{n}\{Y_{j} - \mu_{1}(X_{i})\}1(A_{j} = 1)\kappa_{1,h_{1},j}(B_{1}^{T}X_{i})
\]

\[ \triangleq J_{0} + J_{1} + J_{2} + J_{3}. \] (S2)

To bound \( J_{1} \), we re-write it as

\[
J_{1} = \frac{1}{n} \sum_{i=1}^{n}\varepsilon_{1,i} \left( \sum_{j=1}^{n}\{1 - \pi(X_{j})\}\omega_{h,j}(u; B)\kappa_{1,h_{1},j}(B_{1}^{T}X_{i}) - \{1 - \pi(X_{i})\}\omega_{h,i}(u; B) \right).
\]

Since \( E(\varepsilon_{1,i} | X_{i}) = 0 \), we can show that \( J_{1} \) is a degenerate U-process indexed by \((u, B)\). An application of Theorem 6 in Nolan and Pollard (1987) ensures that \( E(\text{sup}_{(u,B)} | J_{1}) \leq C / (n^{2}h_{1}^{d_{1}}h^{d}) \). Thus, by selecting \( h_{1} \) in an optimal rate \( O\{n^{-1/(2q_{1}+d_{1})}\} \) and coupled with Conditions A3 and A6,
we have
\[
\sup_{(u,B)} |J_1| = o_p \left\{ h^q + \left( \frac{\log n}{nh^d} \right)^{1/2} \right\}. \tag{S3}
\]

Second, similar to the proofs in [Huang and Chiang (2017)], standard arguments in kernel smoothing estimation show that
\[
\sup_{i} \left| \sum_{j=1}^{n} \{ \mu_1(X_j) - \mu_1(X_i) \} 1(A_j = 1) \kappa_{1,h_1,j}(B_1^T X_i) \right|
= O_p \left\{ h^{q_1} \left( \frac{\log n}{nh_{1}^{d_1}} \right)^{1/2} \right\} = O_p \{ n^{-q_1/(2q_1+d_1)} \}
\]
by selecting \( h_1 \) in an optimal rate \( O\{n^{-1/(2q_1+d_1)}\} \). Under Conditions A3 and A6, one can further show that this rate is \( o_p [h^q + \{ \log n/(nh^d) \}]^{1/2} \). Thus, we have
\[
\sup_{(u,B)} |J_2| = o_p \left\{ h^q + \left( \frac{\log n}{nh^d} \right)^{1/2} \right\}. \tag{S4}
\]

Finally, note that \( J_3 \) is also a degenerate U-process indexed by \((u, B)\). Thus, by the same argument for \( J_1 \), we can show that
\[
\sup_{(u,B)} |J_3| = o_p \left\{ h^q + \left( \frac{\log n}{nh^d} \right)^{1/2} \right\}. \tag{S5}
\]

By substituting (S3)–(S5) into (S2), we then have
\[
\sup_{(u,B)} |I_1 - \frac{1}{n} \sum_{i=1}^{n} (1 - A_i) \varepsilon_{1,i} \omega_{h,i}(u; B)| = o_p \left\{ h^q + \left( \frac{\log n}{nh^d} \right)^{1/2} \right\}. \tag{S6}
\]

Following the same arguments above, we can also show that
\[
\sup_{(u,B)} |I_2 - \frac{1}{n} \sum_{i=1}^{n} A_i \varepsilon_{0,i} \omega_{h,i}(u; B)| = o_p \left\{ h^q + \left( \frac{\log n}{nh^d} \right)^{1/2} \right\}. \tag{S7}
\]

Substituting (S6)–(S7) into (S1) completes the proof.

Now we derive the independent and identically distributed representations of \( \tilde{\tau}(B^T x; B) - \)
\( \tau^{[0]}(x; B) \) and \( \partial_{\text{vecl}(B)} \hat{\tau}(B^T x; B) - \tau^{[1]}(x; B) \).

**Lemma S2.** Suppose that Assumption 1 and Conditions A1–A6 are satisfied. Then,

\[
\begin{align*}
\sup_{(x, B)} |\hat{\tau}(B^T x; B) - \tau^{[0]}(x; B) - \frac{1}{n} \sum_{i=1}^{n} \eta^{[0]}_{h, i}(x; B)| &= o_p \left( h^{2q} + \frac{\log n}{nh^{d+1}} \right), \tag{S8}
\end{align*}
\]

\[
\begin{align*}
\sup_{(x, B)} \|\partial_{\text{vecl}(B)} \hat{\tau}(B^T x; B) - \tau^{[1]}(x; B) - \frac{1}{n} \sum_{i=1}^{n} \eta^{[1]}_{h, i}(x; B)\| &= o_p \left( h^{2q} + \frac{\log n}{nh^{d+1}} \right), \tag{S9}
\end{align*}
\]

where

\[
\begin{align*}
\eta^{[0]}_{h, i}(x; B) &= \frac{\xi_i(x; B)}{f_{B^T X}(B^T x)} K_{q, h}(B^T X_i - B^T x), \\
\eta^{[1]}_{h, i}(x; B) &= \frac{\xi_i(x; B)}{f_{B^T X}(B^T x)} \partial_{\text{vecl}(B)} K_{q, h}(B^T X_i - B^T x) \\
&- \tau^{[1]}(x; B) K_{q, h}(B^T X_i - B^T x) - \frac{f^{[1]}(x, B^T x; B)}{f_{B^T X}(B^T x)} \eta^{[0]}_{h, i}(x; B),
\end{align*}
\]

and \( \xi_i(x; B) = Z_i - E(Z \mid B^T X = B^T x) \).

**Proof.** First, (S8) is a direct result of Lemma S1. As for (S9), note that

\[
\begin{align*}
\frac{1}{n} \sum_{i=1}^{n} \hat{D}_i \partial_{\text{vecl}(B)} K_{q, h}(B^T X_i - B^T x) - G^{[1]}(x, B^T x; B) \\
= \frac{1}{n} \sum_{i=1}^{n} \xi_i(x; B) \partial_{\text{vecl}(B)} K_{q, h}(B^T X_i - B^T x) + r_{1n}(x; B), \tag{S10}
\end{align*}
\]

where \( \sup_{(x, B)} |r_{1n}(x, B)| = o_p [h^q + \{\log n/(nh^{d+1})\}^{1/2}] \), by paralleling the proof steps of Lemma S1. Now by using the Taylor expansion, we have

\[
\begin{align*}
&\partial_{\text{vecl}(B)} \hat{\tau}(B^T x; B) - \tau^{[1]}(x; B) \\
= \sum_{i=1}^{n} \hat{D}_i \partial_{\text{vecl}(B)} K_{q, h}(B^T X_i - B^T x)/n - \tau^{[0]}(x; B) \sum_{i=1}^{n} \partial_{\text{vecl}(B)} K_{q, h}(B^T X_i - B^T x)/n \\
&- \frac{\tau^{[1]}(x; B)}{n} \sum_{i=1}^{n} K_{q, h}(B^T X_i - B^T x) - \frac{f^{[1]}(x, B^T x; B)}{f_{B^T X}(B^T x)} \{\hat{\tau}(B^T x; B) - \tau^{[0]}(x; B)\} \\
&+ r_{2n}(x; B), \tag{S11}
\end{align*}
\]
where
\[
 r_{2n}(x, B) = \text{O}_P\left(\hat{\tau}(B^T x; B) - \tau^{(0)}(x; B) \right)^2 \\
+ \left\| \sum_{i=1}^n \hat{D}_i \partial_{\text{vec}(B)} \mathbb{K}_{q,h}(B^T X_i - B^T x)/n - G^{[1]}(x, B^T x; B) \right\|^2.
\]

Finally, substituting the result in Lemma $\text{S1}$ and $(\text{S10})$ into $(\text{S11})$ completes the proof. \hfill \Box

**Corollary 1.** Suppose that Assumption 1 and Conditions A1–A6 are satisfied. Then,
\[
\sup_{(x,B)} \left| \hat{\tau}(B^T x; B) - \tau^{(0)}(x; B) \right| = \text{O}_P \left\{ h^q + \left( \frac{\log n}{nh^d} \right)^{1/2} \right\},
\]
\[
\sup_{(x,B)} \left\| \partial_{\text{vec}(B)} \hat{\tau}(B^T x; B) - \tau^{[1]}(x; B) \right\| = \text{O}_P \left\{ h^q + \left( \frac{\log n}{nh^{d+1}} \right)^{1/2} \right\}.
\]

**S3 Proofs of Theorems 2 and 3**

**S3.1 Proof of Theorem 2**

*Proof.* Let $\hat{\tau}^{-i}(B^T X_i; B) = \sum_{j \neq i} Z_j \mathbb{K}_{q,h}(B^T X_j - B^T X_i)/\sum_{j \neq i} \mathbb{K}_{q,h}(B^T X_j - B^T X_i)$. We can decompose $\text{CV}(d, B, h)$ into
\[
\text{CV}(d, B, h) = \frac{1}{n} \sum_{i=1}^n \left\{ Z_i - \hat{\tau}^{-i}(B^T X_i; B) \right\}^2 + \frac{1}{n} \sum_{i=1}^n \left( \hat{D}_i - Z_i \right)^2 \\
+ \frac{1}{n} \sum_{i=1}^n \left\{ \hat{\tau}^{-i}(B^T X_i; B) - \hat{\tau}^{-i}(B^T X_i; B) \right\}^2 \\
+ \frac{2}{n} \sum_{i=1}^n \left( \hat{D}_i - Z_i \right) \{ \hat{\tau}^{-i}(B^T X_i; B) - \hat{\tau}^{-i}(B^T X_i; B) \} \\
+ \frac{2}{n} \sum_{i=1}^n \left( \hat{D}_i - Z_i \right) \{ Z_i - \tau(X_i) \} + \frac{2}{n} \sum_{i=1}^n \left( \hat{D}_i - Z_i \right) \{ \tau(X_i) - \hat{\tau}^{-i}(B^T X_i; B) \} \\
+ \frac{2}{n} \sum_{i=1}^n \left\{ Z_i - \tau(X_i) \right\} \{ \hat{\tau}^{-i}(B^T X_i; B) - \hat{\tau}^{-i}(B^T X_i; B) \} \\
+ \frac{2}{n} \sum_{i=1}^n \left\{ \tau(X_i) - \hat{\tau}^{-i}(B^T X_i; B) \right\} \{ \hat{\tau}^{-i}(B^T X_i; B) - \hat{\tau}^{-i}(B^T X_i; B) \} \\
\triangleq SS_1 + SS_2 + SS_3 + SC_1 + SC_2 + SC_3 + SC_4 + SC_5.
\]
By using first-ordered Taylor expansion, we have

\[ \text{Proof.} \]

Note that

\[ \sup_i |\hat{D}_i - Z_i| \leq \sum_{a=0}^{1} \sup_{u(B)} |\hat{\mu}_a(u; B) - \mu_a(u; B)| = o_p \left\{ h^q + \left( \frac{\log n}{nh^d} \right)^{1/2} \right\}, \quad (S12) \]

\[ \sup_{(i,B)} |\tilde{\tau}^{-i}(B^T X_i; B) - \tilde{\tau}^{-i}(B^T X_i; B)| \leq C \sum_{a=0}^{1} \sup_{u(B)} |\hat{\mu}_a(u; B) - \mu_a(u; B)| = o_p \left\{ h^q + \left( \frac{\log n}{nh^d} \right)^{1/2} \right\} \quad (S13) \]

for some positive constant \( C \), by using Conditions A1–A3, Condition A6, and standard arguments in kernel smoothing estimation.

When \( \text{span}(B) \supseteq \text{span}(B_\tau) \), Theorem 1 of Huang and Chiang (2017) implies that \( SS_1 = \sigma^2 + O_p \{ h^2q + \log n/(nh^d) \} \), where \( \sigma^2 = \mathbb{E} \{ \tau(X)^2 \} \). From \( (S12)-(S13) \), \( \sup_B |SS_3| \) and \( \sup_B |SC_1| \) are of order \( o_p \{ h^2q + \log n/(nh^d) \} \). Further, by using \( \sup_{(x,B)} |\tilde{\tau}(B^T x; B) - \tau(x)| = O_p \{ h^q + \{ \log n/(nh^d) \}^{1/2} \} \), \( \sup_B |SC_3| \) and \( \sup_B |SC_5| \) are also of order \( o_p \{ h^2q + \log n/(nh^d) \} \). Now note that \( SC_4 \) can be expressed a U-process indexed by \( B \) asymptotically. By using the same proof steps for the cross term in Theorem 1 of Huang and Chiang (2017), one can immediately conclude that \( \sup_B |SC_4| = o_p \{ h^2q + \log n/(nh^d) \} \). Combining the results above, we have \( \text{cv}(d,B,h) = SS_1 + SS_2 + SC_2 + o_p(SS_1) \) uniformly in \( B \). When \( \text{span}(B) \not\supseteq \text{span}(B_\tau) \), Theorem 1 of Huang and Chiang (2017) implies that \( SS_1 = \sigma^2 + b_\tau^2(B) + o_p(1) \). By using \( (S12)-(S13) \) again, we have \( \text{cv}(d,B,h) = SS_1 + SS_2 + SC_2 + o_p(1) \) uniformly in \( B \). Finally, since \( SS_2 \) and \( SC_2 \) are independent of \( B \), the minimizer of \( \text{cv}(d,B,h) \) has the same asymptotic distribution as the minimizer of \( SS_1 \). Thus, Theorem 2 is a direct result of Theorem 2 in Huang and Chiang (2017).

S3.2 Proof of Theorem 3

Proof. By using first-ordered Taylor expansion, we have

\[ \tilde{\tau}(\hat{B}^T x; \hat{B}) - \tau(x) = \tilde{\tau}(\hat{B}^T x; \hat{B}) - \tilde{\tau}(B_\tau^T x; B_\tau) + \tilde{\tau}(B_\tau^T x; B_\tau) - \tau(x) \]

\[ = \partial_{\text{vecl}(B)} \tilde{\tau}(\hat{B}^T x; \hat{B}) \text{vecl}(\hat{B} - B_\tau) + \tilde{\tau}(B_\tau^T x; B_\tau) - \tau(x), \]

S8
where $\bar{B}$ lies on the line segment between $\hat{B}$ and $B_\tau$. From Theorem 2, vec$\ell(\hat{B} - B_\tau) = O_P(n^{-1/2})$. Coupled with Corollary [1] and continuous mapping theorem, $\partial_{\text{vec}(B)} \hat{\tau}(\bar{B}^T x; \bar{B}) = O_P(1)$. Moreover, from [SS], we have

$$(nh_\tau^{d_\tau})^{1/2} \{ \hat{\tau}(B_\tau^T x; B_\tau) - \tau(x) \} - h_\tau^{d_\tau} \gamma(x) \to N\{0, \sigma_\tau^2(x)\}$$

in distribution as $n \to \infty$. Combining the results above completes the proof of Theorem 3. \qed