Identification and Estimation of Conditional Average Partial Causal Effects via Instrumental Variable

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Abstract

There has been considerable recent interest in estimating heterogeneous causal effects. In this paper, we study conditional average partial causal effects (CAPCE) to reveal the heterogeneity of causal effects with continuous treatment. We provide conditions for identifying CAPCE in an instrumental variable setting. Notably, CAPCE is identifiable under a weaker assumption than required by a commonly used measure for estimating heterogeneous causal effects of continuous treatment. We develop three families of CAPCE estimators: sieve, parametric, and reproducing kernel Hilbert space (RKHS)-based, and analyze their statistical properties. We illustrate the proposed CAPCE estimators on synthetic and real-world data.

1 INTRODUCTION

Instrumental variable (IV) analysis is a powerful tool used to elucidate causal relationships between treatment (X) and outcome (Y) when a controlled experiment is not feasible [\[Imbens, 2014,](#page-10-0) [Angrist and Krueger, 2001\]](#page-9-0). Traditionally, there are a large number of works focusing on binary or categorical treatment variables [\[Imbens and Angrist, 1994,](#page-10-1) [Balke and Pearl, 1997\]](#page-9-1); recently, there has been a growing interest in continuous treatment variables [\[Hirano and Imbens,](#page-10-2) [2005,](#page-10-2) [Kennedy et al., 2017,](#page-10-3) [Bahadori et al., 2022\]](#page-9-2). There is also considerable recent interest in estimating heterogeneous causal effects across subsets of the population [\[Athey](#page-9-3) [and Imbens, 2016,](#page-9-3) [Ding et al., 2016,](#page-9-4) [Athey and Imbens,](#page-9-5) [2019,](#page-9-5) [Künzel et al., 2019,](#page-10-4) [Wager and Athey, 2018,](#page-11-0) [Zhang](#page-11-1) [et al., 2022,](#page-11-1) [Singh et al., 2023\]](#page-10-5), including IV-based methods [\[Angrist, 2004,](#page-8-0) [Syrgkanis et al., 2019,](#page-10-6) [Huntington-Klein,](#page-10-7) [2020,](#page-10-7) [Bargagli-Stoffi et al., 2022\]](#page-9-6). Most of the works focus on *conditional average causal effect (CACE)* $\mathbb{E}[Y_1 - Y_0 | \boldsymbol{w}]$, also known as conditional average treatment effect (CATE),

for evaluating heterogeneous causal effects of a binary X , where Y_x denotes the potential outcome under treatment $X = x$, and W are covariates (e.g. gender, age, and race).

In this work, we study estimating heterogeneous causal effects of a *continuous* treatment via the IV method. Existing work in this direction has focused on estimating $\mathbb{E}[Y_x|\boldsymbol{w}]$. The most widely used methods include parametric two-stage least squared (PTSLS) [\[Wright, 1928,](#page-11-2) [Angrist and Pischke,](#page-9-7) [2009,](#page-9-7) [Wooldridge, 2010\]](#page-11-3), sieve nonparametric two-stage least squared (sieve NTSLS) [\[Newey and Powell, 2003,](#page-10-8) [Chen and Christensen, 2018\]](#page-9-8), and Kernel IV [\[Singh et al.,](#page-10-9) [2019\]](#page-10-9). The line of works in [\[Syrgkanis et al., 2019,](#page-10-6) [Dikkala](#page-9-9) [et al., 2020,](#page-9-9) [Muandet et al., 2020,](#page-10-10) [Bennett et al., 2023\]](#page-9-10) focus on the efficiency of estimators assuming simple additive errors. All these methods rely on a *separability* assumption for identifying $\mathbb{E}[Y_x|\boldsymbol{w}]$ [\[Newey and Powell, 2003\]](#page-10-8).

Another quantity for evaluating the causal effects of a continuous treatment is average partial causal effect (APCE) $\mathbb{E}[\partial_x Y_x]$ [\[Chamberlain, 1984,](#page-9-11) [Wooldridge, 2005,](#page-11-4) [Graham](#page-9-12) [and Powell, 2012\]](#page-9-12). [Wong](#page-11-5) [\[2022\]](#page-11-5) provided a condition for identifying $\mathbb{E}[\partial_x Y_x]$ and [Kawakami et al.](#page-10-11) [\[2023\]](#page-10-11) presented APCE estimators.

In this paper, we consider $\mathbb{E}[\partial_x Y_x|\boldsymbol{w}]$, termed *conditional average partial causal effect (CAPCE)*, to capture the heterogeneous causal effects of a continuous treatment. CAPCE extends APCE and is a natural generalization of the CACE of a binary treatment. The quantity represented by CAPCE has been implicitly studied in the literature (e.g. [\[Galagate,](#page-9-13) [2016\]](#page-9-13)). Still existing works have focused on $\mathbb{E}[Y_x|\boldsymbol{w}]$. One contribution of this work is to show that under the IV model, CAPCE is identifiable under a *weaker* separability assumption than required by the previous work (sieve NTSLS, PT-SLS, Kernel IV) for identifying $\mathbb{E}[Y_x|\boldsymbol{w}]$. Thus, computing CAPCE allows scientists to estimate causal effects in a larger class of models. Granted, given an estimated $\mathbb{E}[Y_x|\boldsymbol{w}]$, one can compute its derivative to obtain CAPCE, but not the other way around. However, in practice, the causal effect from a reference point (e.g., CACE) is often the main inter-

Figure 1: A causal graph representing the IV model.

est, and CAPCE is enough to compute causal effects from a ′′

reference point:
$$
\mathbb{E}[Y_{x''} - Y_{x'}|\boldsymbol{w}] = \int_{x'}^{x''} \mathbb{E}[\partial_x Y_x|\boldsymbol{w}] dx.
$$

We then develop three families of methods for estimating CAPCE: sieve, parametric, and reproducing kernel Hilbert space (RKHS)-based, and analyze their statistical properties. Finally, we illustrate the proposed estimators on synthetic data, showing superior performance to existing methods. We also evaluate CAPCE in a real-world dataset.

2 NOTATION AND BACKGROUND

We represent each variable with a capital letter (X) and its realized value with a small letter (x) . Let Ω_X be the domain of X, $\mathbb{E}[Y]$ be the expectation of Y, $\mathbb{P}(X \leq x)$ be the cumulative distribution function (CDF) of X , and $p(X = x)$ be the probability density function (PDF) of X. A metric space $\langle \Omega, d \rangle$, where distance function $d(x, y)$ is defined by a given norm $||x - y||$ for $x, y \in \Omega$, is compact if every sequence in Ω has a convergent sub-sequence whose limit is in Ω. If every Cauchy sequence of points in Ω has a limit in Ω , Ω is called complete.

Sobolev norm [\[Gallant and Nychka, 1987,](#page-9-14) [Leoni,](#page-10-12) [2009\]](#page-10-12). Let λ be a $d + 1$ dimensional vector of non-negative integer, $|\lambda| = \sum_{k=1}^{d+1}$ $D^{\boldsymbol{\lambda}} f(x, \boldsymbol{w}) = \partial^{|\boldsymbol{\lambda}|} f(x, \boldsymbol{w}) / \partial x^{\lambda_1} \partial w_1^{\lambda_2} \cdots \partial w_d^{\lambda_{d+1}}.$ λ_l , and Sobolev norm is defined as follows: $||f||_{W^{l,p}} =$ $\sqrt{ }$ \int \mathcal{L} \sum $|\boldsymbol{\lambda}| \leq l$ $\int {\{D^{\lambda} f(x, \boldsymbol{w})\}^p}dxd\boldsymbol{w}$ \mathcal{L} \mathcal{L} J $1/p$ for $1 \leq p < \infty$,

and $||f||_{W^{l,\infty}} = \max_{|\lambda| \leq l} \sup_{(x,w)} D^{\lambda} f(x, w)$. Note that $W^{0,p}$ norm coincides with L_p norm for $1 \le p \le \infty$.

Structural Causal Models (SCM). We use SCM as our framework [\[Pearl, 2009\]](#page-10-13). An SCM M is a tuple $\langle V, U, \mathcal{F}, \mathbb{P}_U \rangle$, where U is a set of exogenous (unobserved) variables following a joint distribution \mathbb{P}_{U} , and V is a set of endogenous (observable) variables whose values are determined by structural functions $\mathcal{F} = \{f_{V_i}\}_{V_i \in V}$ such that $v_i := f_{V_i}(\mathbf{pa}_{V_i}, \boldsymbol{u}_{V_i})$ where $\mathbf{PA}_{V_i} \subseteq \boldsymbol{V}$ and $U_{V_i} \subseteq \boldsymbol{U}$. Each SCM M induces an observational distribution \mathbb{P}_V

over V, and a causal graph $G(\mathcal{M})$ over V in which there exists a directed edge from every variable in \mathbf{PA}_{V_i} to V_i . An intervention $do(x)$ of setting endogenous variables X to constants x replaces the functions of X by the constants x and induces a *sub-model* \mathcal{M}_x . We denote the potential outcome Y under intervention $do(x)$ by $Y_x(u)$, which is the solution of Y in the sub-model \mathcal{M}_x given $U = u$.

Instrumental Variable (IV) Model with Covariates. We consider the IV model represented by the causal graph in Fig [1,](#page-1-0) with the following SCM \mathcal{M}_{IV} over $\mathbf{V} = \{Z, X, Y, \mathbf{W}\}\$ and $U = \{H, u_X, u_Y, u_Z, u_W\}$:

$$
Y := f_Y(X, \mathbf{W}, \mathbf{H}, \mathbf{u}_Y), \ X := f_X(Z, \mathbf{W}, \mathbf{H}, \mathbf{u}_X),
$$

$$
\mathbf{W} := f_\mathbf{W}(\mathbf{H}, \mathbf{u}_\mathbf{W}), \ Z := f_Z(\mathbf{u}_Z),
$$
 (1)

where $f_{\mathbf{W}}$ is a vector function. We assume all variables are continuous, W are d -dimensional pre-treatment covariates, and H stands for unmeasured confounders. This IV model has been studied in e.g., [\[Hartford et al., 2017,](#page-9-15) [Huntington-](#page-10-7)[Klein, 2020\]](#page-10-7). We further consider an IV model with an additional edge $W \rightarrow Z$ in Appendix [A.2.](#page-13-0)

Related work. Under the IV model, [Newey and Powell](#page-10-8) [\[2003\]](#page-10-8) introduced sieve NTSLS for identifying and estimating $\mathbb{E}[Y_x|\boldsymbol{w}]$ via an integral equation, $\mathbb{E}[Y|Z=z] =$ **Z** $\Omega_{\boldsymbol{W}}$ Ω_X $\mathfrak{p}(X = x, \boldsymbol{W} = \boldsymbol{w} | Z = z) \mathbb{E}[Y_x | \boldsymbol{w}] dxd\boldsymbol{w},$ under the following assumption called *separability*:

$$
f_Y(X, \boldsymbol{W}, \boldsymbol{H}, \boldsymbol{u}_Y) = f_Y^1(X, \boldsymbol{W}, \boldsymbol{u}_Y) + f_Y^2(\boldsymbol{H}, \boldsymbol{u}_Y),
$$

$$
\mathbb{E}[f_Y^2(\boldsymbol{H}, \boldsymbol{u}_Y)|\boldsymbol{W}] = 0,
$$
 (2)

which says the function $f_Y(X, \boldsymbol{W}, \boldsymbol{H}, \boldsymbol{u}_Y)$ is in the form of a summation of two functions, one over (X, \mathbf{W}) and one over H. Parametric PTSLS [\[Angrist and Pischke, 2009,](#page-9-7) [Wooldridge, 2010\]](#page-11-3) and Kernel IV [\[Singh et al., 2019\]](#page-10-9) methods for estimating $\mathbb{E}[Y_x|\boldsymbol{w}]$ have also been developed under the separability assumption.

Recently, [Wong](#page-11-5) [\[2022\]](#page-11-5) introduced an integral equation for identifying APCE $\mathbb{E}[\partial_x Y_x] := \mathbb{E}_{U}[\partial_x Y_x(U)]$ under the IV model with no covariates $W: \mathbb{E}[Y|Z = z] - \mathbb{E}[Y|Z = z]$ $[z_0] = \Omega_X$ $\{\mathbb{P}(X \leq x | Z = z) - \mathbb{P}(X \leq x | Z = z)\}$ z_0 } $\mathbb{E}[\partial_x Y_x]dx$. [Kawakami et al.](#page-10-11) [\[2023\]](#page-10-11) has developed parametric (P-APCE) and Picard iteration-based (N-APCE) estimators for APCE. In this paper, we extend their results and develop three families of methods for estimating CACPE $\mathbb{E}[\partial_x Y_x|\mathbf{w}]$. Our parametric estimator reduces to P-APCE when W is empty. The sieve and RKHS estimators in this paper were not provided in [\[Kawakami et al., 2023\]](#page-10-11). We note that Picard-iteration estimator in [\[Kawakami et al., 2023\]](#page-10-11) is not suitable here because equation [\(3\)](#page-2-0) uses a PDF in the integral kernel instead of a CDF in the equation for APCE.

3 IDENTIFICATION OF CAPCE

First, we formally define *conditional average partial causal effect (CAPCE)* to capture the heterogeneous causal effects of a continuous treatment. Then we present a theorem for identifying CAPCE under the IV model.

Definition 1 (CAPCE).
$$
\mathbb{E}[\partial_x Y_x | w]
$$
 := $\mathbb{E}_U \left[\frac{\partial}{\partial x} Y_x (U) \middle| W = w \right].$

CAPCE is a real-valued function from $x \in \Omega_X$ and $w \in$ Ω_W to R. It is a generalization of CACE for continuous treatment. It is also a generalization of APCE $\mathbb{E}[\partial_x Y_x]$ to represent heterogeneous causal effects. Next, we present conditions for identifying CAPCE under the IV model.

Assumption 3.1. *Under the SCM* M_{IV} *, given* $W = w$ *,*

- *1. Instrument relevance: IV* Z *has a causal effect on* X*, i.e.*, $\mathbb{E}[X_z]$ *is not a constant function of z.*
- *2.* Y_r *is differentiable and bounded in* $x \in \Omega_X$.
- 3. $\sup_{x,z,\boldsymbol{w}} \mathfrak{p}(X_z = x | \boldsymbol{W} = \boldsymbol{w}) < \infty$.
- 4. The set of distributions $P(X|Z=z, \mathbf{W}=\mathbf{w})$ induced *by varying* z *is a complete set.*

The first assumption is standard for the IV setting. The second assumption means that there exists CAPCE for all subjects for $x \in \Omega_X$ and $w \in \Omega_W$. The third assumption means the density function of $X_{z,w}$ is bounded. The fourth assumption implies that h is a zero function if $\mathbb{E}[h(X)|Z] =$ $z, W = w$ does not depend on z for all $w \in \Omega_W$, which is also assumed in [\[Newey and Powell, 2003\]](#page-10-8) for identifying $\mathbb{E}[Y_x|\boldsymbol{w}].$

Assumption 3.2 (Separability on X). $f_Y(X, \mathbf{W}, \mathbf{H}, \mathbf{u}_Y)$ *is in the form of a summation of two functions over* X *and* \boldsymbol{H} separately, i.e., $f_Y(X, \boldsymbol{W}, \boldsymbol{H}, \boldsymbol{u}_Y) = f^1_Y(X, \boldsymbol{W}, \boldsymbol{u}_Y) +$ $f_Y^2(\boldsymbol{W}, \boldsymbol{H}, \boldsymbol{u}_Y).$

We obtain the following result.

Theorem 3.1 (Identification of CAPCE). *Under SCM* M_{IV} *and Assumptions* [3.1](#page-2-1) *and* [3.2,](#page-2-2) *CAPCE* $\mathbb{E}[\partial_x Y_x | \mathbf{w}]$ *is identifiable from distributions* $\mathbb{P}(X, W|Z)$ *and* $\mathbb{P}(Y|Z)$ *via the integral equation:*

$$
\mu(z) = \int_{\Omega_{\boldsymbol{W}}} \int_{\Omega_{\boldsymbol{X}}} k(z, x, \boldsymbol{w}) \mathbb{E}[\partial_x Y_x | \boldsymbol{w}] dx d\boldsymbol{w}, \qquad (3)
$$

where $\mu(z) = \mathbb{E}[Y|Z = z_0] - \mathbb{E}[Y|Z = z], k(z, x, w) =$ $\mathfrak{p}(X \leq x, \mathbf{W} = \mathbf{w}|Z = z) - \mathfrak{p}(X \leq x, \mathbf{W} = \mathbf{w}|Z = z_0)$, *and* z_0 *is a arbitrary fixed value.*

Remark: Assumption [3.2](#page-2-2) is weaker than the assumption [\(2\)](#page-1-1) needed by existing work sieve NTSLS [\[Newey and Powell,](#page-10-8)

[2003\]](#page-10-8), PTSLS [\[Wooldridge, 2010\]](#page-11-3), and Kernel IV [\[Singh](#page-10-9) [et al., 2019\]](#page-10-9) for identifying $\mathbb{E}[Y_x|\boldsymbol{w}]$, which require both covariates W and the treatment X to be separable from the unmeasured confounders H . Assumption [3.2](#page-2-2) is particularly less restrictive when there are many covariates. Theorem [3.1](#page-2-3) states that *CAPCE* $\mathbb{E}[\partial_x Y_x | \boldsymbol{w}]$ *is identifiable under a weaker assumption than required by* $\mathbb{E}[Y_x|\boldsymbol{w}]$. The result enables us to compute causal effects in IV models where Assumption [3.2](#page-2-2) holds but assumption [\(2\)](#page-1-1) does not such that existing methods are not applicable. Theorem [3.1](#page-2-3) extends the results in [\[Wong, 2022,](#page-11-5) [Kawakami et al., 2023\]](#page-10-11) for identifying APCE $\mathbb{E}[\partial_x Y_x]$; however, it is worth noting that this important point about weaker separability assumption does not arise in the work of [Wong](#page-11-5) [\[2022\]](#page-11-5) and [Kawakami et al.](#page-10-11) [\[2023\]](#page-10-11) because they study the setting with no covariates W .

4 ESTIMATION OF CAPCE

In this section, we develop three families of methods for estimating CAPCE from data based on Theorem [3.1.](#page-2-3) We do not need samples from the joint $p(Z, X, Y, W)$, but rather two datasets $\mathcal{D}^{(1)} = \{x_i^{(1)}, w_i^{(1)}, z_i^{(1)}\}_{i=1}^{N_1}$ and $\mathcal{D}^{(2)} = \{y_i^{(2)}, z_i^{(2)}\}_{i=1}^{N_2}$ known as two-samples IV methods [\[Singh et al., 2019,](#page-10-9) [Angrist and Krueger, 1992\]](#page-9-16).

4.1 SIEVE CAPCE ESTIMATOR

Sieve estimators are a class of non-parametric estimators that use progressively more complex models to estimate an unknown function as more data becomes available [\[Geman](#page-9-17) [and Hwang, 1982\]](#page-9-17).

Approximation by Orthonormal Basis Functions. We approximate the CAPCE $\mathbb{E}[\partial_x Y_x | \boldsymbol{w}]$ by a set of orthonormal basis functions, such as Hermite polynomial functions [\[Hermite, 2009\]](#page-10-14). Specifically,

$$
\mathbb{E}[\partial_x Y_x | \boldsymbol{w}] \equiv g_0(x, \boldsymbol{w}) \approx g(x, \boldsymbol{w}) = \sum_{j=1}^J \beta_j \phi_j(x, \boldsymbol{w}),
$$
\n(4)

where $\{\phi_j(x, \mathbf{w})\}_{j=1}^{\infty}$ is a set of infinite basis functions that satisfy the following conditions where Sobolev norm $W^{l,2}$ norm $(0 < l < \infty)$ is used:

Assumption 4.1. *The basis functions* $\{\phi_j(x, \mathbf{w})\}_{j=1}^{\infty}$ *are orthonormal basis functions, and satisfy* $\|\phi_j(x, \mathbf{w})\|_{W^{l,2}} <$ ∞ *for all* $j = 1, 2, \ldots$

Assumption 4.2. $\sum_{i=1}^{J}$ $j=1$ $\beta_j \phi_j(x, \mathbf{w})$ convergences uniformly *to* $q_0(x, \mathbf{w})$ *if* $J \to \infty$ *.*

We note that Hermite polynomial functions satisfy As-sumption [4.2](#page-2-4) for any bounded and continuous function g_0 [\[Damelin et al., 2001\]](#page-9-18).

Compactness Restriction. The integral equation [\(3\)](#page-2-0), known as a "Fredholm Integral Equation of the First Kind" [\[Bôcher, 1926\]](#page-9-19), is ill-posed since the integral operator K, where $\mathcal{K}(f)(z) = \int$ $\Omega_{\boldsymbol{W}}$ Z Ω_X $k(z,x,\boldsymbol{w})f(x,\boldsymbol{w})dxd\boldsymbol{w},$ is not guaranteed to be compact. Problems where one or more of the three properties - existence, uniqueness, and stability of the solution - do not hold are called ill-posed problems [\[Tikhonov et al., 1995\]](#page-10-15) and lead to severe estimation difficulties. To relieve the issue, we put restrictions on the functional space of $g_0(x, \mathbf{w})$. Let $g(X, \mathbf{W}) = \mathbf{X}$ $\Omega_{\boldsymbol{W}}$ Z Ω_X $\{\mathbb{1}_{X\leq x,\mathbf{W}=\mathbf{w}}-\mathbb{E}[\mathbb{1}_{X\leq x,\mathbf{W}=\mathbf{w}}|Z=$ z_0]} $g(X, \boldsymbol{W})dxd\boldsymbol{w}$, and define regularized Sobolev norm $\tilde{W}^{l,2}$, which is called "consistency norm" in [\[Gallant and](#page-9-14) [Nychka, 1987\]](#page-9-14), as follows

$$
\|\mathfrak{g}(x,\mathbf{w})\|_{\tilde{W}^{l,2}}^2 = \sum_{|\lambda| \leq l} \int {\{D^{\lambda}\mathfrak{g}(x,\mathbf{w})\}}^2
$$

$$
\times {1 + (x,\mathbf{w}^T)(x,\mathbf{w}^T)^T}^k dx d\mathbf{w},
$$
 (5)

where $l \geq 1$ is an integer and κ is a constant satisfying $\kappa > (1+d)/2$ where d is the dimension of W. We make the following assumption:

Assumption 4.3. *Given a positive regularization parameter* B_S , $g_0(x, \mathbf{w})$ *is in the functional space* $\mathcal{G}_{B_S} = \{g : S\}$ $\|\mathfrak{g}(x,\mathbf{w})\|_{\tilde{W}^{l,2}}^2 \leq B_S\}.$

Using the approximation in [\(4\)](#page-2-5), equation [\(3\)](#page-2-0) reduces to

$$
\mu(z) = \sum_{j=1}^{J} \beta_j \int_{\Omega_{\mathbf{W}}} \int_{\Omega_{X}} k(z, x, \mathbf{w}) \phi_j(x, \mathbf{w}) dxd\mathbf{w}.
$$
 (6)

Letting the anti-derivative of the basis functions be $\varphi_j(x, \mathbf{w}) = \int \phi_j(x, \mathbf{w}) dx$ ^{[1](#page-3-0)} Then, the equation becomes $\mathbb{E}[Y|Z=z] - \mathbb{E}[Y|Z=z_0] =$

$$
\sum_{j=1}^{J} \beta_j \{ \mathbb{E}[\varphi_j(X, \mathbf{W}) | Z = z] - \mathbb{E}[\varphi_j(X, \mathbf{W}) | Z = z_0] \}
$$
\n(7)

Let $c = \mathbb{E}[Y|Z = z] - \mathbb{E}[Y|z = z_0], \beta = (\beta_1, ..., \beta_J)^T$, and $\mathbf{d} = (d^1, \dots, d^J)^T$ where $d^j = \mathbb{E}[\varphi_j(X, \mathbf{W}) | Z]$ $|z| - \mathbb{E}[\varphi_i(X, \boldsymbol{W})|Z = z_0]$. Then, the integral equation [\(3\)](#page-2-0) finally reduces to a linear equation $c = \beta^T d$.

Sieve CAPCE (S-CAPCE) estimator. Given datasets $\mathcal{D}^{(1)} = \{x_i^{(1)}, w_i^{(1)}, z_i^{(1)}\}_{i=1}^{N_1}$ and $\mathcal{D}^{(2)} = \{y_i^{(2)}, z_i^{(2)}\}_{i=1}^{N_2}$, our S-CAPCE estimator consists of two stages. In Stage 1, we learn models $\mathbb{E}[Y|Z=z]$ and $\mathbb{E}[\varphi_i(X, \mathbf{W})|Z=z]$ from the datasets by regression. Then in Stage 2, we estimate parameters β by solving Eq. [\(7\)](#page-3-1).

 \int_0^x ¹We will simply write the antiderivative $\varphi_i(x, \mathbf{w})$ = $\int_{-\infty}^{\infty} \phi_j(x', \mathbf{w}) dx'$ as $\varphi_j(x, \mathbf{w}) = \int \phi_j(x, \mathbf{w}) dx$ in the paper.

Stage 1. We learn prediction models $\mathbb{E}[Y|Z = z]$ using $\mathcal{D}^{(2)}$ and $\mathbb{E}[\varphi_i(X, \boldsymbol{W})|Z = z]$ for $j = 1, \ldots, J$ using $\mathcal{D}^{(1)}$. Any regression method can be used. We select an IV value z_0 . Denote $\hat{c}_i = \mathbb{\hat{E}}[Y|Z = z_i] - \mathbb{\hat{E}}[Y|Z = z_0]$ and $\hat{d}_i^j = \mathbb{\hat{E}}[\varphi_j(X, \boldsymbol{W})|Z = z_i] - \mathbb{\hat{E}}[\varphi_j(X, \boldsymbol{W})|Z = z_0].$

Specifically, we perform the regression using the power series basis functions in this paper. Let basis functions be $q(z) = (q_1(z), q_2(z), \dots, q_P(z))^T$, and consider the model $\mathbb{\hat{E}}[Y|Z=z] = \sum_{p=1}^P \omega_p q_p(z)$, $\mathbb{\hat{E}}[\varphi_j(X, \boldsymbol{W})|Z=z]$ $[z] = \sum_{p=1}^{P} \nu_p^j q_p(z)$ for $j = 1, \ldots, J$. Denote $\omega =$ $(\omega_1, \dots, \omega_P)^T$ and $\nu^j = (\nu_1^j, \dots, \nu_P^j)^T$. Then, we optimize the error functions below:

$$
Q_1(\boldsymbol{\nu}^j; \mathcal{D}^{(1)})
$$

= $\frac{1}{N_1} \sum_{i=1}^{N_1} (\varphi_j(x_i^{(1)}, \boldsymbol{w}_i^{(1)}) - \boldsymbol{q}(z_i^{(1)})^T \boldsymbol{\nu}^j)^2$, (8)

$$
Q_2(\boldsymbol{\omega}; \mathcal{D}^{(2)}) = \frac{1}{N_2} \sum_{i=1}^{N_2} (y_i^{(2)} - \boldsymbol{q}(z_i^{(2)})^T \boldsymbol{\omega})^2.
$$
 (9)

Let variance-covariance matrices be $\sum_{i=1}^{N_1} N_1^{-1} q(z_i^{(1)}) q(z_i^{(1)})^T$ and $\hat{\mathbf{M}}^{(2)}$ = be $\hat{\mathbf{M}}^{(1)}$ = $\sum_{i=1}^{N_2} N_2^{-1} q(z_i^{(2)}) q(z_i^{(2)})^T$. We obtain

$$
\begin{cases}\n\hat{c}_i = (\mathbf{q}(z_i) - \mathbf{q}(z_0))^T \hat{\mathbf{M}}^{(2)-} \sum_{l=1}^{N_2} \frac{1}{N_2} \mathbf{q}(z_l^{(2)}) y_l^{(2)} \\
\hat{d}_i^j = (\mathbf{q}(z_i) - \mathbf{q}(z_0))^T \hat{\mathbf{M}}^{(1)-} \\
\times \sum_{l=1}^{N_1} \frac{1}{N_1} \mathbf{q}(z_l^{(1)}) \varphi_j(x_l^{(1)}, \mathbf{w}_l^{(1)})\n\end{cases} (10)
$$

for $j = 1, \ldots, J$, where M⁻ denotes the generalized inverse that satisfies $\hat{\mathbf{M}}\hat{\mathbf{M}} = \hat{\mathbf{M}}$, Let $\overline{N} = N_1 + N_2$ and $(z_1, \ldots, z_N) = (z_1^{(1)}, \ldots, z_{N_1}^{(1)})$ $z_{N_1}^{(1)}, z_1^{(2)}, \ldots, z_{N_2}^{(2)}$ $\binom{2}{N_2}$. We will compute predicted values in [\(10\)](#page-3-2) for all $i = 1, \ldots, N$.

Stage 2. Estimate parameters β based on the linear equation $c \ =\ \bm{\beta}^T\bm{d}. \ \text{Let} \ \hat{\bm{c}} \ =\ (\hat{c}_1, \ldots, \hat{c}_N)^T, \ \hat{\bm{d}}_i \ =\ (\hat{d}_i^1, \ldots, \hat{d}_i^J)^T,$ $\hat{\mathbf{D}} = (\hat{d}_1, \dots, \hat{d}_N)^T$, and the empirical risk be

$$
Q_3(\boldsymbol{\beta}; \mathcal{D}^{(1)}, \mathcal{D}^{(2)}) = \frac{1}{N} \sum_{i=1}^N (\hat{c}_i - \hat{d}_i^T \boldsymbol{\beta})^2.
$$
 (11)

Under Assumption [4.3,](#page-3-3) our estimator $\hat{\beta}$ is given by the optimization problem below:

$$
\min_{\boldsymbol{\beta}} Q_3(\boldsymbol{\beta}; \mathcal{D}^{(1)}, \mathcal{D}^{(2)}) \text{ subject to } \boldsymbol{\beta}^T \boldsymbol{\Lambda} \boldsymbol{\beta} \leq B_S, \quad (12)
$$

where

$$
\Lambda_{i,j} = \sum_{|\lambda| \le l} \int \{ D^{\lambda} \varphi_i(x, \mathbf{w}) - D^{\lambda} \mathbb{E}[\varphi_i(X, \mathbf{W}) | Z = z_0] \} \times \{ D^{\lambda} \varphi_j(x, \mathbf{w}) - D^{\lambda} \mathbb{E}[\varphi_j(X, \mathbf{W}) | Z = z_0] \} \times \{ 1 + \| (x, \mathbf{w}^T) \|^2 \}^{\kappa} dx d\mathbf{w}
$$
\n(13)

for $i, j = 1, \dots, J$, and $\mathbf{\Lambda} = {\Lambda_{i,j}}_{i,j=1}^J$. $\mathbf{\Lambda}$ can be calculated by Monte Carlo integration $\hat{\Lambda}$ [\[Kroese et al., 2011\]](#page-10-16). The optimization problem [\(12\)](#page-3-4) can be solved by a ridge regression method with the following solution [\[Hilt et al.\]](#page-10-17):

$$
\hat{\boldsymbol{\beta}} = (\hat{\mathbf{D}}^T \hat{\mathbf{D}} + \zeta_S \text{diag}[\mathbf{\Lambda}])^{-1} \hat{\mathbf{D}}^T \hat{\mathbf{c}},
$$
(14)

where ζ_S is a regularization parameter called Lagrange multipliers. Then, our proposed sieve CAPCE estimator is given

by
$$
\hat{\mathbb{E}}[\partial_x Y_x | \boldsymbol{w}] = \sum_{j=1}^J \hat{\beta}_j \phi_j(x, \boldsymbol{w}).
$$

Model Selection. The model selection in Stage 1 is a standard regression problem, and we presume the models in Stage 1 have been selected appropriately according to standard machine learning methods. We can use the empirical risk in equation [\(11\)](#page-3-5) as a performance metric of the trained model in Stage 2 with parameters β if given separate test datasets $\mathcal{D}^{(1)'} = \{x_i^{(1)'}, z_i^{(1)'}, \mathbf{w}_i^{(1)'}\}_{i=1}^{N'_1}$ and $\mathcal{D}^{(2)'} = \{y_i^{(2)'}, z_i^{(2)'}\}_{i=1}^{N_2'}$. Let $N' = N_1' + N_2'$. Assume \hat{c}_i' and \hat{d}_i' for $i = 1, ..., N'$ are computed using $\mathcal{D}^{(1)'}$ and $\mathcal{D}^{(2)'}$. Then, we can evaluate the trained model by the test

error $\hat{Q}_3(\hat{\boldsymbol{\beta}}~; \mathcal{D}^{(1)'}, \mathcal{D}^{(2)'}) = \frac{1}{N'}$ \sum N' $i=1$ $(\hat{c}_i' - \hat{d}_i^{'T} \hat{\beta})^2$. Given

separate datasets, this performance metric can be used for model selection from various candidate basis functions or the number J or P of basis terms.

Property of sieve CAPCE estimator. We show that sieve CAPCE estimator is consistent under assumptions similar to sieve NTSLS [\[Newey and Powell, 2003\]](#page-10-8). Assumptions B.1 - 4 are shown in Appendix [B.](#page-16-0)

Theorem 4.1 (Consistency). *Under SCM M_{IV} and Assumptions [3.1,](#page-2-1) [3.2,](#page-2-2) [4.1,](#page-2-6) [4.2,](#page-2-4) [4.3,](#page-3-3) [B.1,](#page-16-1) [B.2,](#page-16-2) [B.3,](#page-17-0) and [B.4,](#page-17-1) letting* $P \to \infty$ *and* $J \to \infty$ *, then* $\|\hat{g} - g_0\|_{W^{l,\infty}} \xrightarrow{p} 0$.

Theorem 4.2 (Rate of Convergence). *Under SCM* M_{IV} *and Assumptions [3.1,](#page-2-1) [3.2,](#page-2-2) [4.1,](#page-2-6) [4.2,](#page-2-4) [4.3,](#page-3-3) [C.1,](#page-18-0) [C.2,](#page-18-1) [C.3,](#page-18-2) [C.4,](#page-18-3) [C.5,](#page-18-4) C.6,* and *C.7, setting* $N = N_1 = N_2$ *, then* $\|\hat{g} - g_0\|_A =$ $o_p(N^{-1/4})$.

Assumpts. [C.](#page-17-2)1-7 and norm $\|\cdot\|_A$ are defined in Appendix C.

4.2 PARAMETRIC CAPCE ESTIMATOR

Next, we develop a parametric CAPCE (P-CAPCE) estimator. We consider the setting that the CAPCE $\mathbb{E}[\partial_x Y_x|\mathbf{w}]$ takes the form of the following parametric model:

$$
\mathbb{E}[\partial_x Y_x | \boldsymbol{w}] = \sum_{k=1}^K \gamma_k \theta_k(x, \boldsymbol{w}), \qquad (15)
$$

where $\{\theta_k(x, \mathbf{w})\}_{k=1}^K$ are a set of known functions, and $\boldsymbol{\gamma} = (\gamma_1, \dots, \gamma_K)^T$ are unknown model parameters to be estimated from data.

The derivation of the P-CAPCE estimator is very similar to that of the sieve CAPCE estimator, so we skip the details in the following. Denote the anti-derivatives $\vartheta_k(x, \mathbf{w}) = \int \theta_k(x, \mathbf{w}) dx$ for $k = 1, \ldots, K$. Let $c =$ $\mathbb{E}[Y|Z=z] - \mathbb{E}[Y|z=z_0]$, and $e = (e^1, \dots, e^K)^T$ where $e^{\vec{k}} = \mathbb{E}[\vartheta_k(X, \hat{\boldsymbol{W}})|Z = z] - \mathbb{E}[\vartheta_k(X, \boldsymbol{W})|Z = z_0].$ Then, equation [\(3\)](#page-2-0) reduces to a linear equation $c = \gamma^T e$.

P-CAPCE estimator. Given datasets $\mathcal{D}^{(1)}$ = ${x_1^{(1)}, w_i^{(1)}, z_i^{(1)}\}_{i=1}^{N_1}$ and $\mathcal{D}^{(2)} = {y_i^{(2)}, z_i^{(2)}\}_{i=1}^{N_2}$, our P-CAPCE estimator consists of two stages.

Stage 1. Let basis functions be $q(z)$ = $(q_1(z), q_2(z), \ldots, q_p(z))^T$. Denote $\hat{c}_i = \mathbb{E}[Y|Z =$ z_i] – $\mathbb{E}[Y|Z = z_0]$ and $\hat{e}_i^k = \mathbb{E}[\vartheta_k(X, \boldsymbol{W})|Z =$ z_i] – $\mathbb{E}[\vartheta_k(X, \boldsymbol{W})|Z = z_0]$. Let variance-covariance matrices $\hat{\mathbf{M}}^{(1)} = \sum_{i=1}^{N_1} N_1^{-1} \mathbf{q} (z_i^{(1)}) \mathbf{q} (z_i^{(1)})^T$ and $\hat{\mathbf{M}}^{(2)}$ = $\sum_{i=1}^{N_2} N_2^{-1} \mathbf{q}(z_i^{(2)}) \mathbf{q}(z_i^{(2)})^T$. We obtain the following predication values

$$
\begin{cases}\n\hat{c}_i = (\mathbf{q}(z_i) - \mathbf{q}(z_0))^T \hat{\mathbf{M}}^{(2)-} \sum_{l=1}^{N_2} \frac{1}{N_2} \mathbf{q}(z_l^{(2)}) y_l^{(2)} \\
\hat{e}_i^k = (\mathbf{q}(z_i) - \mathbf{q}(z_0))^T \hat{\mathbf{M}}^{(1)-} \\
\times \sum_{l=1}^{N_1} \frac{1}{N_1} \mathbf{q}(z_l^{(1)}) \vartheta_k(x_l^{(1)}, \mathbf{w}_l^{(1)})\n\end{cases}
$$
\n(16)

for $k = 1, ..., K$. Let $N = N_1 + N_2$ and $(z_1, ..., z_N) =$ $(z_1^{(1)}, \ldots, z_{N_1}^{(1)})$ $z_1^{(1)}, z_1^{(2)}, \ldots, z_{N_2}^{(2)}$ $\binom{2}{N_2}$. We will compute predicted values in [\(16\)](#page-4-0) for all $i = 1, \ldots, N$.

Stage 2. Estimate parameters γ based on the linear equation $c = \boldsymbol{\gamma}^T \boldsymbol{e}$. Let $\hat{\boldsymbol{c}} = (\hat{c}_1, \dots, \hat{c}_N)^T$, $\hat{\boldsymbol{e}}_i = (\hat{e}_i^1, \dots, \hat{e}_i^K)^T$, $\hat{\mathbf{E}} = (\hat{e}_1, \dots, \hat{e}_N)^T$, and the empirical risk be

$$
Q_4(\gamma;\mathcal{D}^{(1)},\mathcal{D}^{(2)}) = \sum_{i=1}^N \frac{1}{N} (\hat{c}_i - \hat{e}_i^T \gamma)^2.
$$
 (17)

We make the following assumption:

Assumption 4.4. *Given a positive regularization parameter* B_P , γ *satisfies* $\gamma^T \gamma \leq B_P$.

Under Assumption [4.4,](#page-4-1) our estimator $\hat{\gamma}$ is given by the optimization problem below:

$$
\min_{\gamma} Q_4(\gamma; \mathcal{D}^{(1)}, \mathcal{D}^{(2)})
$$
 subject to $\gamma^T \gamma \leq B_P.$ (18)

This problem can be solved by the ridge regression method with the following solution [\[Hilt et al.\]](#page-10-17):

$$
\hat{\boldsymbol{\gamma}} = (\hat{\mathbf{E}}^T \hat{\mathbf{E}} + \zeta_P \mathbf{I}_K)^{-1} \hat{\mathbf{E}}^T \hat{\mathbf{c}},\tag{19}
$$

where ζ_P is a regularization parameter, and \mathbf{I}_K is a $K \times K$ identity matrix. Then, our proposed P-CAPCE estimator is

given by
$$
\hat{\mathbb{E}}[\partial_x Y_x | \boldsymbol{w}] = \sum_{k=1}^K \hat{\gamma}_k \theta_k(x, \boldsymbol{w}).
$$

Model Selection. We presume the models in Stage 1 have been selected appropriately. We can use the empirical risk in equation [\(17\)](#page-4-2) as a performance metric of the

trained model in Stage 2 with parameters $\hat{\gamma}$ if given separate test datasets $\mathcal{D}^{(1)'} = \{x_i^{(1)'}, z_i^{(1)'}, \mathbf{w}_i^{(1)}\}^{N'_1}_{i=1}$ and $\mathcal{D}^{(2)'} = \{y_i^{(2)'}, z_i^{(2)'}\}_{i=1}^{N_2'}$. Let $N' = N_1' + N_2'$. Assume \hat{e}'_i and \hat{e}'_i for $i = 1, ..., N$ are computed using $\mathcal{D}^{(1)'}$ and $\mathcal{D}^{(2)'}$. Then, we can evaluate the trained model by the test

error $\hat{Q}_4(\hat{\gamma}; \mathcal{D}^{(1)'}, \mathcal{D}^{(2)'}) = \frac{1}{N'}$ \sum N' $i=1$ $(\hat{c}_i' - \hat{e}_i^{'T}\hat{\gamma})^2$. Given a

separate dataset, this performance metric can be used for model selection from various candidate basis functions or the number K or P of basis terms.

Property of P-CAPCE estimator. We show that P-CAPCE estimator is consistent.

Theorem 4.3 (Consistency). *Under SCM M_{IV} and Assumptions [3.1,](#page-2-1) [3.2,](#page-2-2) [4.4,](#page-4-1) [D.1,](#page-19-0) [D.2,](#page-19-1) [D.3,](#page-19-2) and [D.4,](#page-19-3) letting* $P \to \infty$ *, then* $\|\hat{\gamma} - \gamma\| \xrightarrow{p} 0$.

Theorem 4.4 (Rate of Convergence). *Under SCM* M_{IV} *and Assumptions [3.1,](#page-2-1) [3.2,](#page-2-2) [4.4,](#page-4-1) [E.1,](#page-20-0) [E.2,](#page-20-1) [E.3,](#page-20-2) [E.4,](#page-20-3) and [E.5,](#page-20-4) setting* $N = N_1 = N_2$ *, then* $\|\hat{\gamma} - \gamma\| = o_p(N^{-1/4})$ *.*

Assumptions D.1 - 4 are shown in Appendix [D.](#page-19-4) Assumptions E.1 - 5 are in Appendix [E.](#page-20-5)

4.3 RKHS CAPCE ESTIMATOR

Finally, we develop a reproducing kernel Hilbert space (RKHS) CAPCE estimator. RKHS models are popular and widely used in nonparametric regression [\[Theodoridis and](#page-10-18) [Koutroumbas, 2006,](#page-10-18) [Schölkopf et al., 2013\]](#page-10-19).

RKHS model. Let $k_{X,W}$: $\Omega_{X,W} \times \Omega_{X,W} \rightarrow \mathbb{R}$ and k_Z : $\Omega_Z \times \Omega_Z \to \mathbb{R}$ be measurable positive definitive kernels corresponding to RKHSs $\mathcal{H}_{X,\boldsymbol{W}}$ and \mathcal{H}_Z . A symmetric function $k : \Omega \times \Omega \to \mathbb{R}$ is called positive-definite kernel if $\sum_{n=1}^n$ $i=1$ $\sum_{n=1}^{\infty}$ $j=1$ $c_i c_j k(\boldsymbol{a}_i, \boldsymbol{a}_j) \geq 0$ for all $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n \in \Omega$ given any $n\in\mathbb{N}$ and $c_1,\ldots,c_n\in\mathbb{R}$ [\[Shawe-Taylor and](#page-10-20) [Cristianini, 2004\]](#page-10-20). Denote the feature map $\eta : \Omega_{X,W} \rightarrow$ $\mathcal{H}_{X,\boldsymbol{W}},\,(x,\boldsymbol{w})\,\mapsto\,k'_{X,\boldsymbol{W}}(x,\boldsymbol{w},\cdot,\cdot)$ and $\psi\,:\,\Omega_{Z}\,\to\,\mathcal{H}_{Z},$ $z \mapsto k_Z(z, \cdot)$. In addition, we denote the antiderivative feature function π : $\Omega_{X,\mathbf{W}} \to \mathcal{H}_{X,\mathbf{W}}$, $(x,\mathbf{w}) \mapsto$ $k_{X,\boldsymbol{W}}(x,\boldsymbol{w},\cdot,\cdot)$ with $\pi(x,\boldsymbol{w}) = -\int \eta(x,\boldsymbol{w})dx$ and the antiderivative kernel function $k_{X,\mathbf{W}}(x,\mathbf{w},x',\mathbf{w}')$ = $\int k'_{X,W}(x, \boldsymbol{w}, x', \boldsymbol{w}') dxdx'$. Assume that the CAPCE takes the form

$$
\mathbb{E}[\partial_x Y_x | \mathbf{w}] = H(\pi(x, \mathbf{w})) \tag{20}
$$

for some operator $H \in \mathcal{L}_2(\mathcal{H}_{X,\mathbf{W}}, \Omega_Y)$, where $\mathcal{L}_2(\Omega_1, \Omega_2)$ is the \mathcal{L}_2 measurable function space from Ω_1 to Ω_2 , and $H(\pi(x, \mathbf{w}))$ is a composition function $H \circ \pi : \Omega_{X, \mathbf{W}} \to$

 Ω_V . Our RKHS CAPCE estimator consists of two stages (a detailed derivation is provided in Appendix [A.2\)](#page-13-0).

Stage 1. We learn an operator $G_1 \in \mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_{X,W})$ that satisfies $\mathbb{E}[\pi(X, \mathbf{W})|Z = z] = G_1(\psi(z))$, and learn an operator $G_2 \in \mathcal{L}_2(\mathcal{H}_Z, \Omega_Y)$ that satisfies $\mathbb{E}[Y|Z=z] =$ $G_2(\psi(z)).$

Stage 2. We learn an operator $H \in \mathcal{L}_2(\mathcal{H}_{X,\mathbf{W}}, \Omega_Y)$ that satisfies $\mathbb{E}[Y|Z=z] - \mathbb{E}[Y|Z=z_0] = H(\mathbb{E}[\pi(X, \mathbf{W})|Z =$ $|z| - \hat{\mathbb{E}}[\pi(X, \boldsymbol{W})|Z = z_0] \rangle \Leftrightarrow \hat{G}_1(\psi(z) - \psi(z_0)) =$ $H(\hat{G}_2(\psi(z) - \psi(z_0)))$, where \hat{G}_1 and \hat{G}_2 are learned in Stage 1.

We learn \hat{G}_1 , \hat{G}_2 , and \hat{H} by the following optimization problems using datasets $\mathcal{D}^{(1)}$ and $\mathcal{D}^{(2)}$:

$$
\min_{G_1} \frac{1}{N_1} \sum_{i=1}^{N_1} \left\| \pi(x_i^{(1)}, \boldsymbol{w}_i^{(1)}) - G_1(\psi(z_i^{(1)})) \right\|_{\mathcal{H}_{X,\boldsymbol{W}}}^2
$$
\n
$$
+ \lambda_1 \| G_1 \|_{\mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_{X,\boldsymbol{W}})}^2,
$$
\n(21)

$$
\min_{G_2} \frac{1}{N_2} \sum_{i=1}^{N_2} \left\| y_i^{(2)} - G_2(\psi(z_i^{(2)})) \right\|^2 + \lambda_2 \left\| G_2 \right\|_{\mathcal{L}_2(\mathcal{H}_Z, \Omega_Y)}^2,
$$
\n(22)

$$
\begin{split} \min_{H} \frac{1}{N_2} \sum_{i=1}^{N_2} \left\| \hat{G}_2(\psi(z_i^{(2)}) - \psi(z_0)) - H(\hat{G}_1(\psi(z_i^{(2)}) - \psi(z_0))) \right\|^2 \\ + \xi \left\| H \right\|_{\mathcal{L}_2(\mathcal{H}_{X,\mathbf{W}},\Omega_Y)}^2 + \lambda_3 \left\| H \circ \hat{G}_1 \right\|_{\mathcal{L}_2(\mathcal{H}_Z,\Omega_Y)}^2, \end{split} \tag{23}
$$

where $(\lambda_1, \lambda_2, \lambda_3, \xi)$ are regularization parameters. From the representer theorem [\[Schölkopf et al., 2001\]](#page-10-21), the optimal G_1 exists in span $\{\psi(z_1^{(1)}), \dots, \psi(z_{N_1}^{(1)})\}$ $\binom{1}{N_1}$, and the optimal G_2 and H exist in span $\{\psi(z_1^{(2)}), \dots, \psi(z_{N_2}^{(2)})\}$ $\binom{(2)}{N_2}$.

We denote gram matrices $K_{Z^{(1)}Z^{(1)}}$ = ${k_Z(z_i^{(1)}, z_j^{(1)})\}_{i,j=1}^{N_1};$ $\mathbf{K}_{Z^{(1)}z_0}$ is $N_1 \times N_1$ matrix ${k_Z(z_i^{(1)}, z_0)}_{i,j=1}^{N_1}$; and ${\bf K}_{(X,W)^{(1)}(x,w)}$ is N_1 -dimension vector ${k_{X,W}(x_i^{(1)}, w_i^{(1)}, x, w)}_{i=1}^{N_1}$. Then, the RKHS CAPCE estimator is given by

$$
\hat{\mathbb{E}}[\partial_x Y_x | \boldsymbol{w}] = \hat{\boldsymbol{\alpha}}^T \mathbf{K}_{(X, \boldsymbol{W})^{(1)}(x, \boldsymbol{w})},
$$
(24)

where

$$
\hat{\alpha} = (\hat{\mathbf{O}}\hat{\mathbf{O}}^T + N_2 \xi \mathbf{K}_{(X,\mathbf{W})^{(1)}(X,\mathbf{W})^{(1)}} + N_2 \lambda_3 \mathbf{I}_{N_2})^{-1} \times \hat{\mathbf{O}} \{ \mathbf{y}^{(2)T} (\mathbf{K}_{Z^{(2)}Z^{(2)}} + N_2 \lambda_2 \mathbf{I}_{N_2})^{-1} \times (\mathbf{K}_{Z^{(2)}Z^{(2)}} - \mathbf{K}_{Z^{(2)}z_0}) \},
$$
\n(25)

$$
\hat{\mathbf{O}} = \mathbf{K}_{(X,W)^{(1)}(X,W)^{(1)}} (\mathbf{K}_{Z^{(1)}Z^{(1)}} + N_1 \lambda_1 \mathbf{I}_{N_1})^{-1} \times (\mathbf{K}_{Z^{(1)}Z^{(2)}} - \mathbf{K}_{Z^{(1)}z_0}),
$$
\n(26)

and \mathbf{I}_N is a $N \times N$ identity matrix.

Model Selection. We presume the models in Stage 1 have been selected appropriately, and introduce a model selection method in Stage 2 following [\[Singh et al., 2019\]](#page-10-9). Assume we have separate datasets $\mathcal{D}^{(1)'} = \{x_i^{(1)'}, \mathbf{w}_i^{(1)'}, z_i^{(1)'}\}_{i=1}^{N'_1}$ and $\mathcal{D}^{(2)} = \{y_i^{(2)'} , z_i^{(2)'}\}_{i=1}^{N_2'}$. We determine the optimal λ_1^* by minimizing

$$
L_1(\lambda_1) = \frac{1}{N'_1} \text{Trace}\Big[\mathbf{K}_{(X,W)^{(1)'}(X,W)^{(1)'}} - 2\mathbf{K}_{(X,W)^{(1)'}(X,W)^{(1)}}\mathbf{P}_1 + \mathbf{P}_1^T\mathbf{K}_{(X,W)^{(1)}(X,W)^{(1)}}\mathbf{P}_1\Big],
$$
\n(27)

where $P_1 = (\mathbf{K}_{Z^{(1)}Z^{(1)}} + N'_1 \lambda_1 \mathbf{I}_{N_1})^{-1} \mathbf{K}_{Z^{(1)}Z^{(2)}}$. We determine the optimal λ_2^* by minimizing

$$
L_2(\lambda_2) = \frac{1}{N'_2} \text{Trace} \Big[\mathbf{y}^{(2)'} \mathbf{y}^{(2)'T} - 2 \mathbf{y}^{(2)'} \mathbf{y}^{(2)T} \mathbf{P}_2 + \mathbf{P}_2^T \mathbf{y}^{(2)} \mathbf{y}^{(2)T} \mathbf{P}_2 \Big], \tag{28}
$$

where $P_2 = (K_{Z^{(1)}Z^{(1)}} + N_1\lambda_2 I_{N_1})^{-1}K_{Z^{(1)}Z^{(2)}}$. Finally, we determine the optimal ξ^* and λ_3^* minimizing test error $L(\lambda_3, \xi)$ 1 N_2' $\sum_{i=1}^{N_{\mathbf{Z}}'}\|\boldsymbol{y}^{(2)'T}(\mathbf{K}_{Z^{(2)'}Z^{(2)'}}+N_{2}'\lambda_{2}^{*}\mathbf{I}_{N_{2}'})^{-1}(\mathbf{K}_{Z^{(2)'}Z^{(2)'}}-1)$ $i=1$

 $\mathbf{K}_{Z^{(2)'z_0}})-\hat{H}_{\lambda_3,\xi}(x^{(1)'}_i,w^{(1)'}_i)\|^2$ where $\hat{H}_{\lambda_3,\xi}$ is learned with $\lambda_1 = \lambda_1^*$ and $\lambda_2 = \lambda_2^*$ using $\mathcal{D}^{(1)}$ and $\mathcal{D}^{(2)}$.

Properties of RKHS CAPCE estimator. The RKHS CAPCE estimator requires $\mathcal{O}(N_1^3) + \mathcal{O}(N_2^3)$ time [\[Saun](#page-10-22)[ders et al., 1998\]](#page-10-22). We show that RKHS CAPCE is consistent under assumptions similar to Kernel IV [\[Singh et al., 2019\]](#page-10-9). Assumptions F.1 - 8 are shown in Appendix [F.](#page-20-6)

Theorem 4.5 (Consistency). *Under SCM M_{IV} and Assumptions [3.1,](#page-2-1) [3.2,](#page-2-2) [F.1,](#page-22-0) [F.2,](#page-22-1) [F.3,](#page-22-2) [F.4,](#page-22-3) [F.5,](#page-22-4) [F.6,](#page-22-5) [F.7](#page-22-6) and [F.8,](#page-22-7) the RKHS CAPCE estimator in [\(24\)](#page-5-0) converges pointwise to CAPCE when* $\lambda_3 = 0$ *.*

When $\lambda_3 = 0$, the inverse of the matrix $\hat{O}\hat{O}^T$ + $N_2 \xi \mathbf{K}_{(X,W)^{(1)}(X,W)^{(1)}}$ in Eq. [\(25\)](#page-5-1) is numerically unstable. In practice, regularization leads to bias, but we must consider the bias-variance trade-off.

5 EXPERIMENTS

In this section, we present numerical experiments to demonstrate the performance of the proposed P-CAPCE, sieve CAPCE, and RKHS CAPCE estimators. Detailed settings

are in Appendix [G.](#page-23-0) The experiments are performed using an Apple M1 (16GB).

Baselines. We compare with the most widely used methods PTSLS (parametric), NTSLS (sieve), and Kernel IV. These methods compute $\mathbb{E}[Y_x|w]$ which we differentiate to compute CAPCE $\mathbb{E}[\partial_x Y_x|w]$.

SCM Settings. We consider the following two SCMs: $W :=$ $H + E_1, X := Z + W + H + E_2$, and

$$
\begin{cases}\nY := 10X^2 + WX + X + W + 50f(W)H + E_3 \text{ (A)} \\
Y := \exp(X)\exp(W) + 25f(W)H + E_3 \text{ (B)}\n\end{cases}
$$
\n(29)

where $f(W) = W^5 + W^4 + W^3 + W^2$. The SCMs satisfy separability Assumption [3.2](#page-2-2) but not [\(2\)](#page-1-1). We use setting (A) as a parametric setting and setting (B) as a nonparametric setting. Values of Z , H , E_1 , E_2 , and E_3 are sampled i.i.d. from a uniform distribution on $[-1, 1]$. True CAPCE is $20x + w + 1$ in setting (A) and $exp(x)exp(w)$ in setting (B).

Setting of P-CAPCE and PTSLS. We used the basis terms $\{1, W, X\}$ for P-CAPCE and $\{1, W, X, W X, X^2\}$ for PT-SLS, which match setting (A).

Setting of NTSLS and sieve CAPCE. We consider the basis terms $h_p(X)h_q(W)$ for $p = 0, 1, 2$ and $q = 0, 1, 2$, where h_p is Hermite polynomial functions: $h_0(t) = 1$, $h_1(t) = t$, $h_2(t) = t^2 - 1$, and $h_3(t) = t^3 - 3t$.

Setting of Kernel IV and RKHS CAPCE. We use polynomial kernel function $k_Z(z, z') = (z^T z' + C_1)^{C_2}$ and $k_{X,W}(x, w, x', w') = ((x, w)^T (x', w') + C_3)^{C_4}.$

Results. The means of estimated coefficients by PTSLS and P-CAPCE in the parametric setting (A) are shown in Table [1.](#page-7-0) We observe that, when $N = 1000$, both P-CAPCE and PTSLS estimates have large standard deviations (SD) (shown in Appendix [G\)](#page-23-0) such that the differences in estimated values are not statistically significant. The estimated coefficients of P-CAPCE are converging to the true values when the sample size $N = 10000$, while the coefficient for W estimated by PTSLS is still biased. We plotted the true and estimated CAPCE curves given $W = 1$ in Figure [2\(](#page-8-1)a). It is clear that the estimated curve by P-CAPCE is much closer to the true curve than PTSLS. The true and estimated CAPCE surfaces over (X, W) are shown in Appendix [G.](#page-23-0)

We computed the mean-squared-error (MSE) between estimated and true CAPCE values for each estimator,

where MSE is computed as $\frac{1}{N_1'}$ $\sum_{1}^{N_1'}$ $i=1$ $\{\hat{g}(x_i^{(1)'}, w_i^{(1)'}) -$

 $g(x_i^{(1)'}, w_i^{(1)'})\}^2$ with test dataset $\mathcal{D}^{(1)'}$, and the results are shown in Table [2.](#page-7-1) We observed that our sieve and RKHS CAPCE estimators are superior to the existing methods; sieve and RKHS CAPCE estimators are superior to P-CAPCE in the nonparametric setting (B); and kernel-based methods are much slower than other methods. We plotted the true and estimated CAPCE curves given $W = 1$ in Figure

Estimated coefficients		$N = 1000$		$N = 10000$			
Terms		W					
PTSLS	1.248		50.032 27.862 1.101 51.181			- 19.763	
P-CAPCE	-1.651	10.383	19.293	1.226	0.963	19 971	
True Coefficients							

Table 1: Means of estimated coefficients by PTSLS and P-CAPCE estimators in setting (A).

Table 2: MSE and run time of estimators in settings (A) and (B).

MSE	PTSLS	NTSLS	Kernel IV	P-CAPCE	S-CAPCE	RKHS CAPCE
(A) $N = 1000$	925.139	418.396	548.821	104.990	203.079	87.853
Time (second)	0.126	0.361	6.105	0.132	0.596	6.410
(A) $N = 10000$	817.074	357.777	495.742	69.185	185.056	71.276
Time (second)	0.372	1.127	2814.018	0.452	1.883	4530.765
(B) $N = 1000$	290.340	46.405	45.734	202.313	8.600	11.612
Time (second)	0.127	0.356	6.019	0.143	0.454	6.540
(B) $N = 10000$	265.400	20.990	51.470	54.124	3.579	8.985
Time (second)	0.367	1.031	2951.841	0.485	1.836	4360.991

[2\(](#page-8-1)b), which shows the estimated curves by sieve and RKHS CAPCE are much closer to the true curve than NTSLS and Kernel IV. The true and estimated CAPCE surfaces over (X, W) are shown in Appendix [G.](#page-23-0)

Overall, the results of settings (A) and (B) show that our proposed methods (P-CAPCE, sieve CAPCE, RKHS CAPCE) are superior to the previous works (PTSLS, NTSLS, Kernel IV). The advantage of our proposed methods stems from that the underlying models (A) and (B) do not satisfy the separability assumption [\(2\)](#page-1-1) needed by the existing works. Indeed, we have performed experiments in settings where the interaction between the covariates W and unobserved confounders H (the $f(W)H$ term in [\(29\)](#page-6-0)) is absent, and the results (presented in Appendix [G\)](#page-23-0) show that the performances of the existing methods PTSLS, NTSLS, Kernel IV are comparable with our proposed methods under this situation. Among the three proposed methods, the performance of P-CAPCE relies on correct parametric model assumption, and RKHS CAPCE is computationally expensive and requires tuning many regularization parameters.

6 APPLICATION IN A REAL-WORLD DATASET

In this section, we present an application of our CAPCE estimators to a real-world dataset in economics.

Real-world Dataset. We take up an open dataset "the National Longitudinal Survey of Young Men" in the R package "wooldridge" ([https://cran.r-project.org/](https://cran.r-project.org/package=wooldridge) [package=wooldridge](https://cran.r-project.org/package=wooldridge)), which has been analyzed by

many works, e.g., in [\[Griliches, 1977,](#page-9-20) [Blackburn and Neu](#page-9-21)[mark, 1992\]](#page-9-21). The sample size is 935 with 857 left after excluding missing values. We evaluate the heterogeneity of the effect of years of education on monthly wages, which is of great interest in economics [\[Angrist and Krueger, 1991,](#page-9-22) [Card, 1999\]](#page-9-23). We followed [Blackburn and Neumark](#page-9-21) [\[1992\]](#page-9-21) to use mother's education as an instrument to uncover the effect of education on wages. The use of mother's education as an instrument in this dataset has been subjected to debate in the literature (e.g., [\[Card, 1999,](#page-9-23) [Kling, 2001,](#page-10-23) [Wooldridge,](#page-11-3) [2010\]](#page-11-3)). We take the subject's years of education as the treatment variable (X) , their monthly wage as the outcome (Y) , their mother's years of education as the IV (Z) , and their IQ as a covariate (W) . The domains of X and Z are [9, 18], ranging from the 1st year of high school to the 2nd year of a master's degree. The domain of W is [50, 145].

Settings. We applied P-CAPCE and PTSLS. Other estimators are not used due to the small sample size. We use terms $\{1, W, W^2, X, XW, XW^2\}$ for P-CAPCE and $\{1, W, W^2, X, XW, XW^2, X^2, X^2W, X^2W^2\}$ for PT-SLS. Detailed settings are in Appendix [G.](#page-23-0)

Results. The estimated CAPCE values are shown in Appendix [G.](#page-23-0) For subjects with IQ 100, the estimated CAPCE $\mathbb{E}[\partial_x Y_x|W = 100]$ of years of education (X) on wages (Y) is given by $94.905 - 5.618x$ by P-CAPCE and $108.491 5.882x$ by PTSLS. Both predict that years of education increase wages, which is consistent with previous works [\[Blackburn and Neumark, 1992,](#page-9-21) [Wooldridge, 2010\]](#page-11-3). The results also show that education significantly affects wages at the compulsory school level, but the effect gets weaker with more years of education, consistent with the results

(a) Parametric setting (A) (Means, 95% CI)

(b) Nonparametric setting (B) (Means)

Figure 2: Plots of CAPCE curves with $W = 1$. X-axis represents treatment (X) ; Y-axis is CAPCE value. Dot-dashed curves in (a) represent 95% pointwise confidence interval (CI).

in [\[Angrist and Krueger, 1991,](#page-9-22) [Caplan, 2018\]](#page-9-24). On the other hand, for subjects with IQ 80, the estimated CAPCE $\mathbb{E}[\partial_x Y_x|W = 80]$ is 60.740 – 3.598x by P-CAPCE and $69.465 - 3.057x$ by PTSLS. For subjects with IQ 120, the estimated CAPCE $\mathbb{E}[\partial_x Y_x|W = 120]$ is 136.662 – 8.086x by P-CAPCE and $156.181 - 9.531x$ by PTSLS.

While we estimate the heterogeneity of causal effects of education on wages across subjects with different IQs, existing works [\[Blackburn and Neumark, 1992,](#page-9-21) [Card, 1999,](#page-9-23) [Kling,](#page-10-23) [2001,](#page-10-23) [Wooldridge, 2010,](#page-11-3) [Kawakami et al., 2023\]](#page-10-11) using this dataset have focused on the effects of education on wages over the whole population. [Card](#page-9-23) [\[1999\]](#page-9-23) and [Wooldridge](#page-11-3) [\[2010\]](#page-11-3) provided a summary of the early works on IV estimates and showed that the estimates of all studies were positive implying education increases wages. On the other hand, our results give two new insights into the effects of education on wages. First, our results suggest that for each sub-population $IQ = 80, 100, 120$, education significantly affects wages at the compulsory school level; but has little effect at the college level. This result is consistent with the

result of APCE estimates for the whole population given in [\[Kawakami et al., 2023\]](#page-10-11). Second, we reveal that the effect of education on wages is more significant for high IQ students, especially at the compulsory school level. To the best of our knowledge, this result has not been revealed in previous studies of this dataset, but it is consistent with the panel data analysis result in [\[Altonji and Dunn, 1996\]](#page-8-2).

7 CONCLUSION

We study conditional average partial causal effect (CAPCE) to represent the heterogeneous causal effects of a continuous treatment. We present a method for identifying CAPCE in the IV model. Notably, CAPCE $\mathbb{E}[\partial_x Y_x|\mathbf{w}]$ is identifiable under a weaker assumption than required by $\mathbb{E}[Y_x|\boldsymbol{w}]$, showing the merit of studying CAPCE instead of $\mathbb{E}[Y_x|\boldsymbol{w}]$, which has been the focus of existing work. We develop three families of CAPCE estimators: sieve, parametric, and RKHS, and analyze their statistical properties. We empirically demonstrate that the proposed CAPCE estimators are superior to the existing widely used IV methods PT-SLS [\[Angrist and Pischke, 2009,](#page-9-7) [Wooldridge, 2010\]](#page-11-3), sieve NTSLS [\[Newey and Powell, 2003\]](#page-10-8), and Kernel IV [\[Singh](#page-10-9) [et al., 2019\]](#page-10-9) in settings where the standard separability assumption [\(2\)](#page-1-1) is violated. The work provides scientists with a new tool for analyzing the heterogeneous causal effects of a continuous treatment. The results can be extended to an IV model with an additional edge $W \to Z$. An identification theorem similar to Theorem [3.1](#page-2-3) can be derived, which uses $\mathbb{P}(Y|Z, W)$ as input instead of $\mathbb{P}(Y|Z)$. We present this result in Appendix [A.2.](#page-13-0)

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References

- Chunrong Ai and Xiaohong Chen. Efficient estimation of models with conditional moment restrictions containing unknown functions. *Econometrica*, 71(6):1795–1843, 2003.
- Joseph G. Altonji and Thomas A. Dunn. The effects of family characteristics on the return to education. *The Review of Economics and Statistics*, 78(4):692–704, 1996.
- Joshua D. Angrist. Treatment effect heterogeneity in theory and practice. *The Economic Journal*, 114(494):C52–C83, 2004.
- Joshua D. Angrist and Alan B. Krueger. Does compulsory school attendance affect schooling and earnings? *The Quarterly Journal of Economics*, 106(4):979–1014, 1991.
- Joshua D. Angrist and Alan B. Krueger. The effect of age at school entry on educational attainment: An application of instrumental variables with moments from two samples. *Journal of the American Statistical Association*, 87(418): 328–336, 1992.
- Joshua D. Angrist and Alan B. Krueger. Instrumental variables and the search for identification: From supply and demand to natural experiments. *Journal of Economic Perspectives*, 15(4):69–85, December 2001.
- Joshua D Angrist and Jörn-Steffen Pischke. *Mostly harmless econometrics: An empiricist's companion*. Princeton university press, 2009.
- Susan Athey and Guido Imbens. Recursive partitioning for heterogeneous causal effects. *Proceedings of the National Academy of Sciences*, 113(27):7353–7360, 2016.
- Susan Athey and Guido W. Imbens. Machine learning methods that economists should know about. *Annual Review of Economics*, 11(1):685–725, 2019.
- Mohammad Taha Bahadori, Eric J. Tchetgen Tchetgen, and David E. Heckerman. End-to-end balancing for causal continuous treatment-effect estimation. In *ICML 2022, UAI 2022 Workshop on Advances in Causal Inference*, 2022.
- Alexander Balke and Judea Pearl. Bounds on treatment effects from studies with imperfect compliance. *Journal of the American Statistical Association*, 92(439):1171– 1176, 1997.
- Falco J. Bargagli-Stoffi, Kristof De Witte, and Giorgio Gnecco. Heterogeneous causal effects with imperfect compliance: A Bayesian machine learning approach. *The Annals of Applied Statistics*, 16(3):1986 – 2009, 2022.
- Andrew Bennett, Nathan Kallus, Xiaojie Mao, Whitney Newey, Vasilis Syrgkanis, and Masatoshi Uehara. Minimax Instrumental Variable Regression and L_2 Convergence Guarantees without Identification or Closedness. Papers 2302.05404, arXiv.org, February 2023.
- McKinley Blackburn and David Neumark. Unobserved ability, efficiency wages, and interindustry wage differentials. *The Quarterly Journal of Economics*, 107(4):1421–1436, 1992.
- Maxime Bôcher. *An introduction to the study of integral equations*. Number 10. University Press, 1926.
- Bryan Caplan. *The Case against Education: Why the Education System Is a Waste of Time and Money*. Princeton University Press, 2018.
- David Card. Chapter 30 - the causal effect of education on earnings. volume 3 of *Handbook of Labor Economics*, pages 1801–1863. Elsevier, 1999.
- Gary Chamberlain. Panel data. In Z. Griliches† and M. D. Intriligator, editors, *Handbook of Econometrics*, volume 2, chapter 22, pages 1247–1318. Elsevier, 1 edition, 1984.
- Xiaohong Chen and Timothy M. Christensen. Optimal sup-norm rates and uniform inference on nonlinear functionals of nonparametric iv regression. *Quantitative Economics*, 9(1):39–84, 2018.
- S.B. Damelin, H.S. Jung, and K.H. Kwon. Convergence of hermite and hermite–fejér interpolation of higher order for freud weights. *Journal of Approximation Theory*, 113 (1):21–58, 2001.
- Nishanth Dikkala, Greg Lewis, Lester Mackey, and Vasilis Syrgkanis. Minimax estimation of conditional moment models. In *Proceedings of the 34th International Conference on Neural Information Processing Systems*, NIPS'20, Red Hook, NY, USA, 2020. Curran Associates Inc.
- Peng Ding, Avi Feller, and Luke Miratrix. Randomization inference for treatment effect variation. *Journal of the Royal Statistical Society. Series B (Statistical Methodology)*, 78(3):655–671, 2016.
- Douglas Galagate. *Causal inference with a continuous treatment and outcome: Alternative estimators for parametric dose-response functions with applications*. PhD thesis, University of Maryland, College Park, 2016.
- A. Ronald Gallant and Douglas W. Nychka. Seminonparametric maximum likelihood estimation. *Econometrica*, 55(2):363–390, 1987.
- Stuart Geman and Chii-Ruey Hwang. Nonparametric Maximum Likelihood Estimation by the Method of Sieves. *The Annals of Statistics*, 10(2):401 – 414, 1982.
- Bryan S. Graham and James L. Powell. Identification and estimation of average partial effects in "irregular" correlated random coefficient panel data models. *Econometrica*, 80 (5):2105–2152, 2012.
- Zvi Griliches. Estimating the returns to schooling: Some econometric problems. *Econometrica*, 45(1):1–22, 1977.
- Jason Hartford, Greg Lewis, Kevin Leyton-Brown, and Matt Taddy. Deep IV: A flexible approach for counterfactual prediction. In *Proceedings of the 34th International Conference on Machine Learning*, volume 70 of *Proceedings of Machine Learning Research*, pages 1414–1423. PMLR, 06–11 Aug 2017.
- Charles Hermite. *Sur un nouveau développement en série des fonctions*, volume 2 of *Cambridge Library Collection - Mathematics*, page 293–308. Cambridge University Press, 2009.
- Donald E. Hilt, Donald W. Seegrist, United States. Forest Service., and Pa.) Northeastern Forest Experiment Station (Radnor. *Ridge, a computer program for calculating ridge regression estimates*, volume no.236. Upper Darby, Pa, Dept. of Agriculture, Forest Service, Northeastern Forest Experiment Station, 1977.
- Keisuke Hirano and Guido W. Imbens. *The Propensity Score with Continuous Treatments*, pages 73–84. Wiley-Blackwell, July 2005.
- Nick Huntington-Klein. Instruments with heterogeneous effects: Bias, monotonicity, and localness. *Journal of Causal Inference*, 8(1):182–208, 2020.
- Guido W. Imbens. Instrumental variables: An econometrician's perspective. *Statistical Science*, 29(3):323–358, 2014.
- Guido W. Imbens and Joshua D. Angrist. Identification and estimation of local average treatment effects. *Econometrica*, 62(2):467–475, 1994.
- Masahiro Kato, Masaaki Imaizumi, Kenichiro McAlinn, Shota Yasui, and Haruo Kakehi. Learning causal models from conditional moment restrictions by importance weighting. In *International Conference on Learning Representations*, 2022.
- Yuta Kawakami, Manabu Kuroki, and Jin Tian. Instrumental variable estimation of average partial causal effects. In *Proceedings of the 40th International Conference on Machine Learning*, volume 202 of *Proceedings of Machine Learning Research*, pages 16097–16130. PMLR, 23–29 Jul 2023.
- Edward H. Kennedy, Zongming Ma, Matthew D. McHugh, and Dylan S. Small. Non-parametric methods for doubly robust estimation of continuous treatment effects. *Journal of the Royal Statistical Society. Series B (Statistical Methodology)*, 79(4):1229–1245, 2017.
- Jeffrey R. Kling. Interpreting instrumental variables estimates of the returns to schooling. *Journal of Business & Economic Statistics*, 19(3):358–364, 2001.
- Dirk P. Kroese, Thomas Taimre, and Zdravko I. Botev. Handbook of monte carlo methods. 2011.
- Sören R. Künzel, Jasjeet S. Sekhon, Peter J. Bickel, and Bin Yu. Metalearners for estimating heterogeneous treatment effects using machine learning. *Proceedings of the National Academy of Sciences*, 116(10):4156–4165, 2019.
- G. Leoni. *A First Course in Sobolev Spaces*. Graduate studies in mathematics. American Mathematical Soc., 2009.
- Paul Milgrom and Ilya Segal. Envelope theorems for arbitrary choice sets. *Econometrica*, 70(2):583–601, 2002.
- Krikamol Muandet, Arash Mehrjou, Si Kai Lee, and Anant Raj. Dual instrumental variable regression. In *Proceedings of the 34th International Conference on Neural Information Processing Systems*, NIPS'20, Red Hook, NY, USA, 2020. Curran Associates Inc.
- Whitney K. Newey and James L. Powell. Instrumental variable estimation of nonparametric models. *Econometrica*, 71(5):1565–1578, 2003.
- Judea Pearl. *Causality: Models, Reasoning and Inference*. Cambridge University Press, 2nd edition, 2009.
- Craig Saunders, Alexander Gammerman, and Vladimir Vovk. Ridge regression learning algorithm in dual variables. In *International Conference on Machine Learning*, 1998.
- Bernhard Schölkopf, Ralf Herbrich, and Alex Smola. A generalized representer theorem. In *COLT/EuroCOLT*, 2001.
- Bernhard Schölkopf, Zhiyuan Luo, and Vladimir Vovk. *Empirical inference: Festschrift in honor of Vladimir N. Vapnik*. Springer Science & Business Media, 2013.
- J. Shawe-Taylor and N. Cristianini. *Kernel methods for pattern analysis*. Cambridge University Press, June 2004.
- R Singh, L Xu, and A Gretton. Kernel methods for causal functions: dose, heterogeneous and incremental response curves. *Biometrika*, page asad042, July 2023.
- Rahul Singh, Maneesh Sahani, and Arthur Gretton. Kernel instrumental variable regression. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 32. Curran Associates, Inc., 2019.
- Vasilis Syrgkanis, Victor Lei, Miruna Oprescu, Maggie Hei, Keith Battocchi, and Greg Lewis. Machine learning estimation of heterogeneous treatment effects with instruments. In *Advances in Neural Information Processing Systems*, volume 32. Curran Associates, Inc., 2019.
- Sergios Theodoridis and Konstantinos Koutroumbas. *Pattern recognition*. Elsevier, 2006.
- Andrei Nikolaevich Tikhonov, AV Goncharsky, VV Stepanov, and Anatoly G Yagola. *Numerical methods for the solution of ill-posed problems*, volume 328. Springer Science & Business Media, 1995.
- Stefan Wager and Susan Athey. Estimation and inference of heterogeneous treatment effects using random forests. *Journal of the American Statistical Association*, 113(523): 1228–1242, 2018.
- Wing Hung Wong. An equation for the identification of average causal effect in nonlinear models. *Statistica Sinica*, 32:539–545, 2022.
- Jeffrey M Wooldridge. Unobserved heterogeneity and estimation of average partial effects. *Identification and inference for econometric models: Essays in honor of Thomas Rothenberg*, pages 27–55, 2005.
- Jeffrey M Wooldridge. *Econometric analysis of cross section and panel data*. MIT press, 2010.
- Philip G. Wright. The tariff on animal and vegetable oils. 1928.
- Yichi Zhang, Dehan Kong, and Shu Yang. Towards r-learner of conditional average treatment effects with a continuous treatment: T-identification, estimation, and inference. *arXiv e-prints*, pages arXiv–2208, 2022.

Appendix to "Identification and Estimation of Conditional Average Partial Causal Effects via Instrumental Variable"

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A PROOFS OF THEOREM 3.1 AND RKHS CAPCE ESTIMATOR

A.1 PROOF OF THEOREM [3.1](#page-2-3)

We give proof of Theorem [3.1.](#page-2-3)

Theorem [3.1.](#page-2-3) *(Identification of CAPCE). Under SCM* M_{IV} *and Assumptions* [3.1](#page-2-1) *and* [3.2,](#page-2-2) *CAPCE* $\mathbb{E}[\partial_x Y_x | \boldsymbol{w}]$ *is identifiable from distributions* $\mathbb{P}(X, W|Z)$ *and* $\mathbb{P}(Y|Z)$ *via the integral equation:*

$$
\mu(z) = \int_{\Omega_{\boldsymbol{W}}} \int_{\Omega_{\boldsymbol{X}}} k(z, x, \boldsymbol{w}) \mathbb{E}[\partial_x Y_x | \boldsymbol{w}] dx d\boldsymbol{w}, \tag{30}
$$

where $\mu(z) = \mathbb{E}[Y|Z = z_0] - \mathbb{E}[Y|Z = z]$, $k(z, x, w) = p(X \le x, W = w|Z = z) - p(X \le x, W = w|Z = z_0)$, and z_0 *is a fixed value.*

Proof. First, we show the following integral equation holds under Assumptions [3.1](#page-2-1) and [3.2](#page-2-2) following the idea in [\[Wong,](#page-11-5) [2022\]](#page-11-5):

$$
\mathbb{E}[Y|Z=z, \mathbf{W}=\mathbf{w}] - \mathbb{E}[Y|Z=z_0, \mathbf{W}=\mathbf{w}]
$$
\n
$$
= -\int_{\Omega_X} {\mathbb{P}(X \le x|Z=z, \mathbf{W}=\mathbf{w}) - \mathbb{P}(X \le x|Z=z_0, \mathbf{W}=\mathbf{w}) } \mathbb{E}[\partial_x Y_x | \mathbf{w}] dx.
$$
\n(31)

From the setting of the IV, the following integral equation holds:

$$
Y_{X_z} = \int_{\Omega_X} \mathbb{1}_{X_z = x} Y_x dx,\tag{32}
$$

given $W = w$ for each subject, where 1 is a delta function or indicator function. This equation means $X_z = x \Rightarrow$ $Y_{X_z} = Y_x$ from the definition of delta function. By substituting the integral equations $Y_{X_z} = \frac{1}{2\pi\epsilon_0 g}$ $\int_{\Omega_X} 1\!\!1_{X_z=x} Y_x dx$ and $Y_{X_{z_0}} =$ $\int_{\Omega_X} 1\!\!1_{X_{z_0}=x} Y_x dx$, then

$$
Y_{X_z} - Y_{X_{z_0}} = \int_{\Omega_X} {\{\mathbb{1}_{X_z = x} - \mathbb{1}_{X_{z_0} = x}\}} Y_x dx
$$
\n(33)

holds. Since the Heaviside step function is the integration of the delta function,

$$
Y_{X_z} - Y_{X_{z_0}} = \left[\{ \mathbb{1}_{X_z = x} - \mathbb{1}_{X_{z_0} = x} \} \partial_x Y_x \right]_{-\infty}^{\infty} - \int_{\Omega_X} \{ \mathbb{1}_{X_z \le x} - \mathbb{1}_{X_{z_0} \le x} \} \partial_x Y_x dx.
$$
 (34)

Figure 3: A causal graph representing the IV setting with covariates when there is an edge $W \to Z$.

Because $\partial_x Y_x < \infty$ for all $x \in \Omega_X$, $\left[\{ \mathbb{1}_{X_z = x} - \mathbb{1}_{X_{z_0} = x} \} \partial_x Y_x \right]_{-\infty}^{\infty} = 0$ holds. Then, the integral equation becomes

$$
Y_{X_z} - Y_{X_{z_0}} = -\int_{\Omega_X} \{ \mathbb{I}_{X_z \le x} - \mathbb{I}_{X_{z_0} \le x} \} \partial_x Y_x dx.
$$
 (35)

From the separability with covariate $f_Y(X, \mathbf{W}, \mathbf{H}, \mathbf{u}_Y) = f_Y^1(X, \mathbf{W}, \mathbf{u}_Y) + f_Y^2(\mathbf{W}, \mathbf{H}, \mathbf{u}_Y)$, random variables $\mathbb{I}_{X_z \leq x}$ $\mathbb{I}_{X_{z_0}\leq x}$ and ∂_xY_x are independent given $W = w$. Thus, we take expectations on both sides:

$$
\mathbb{E}[Y_{X_z}|\boldsymbol{W}=\boldsymbol{w}] - \mathbb{E}[Y_{X_{z_0}}|\boldsymbol{W}=\boldsymbol{w}] \tag{36}
$$

$$
= -\int_{\Omega_X} \mathbb{E}[\{\mathbb{I}_{X_z \le x} - \mathbb{I}_{X_{z_0} \le x}\} \partial_x Y_x | \mathbf{W} = \mathbf{w}] dx \tag{37}
$$

$$
= -\int_{\Omega_X} \{ \mathbb{E}[\mathbb{I}_{X_z \leq x} | \boldsymbol{W} = \boldsymbol{w}] - \mathbb{E}[\mathbb{I}_{X_{z_0} \leq x} | \boldsymbol{W} = \boldsymbol{w}] \} \mathbb{E}[\partial_x Y_x | \boldsymbol{w}] dx.
$$
 (38)

Then, the integral equation becomes

$$
\mathbb{E}[Y|Z=z, \mathbf{W}=\mathbf{w}] - \mathbb{E}[Y|Z=z_0, \mathbf{W}=\mathbf{w}]
$$
\n
$$
= -\int_{\Omega_X} {\mathbb{P}(X \le x|Z=z, \mathbf{W}=\mathbf{w}) - \mathbb{P}(X \le x|Z=z_0, \mathbf{W}=\mathbf{w}) } \mathbb{E}[\partial_x Y_x | \mathbf{w}] dx.
$$
\n(39)

Next, the integral equation can be given by multiplying $p(W = w|Z = z)$ and marginalizing for W, then

$$
\mathbb{E}_{\mathbf{W}}[\mathbb{E}[Y|Z=z,\mathbf{W}=\mathbf{w}]] = \tag{40}
$$

$$
\int_{\Omega_X} \int_{\Omega_W} \mathbb{P}(X \le x | Z = z, \mathbf{W} = \mathbf{w}) \mathfrak{p}(\mathbf{W} = \mathbf{w} | Z = z) \mathbb{E}[\partial_x Y_x | \mathbf{w}] d\mathbf{w} dx \tag{41}
$$

$$
\Leftrightarrow \mathbb{E}[Y|Z=z] = \int_{\Omega_X} \int_{\Omega_W} \mathfrak{p}(X \le x, \mathbf{W}=\mathbf{w}|Z=z) \mathbb{E}[\partial_x Y_x | \mathbf{w}] d\mathbf{w} dx \tag{42}
$$

Finally, we show the uniqueness of the solution. Since X_z is a nontrivial function, there does not exist a function which satisfies $\mathbb{E}[\delta(X)|Z=z, \mathbf{W}=\mathbf{w}]=0$ for any $z \in \Omega_Z$ and $\mathbf{w} \in \Omega_{\mathbf{W}}$. Since $\mathbb{E}[\delta(X)|Z=z, \mathbf{W}=\mathbf{w}]=\mathbb{E}[\delta(X), \mathbf{W}=\mathbf{w}]=0$ $w|Z = z$] $\mathbb{P}(W = w)$, there exists a function which satisfies $\mathbb{E}[\delta(X), W = w|Z = z] = 0$ for any $z \in \Omega_Z$ and $w \in \Omega_W$ if there exists a function which satisfies $\mathbb{E}[\delta(X)|Z=z] = 0$ for any $z \in \Omega_Z$ and $w \in \Omega_W$. Taking a contraposition, there does not exist a function which satisfies $\mathbb{E}[\delta(X), \mathbf{W} = \mathbf{w}|Z = z] = 0$ for any $z \in \Omega_Z$ and $\mathbf{w} \in \Omega_{\mathbf{W}}$. \Box

A.2 IDENTIFICATION THEOREM UNDER IV MODEL IN FIG [3](#page-13-1)

We consider the IV model with covariates represented by the causal graph in Fig [3,](#page-13-1) with the following SCM M'_{IV} over $V = \{Z, X, Y, W\}$ and $U = \{H, u_X, u_Y, u_Z, u_W\}$:

$$
Y := f_Y(X, \mathbf{W}, \mathbf{H}, \mathbf{u}_Y), \ X := f_X(Z, \mathbf{W}, \mathbf{H}, \mathbf{u}_X), \mathbf{W} := f_{\mathbf{W}}(\mathbf{H}, \mathbf{u}_{\mathbf{W}}), \ Z := f_Z(\mathbf{W}, \mathbf{u}_Z), \tag{43}
$$

where f_W is a vector function. We assume all variables are continuous, W are d-dimensional pre-treatment covariates, and H stands for unmeasured confounders. We show a similar identification result to Theorem [3.1.](#page-2-3)

Theorem [3.1](#page-2-1)'. Under SCM M'_{IV} and Assumptions 3.1 and [3.2,](#page-2-2) CAPCE $\mathbb{E}[\partial_x Y_x|\omega]$ is identifiable from distributions $\mathbb{P}(X|Z, \mathbf{W})$ and $\mathbb{P}(Y|Z, \mathbf{W})$ *via the integral equation:*

$$
\mu(z, \mathbf{w}) = \int_{\Omega_X} k(z, x, \mathbf{w}) \mathbb{E}[\partial_x Y_x | \mathbf{w}] dx,
$$
\n(44)

 \Box

where $\mu(z, \mathbf{w}) = \mathbb{E}[Y|Z = z_0, \mathbf{W} = \mathbf{w}] - \mathbb{E}[Y|Z = z, \mathbf{W} = \mathbf{w}], k(z, x, \mathbf{w}) = \mathfrak{p}(X \le x|Z = z, \mathbf{W} = \mathbf{w}) - \mathfrak{p}(X \le x)$ $x|Z = z_0, W = w$, and z_0 *is a fixed value.*

Proof. Eq. [\(44\)](#page-14-0) is guaranteed by Eq. [\(39\)](#page-13-2), which appears in the proof of Theorem [3.1.](#page-2-3)

Based on Theorem 3.1', we have to learn $\mathbb{E}[\partial_x Y_x|w]$ as a function of x for each $w \in \Omega_W$ respectively. In contrast, based on Theorem [3.1,](#page-2-3) we can learn $\mathbb{E}[\partial_x Y_x|\omega]$ directly as a function of x and w.

We perform experiments about estimating CAPCE based on Theorem 3.1' in Appendix [G.5.](#page-27-0)

A.3 DERIVATION OF RKHS CAPCE ESTIMATOR

We show the detailed steps of deriving the RKHS CAPCE estimator.

RKHS estimator. RKHS CAPCE estimator is given as $\mathbb{E}[\partial_x Y_x | \boldsymbol{w}] = \hat{\boldsymbol{\alpha}}^T \mathbf{K}_{(X, \boldsymbol{W})^{(1)}(x, \boldsymbol{w})}$ where

$$
\hat{\alpha} = (\hat{\mathbf{O}}\hat{\mathbf{O}}^T + N_2 \xi \mathbf{K}_{(X,W)^{(1)}(X,W)^{(1)}} + N_2 \lambda_3 \mathbf{I}_{N_2})^{-1} \hat{\mathbf{O}} \times \{ \mathbf{y}^{(2)T} (\mathbf{K}_{Z^{(2)}Z^{(2)}} + N_2 \lambda_2 \mathbf{I}_{N_2})^{-1} (\mathbf{K}_{Z^{(2)}Z^{(2)}} - \mathbf{K}_{Z^{(2)}z_0}) \} \n\hat{\mathbf{O}} = \mathbf{K}_{(X,W)^{(1)}(X,W)^{(1)}} (\mathbf{K}_{Z^{(1)}Z^{(1)}} + N_1 \lambda_1 \mathbf{I}_{N_1})^{-1} (\mathbf{K}_{Z^{(1)}Z^{(2)}} - \mathbf{K}_{Z^{(1)}z_0}),
$$
\n(45)

 $(\lambda_1, \lambda_2, \lambda_3, \xi)$ are regularization parameters, and \mathbf{I}_N is a $N \times N$ identity matrix.

Proof. There are three optimization problems in RKHS estimator, **Stage 1** (A) learning linear operator G_1 , **Stage 1** (B) learning linear operator G_2 , and **Stage 2** learning linear operator H . We explain them respectively.

Stage 1 (A). We denote the feature map be $\psi(z)$ and $\pi(x, w)$, where $\pi(x, w) = -\int_{-\infty}^{x} \eta(x', w) dx'$ for some feature function $\eta(x', \mathbf{w})$. The optimization problem in **Stage 1 (A)** becomes

$$
\min_{G_1 \in \mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_{X, \mathbf{W}})} N_1^{-1} \sum_{i=1}^{N_1} \left\| \pi(x_i^{(1)}, \mathbf{w}_i^{(1)}) - G_1(\psi(z_i^{(1)})) \right\|_{\mathcal{H}_{X, \mathbf{W}}}^2 + \lambda_1 \|G_1\|_{\mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_{X, \mathbf{W}})}^2.
$$
\n(46)

using $\mathcal{D}^{(1)}$. Then, the estimator \hat{G}_1 becomes

$$
\hat{G}_1(\cdot) = \left\langle \pi_{X^{(1)}, \mathbf{W}^{(1)}} (\mathbf{K}_{Z^{(1)}Z^{(1)}} + N_1 \lambda_1 \mathbf{I})^{-1} \psi_Z^{(1)T}, \cdot \right\rangle
$$
\n(47)

where $K_{Z(1)Z(1)}$ and $K_{X(1)X(1)}$ are the empirical kernel matrices, the *i*-th column of $\pi_{X(1),W^{(1)}}$ is − $\int x_i^{(1)}$ −∞ $\eta(x, \mathbf{w})dx$, and the *i*-th column of $\psi_X^{(1)}$ is $\psi(z_i^{(1)})$. The prediction values are

$$
d_0(z) = \pi_{X^{(1)}, \mathbf{W}^{(1)}} (\mathbf{K}_{ZZ} + N_1 \lambda_1 I)^{-1} \psi_Z^{(1)T} \psi(z) = -\sum_{i=1}^{N_1} \gamma_i(z) \int_{-\infty}^{x_i^{(1)}} \eta(x, \mathbf{w}) dx \tag{48}
$$

where $\gamma(z) = (\mathbf{K}_{Z^{(1)}Z^{(1)}} + N_1\lambda_1\mathbf{I})^{-1}\psi_Z^{(1)T}\psi(z) = (\mathbf{K}_{Z^{(1)}Z^{(1)}} + N_1\lambda_1\mathbf{I})^{-1}\mathbf{K}_{Z^{(1)}z}$. Furthermore, the difference in the predication values are

$$
d(z) = d_0(z) - d_0(z_0) = -\sum_{i=1}^{N_1} \{ \gamma_i(z) - \gamma_i(z_0) \} \int_{-\infty}^{x_i^{(1)}} \eta(x, \mathbf{w}) dx
$$
 (49)

and $\gamma(z) - \gamma_i(z_0) = (\mathbf{K}_{Z^{(1)}Z^{(1)}} + N_1\lambda_1\mathbf{I})^{-1}\psi_Z^{(1)T}$ $\mathbf{X}_{Z}^{(1)T} \{ \psi(z) - \psi(z_0) \} = (\mathbf{K}_{Z^{(1)}Z^{(1)}} + N_1 \lambda_1 \mathbf{I})^{-1} (\mathbf{K}_{Z^{(1)}z} - \mathbf{K}_{Z^{(1)}z_0})$ holds. Letting $\hat{G}_1 = \sum_{j=1}^{N_1} \alpha_j \eta(x_j^{(1)}, \mathbf{w}_j^{(1)})$ since the optimal \hat{G}_1 exists in span $(\{\eta(x_j^{(1)}, \mathbf{w}_j^{(1)})\}_{j=1}^{N_1})$ from the representer theorem [\[Schölkopf et al., 2001\]](#page-10-21). Then the functional form of $d(z)$ is restricted by

$$
d(z) = -\left\langle \sum_{j=1}^{N_1} \alpha_j \int_{-\infty}^{x_i^{(1)}} \eta(x, \mathbf{w}_i^{(1)}) dx, -\sum_{i=1}^{N_1} \{ \gamma_i(z) - \gamma_i(z_0) \} \int_{-\infty}^{x_j^{(1)}} \eta(x, \mathbf{w}_j^{(1)}) dx \right\rangle
$$
(50)

$$
= \sum_{i=1}^{N_1} \sum_{j=1}^{N_1} \alpha_j \{ \gamma_i(z) - \gamma_i(z_0) \} \left\langle -\int_{-\infty}^{x_i^{(1)}} \eta(x, \mathbf{w}_i^{(1)}) dx, -\int_{-\infty}^{x_j^{(1)}} \eta(x, \mathbf{w}_j^{(1)}) dx \right\rangle \tag{51}
$$

$$
= \sum_{i=1}^{N_1} \sum_{j=1}^{N_1} \alpha_j \{ \gamma_i(z) - \gamma_i(z_0) \} \left\langle \pi(x_i^{(1)}, \boldsymbol{w}_i^{(1)}), \pi(x_j^{(1)}, \boldsymbol{w}_j^{(1)}) \right\rangle.
$$
 (52)

From the kernel trick, it becomes

$$
= \sum_{i=1}^{N_1} \sum_{j=1}^{N_1} \alpha_j \{ \gamma_i(z) - \gamma_i(z_0) \} k((x_i^{(1)}, \boldsymbol{w}_i^{(1)}), (x_j^{(1)}, \boldsymbol{w}_j^{(1)}))
$$
(53)

$$
= \alpha^T w(z) \tag{54}
$$

where $w(z) = \mathbf{K}_{(X,W)^{(1)}(X,W)^{(1)}} (\mathbf{K}_{ZZ} + N_1 \lambda_1 \mathbf{I})^{-1} (\mathbf{K}_{Z^{(1)}z} - \mathbf{K}_{Z^{(1)}z_0})$. Note that the α will be estimated in **Stage 2.** Stage 1 (B). The optimization problem in Stage 1 (B) is

$$
\min_{G_2 \in \mathcal{L}_2(\mathcal{H}_Z, \Omega_Y)} N_2^{-1} \sum_{i=1}^{N_2} \left\| y_i^{(2)} - G_2(\psi(z_i^{(2)})) \right\|^2 + \lambda_2 \|G_2\|_{\mathcal{L}_2(\mathcal{H}_Z, \Omega_Y)}^2 \tag{55}
$$

using $\mathcal{D}^{(2)}$. As **Stage 1** (A), the estimator of G_2 , \hat{G}_2 , become

$$
\hat{G}_2(\cdot) = \left\langle \mathbf{y}^{(2)} (\mathbf{K}_{Z^{(2)}Z^{(2)}} + N_2 \lambda_2 \mathbf{I})^{-1} \psi_Z^{(2)T}, \cdot \right\rangle
$$
\n(56)

where $\mathbf{K}_{Z^{(2)}Z^{(2)}}$ are the gram matrices, the *i*-th column of $y^{(2)}$ is $y_i^{(2)}$.

$$
u_0(z) = \mathbf{y}^{(2)T} (\mathbf{K}_{Z^{(2)}Z^{(2)}} + N_2 \lambda_2 \mathbf{I})^{-1} \psi_Z^{(2)T} \psi(z) = \sum_{i=1}^{N_2} \gamma_i(z) \psi(z)
$$
(57)

where $\gamma(z) = \mathbf{y}^{(2)T} (\mathbf{K}_{Z^{(2)}Z^{(2)}} + N_2 \lambda_2 I)^{-1} \psi_Z^{(2)T}$ $\chi_Z^{(2)I}$. Then,

$$
u_0(z_0) = \mathbf{y}^{(2)T} (\mathbf{K}_{Z^{(2)}Z^{(2)}} + N_2 \lambda_2 \mathbf{I})^{-1} \mathbf{K}_{Z^{(2)}z_0}
$$
(58)

and, the difference of the predication values are

$$
u(z) = u_0(z) - u_0(z_0) = \mathbf{y}^{(2)T} (\mathbf{K}_{Z^{(2)}Z^{(2)}} + N_2 \lambda_2 \mathbf{I})^{-1} (\mathbf{K}_{Z^{(2)}z} - \mathbf{K}_{Z^{(2)}z_0}).
$$
\n(59)

This is the estimator of $\mathbb{E}[Y|Z=z] - \mathbb{E}[Y|Z=z_0]$.

Stage 2. The optimization problem in **Stage 2** using $\mathcal{D}^{(2)}$ is

$$
\min_{H \in \mathcal{L}_2(\mathcal{H}_{X,W}, \Omega_Y)} N_2^{-1} \sum_{i=1}^{N_2} \left\| \hat{G}_2(\psi(z_i^{(2)}) - \psi(z_0)) - H(\hat{G}_1(\psi(z_i^{(2)}) - \psi(z_0))) \right\|^2
$$

$$
+ \xi \|H\|_{\mathcal{L}_2(\mathcal{H}_{X,W}, \Omega_Y)}^2 + \lambda_3 \|H \circ \hat{G}_1\|_{\mathcal{L}_2(\mathcal{H}_Z, \Omega_Y)}^2.
$$
 (60)

Then, the estimation problem reduces to

$$
\frac{1}{N_2} \sum_{i=1}^{N_2} (y_i^{(2)} - u_0(z_0) - \boldsymbol{\alpha}^T w(z))^2 + \xi \boldsymbol{\alpha}^T \mathbf{K}_{XX} \boldsymbol{\alpha} + \lambda_3 \boldsymbol{\alpha}^T \boldsymbol{\alpha}
$$
\n(61)

$$
= \frac{1}{N_2} \|\mathbf{y}^{(2)} - \mathbf{y}^{(2)T} (\mathbf{K}_{Z^{(2)}Z^{(2)}} + N_2 \lambda_2 \mathbf{I})^{-1} \mathbf{K}_{Z^{(2)}z_0}
$$
(62)

$$
-(\mathbf{K}_{X^{(1)}X^{(1)}}(\mathbf{K}_{Z^{(1)}Z^{(1)}}+N_1\lambda_1\mathbf{I})^{-1}(\mathbf{K}_{Z^{(1)}Z^{(2)}}-\mathbf{K}_{Z^{(1)}z_0}))^T\alpha\|^2
$$
\n(63)

$$
+\xi \alpha^T \mathbf{K}_{(X,W)^{(1)}(X,W)^{(1)}} \alpha + \lambda_3 \alpha^T \alpha, \tag{64}
$$

and the solution to this optimization problem can be represented as

$$
\hat{\alpha} = (\hat{\mathbf{O}}\hat{\mathbf{O}}^T + N_2 \xi \mathbf{K}_{(X, \mathbf{W})^{(1)}(X, \mathbf{W})^{(1)}} + N_2 \lambda_3 \mathbf{I})^{-1} \hat{\mathbf{O}} \tag{65}
$$

$$
\times (\mathbf{y}^{(2)} - \mathbf{y}^{(2)T} (\mathbf{K}_{Z^{(2)}Z^{(2)}} + N_2 \lambda_2 \mathbf{I})^{-1} \mathbf{K}_{Z^{(2)}z_0})
$$
(66)

 \Box

$$
\hat{\mathbf{O}} = \mathbf{K}_{(X,W)^{(1)}(X,W)^{(1)}} (\mathbf{K}_{Z^{(1)}Z^{(1)}} + N_1 \lambda_1 \mathbf{I})^{-1} (\mathbf{K}_{Z^{(1)}Z^{(2)}} - \mathbf{K}_{Z^{(1)}z_0}).
$$
\n(67)

Finally, RKHS CAPCE estimator of $(x, \bm w)$ becomes $\hat{\mathbb{E}}[\partial_x Y_x | \bm w] = \hat{\bm \alpha}^T\mathbf{K}_{(X, \bm W)(x, \bm w)}.$

B CONSISTENCY OF SIEVE CAPCE ESTIMATOR

In this section, we show that sieve CAPCE estimator is consistent under assumptions similar to those guaranteeing the consistency of sieve NTSLS [\[Newey and Powell, 2003\]](#page-10-8).

NOTATIONS

We introduce the notations for the assumptions.

Conditional Moment Restrictions. The estimation problem reduces to the problem called conditional moment restrictions, and properties of the estimator are well studied [\[Newey and Powell, 2003,](#page-10-8) [Ai and Chen, 2003\]](#page-8-3), and it is widely used in machine learning fields [\[Kato et al., 2022\]](#page-10-24). Since $\mathbb{E}[Y|Z=z_0]-\mathbb{E}[Y|Z]=\mathbb{E}[\mathbb{E}[Y|Z=z_0]-Y|Z]$ and $\mathbb{E}[\mathbb{1}_{X\leq x,\mathbf{W}=\mathbf{w}}|Z=z_0]$ z] – $\mathbb{E}[1_{X\leq x, \mathbf{W}=\mathbf{w}}|Z=z_0] = \mathbb{E}[1_{X\leq x, \mathbf{W}=\mathbf{w}} - \mathbb{E}[1_{X\leq x, \mathbf{W}=\mathbf{w}}|Z=z_0]|Z=z_0]$, Theorem 3.1 reduces to

$$
\mathbb{E}\Big[(Y_{X_{z_0}} - Y) - \mathfrak{g}(X, X_{z_0}, \mathbf{W}, g)\Big| Z = z\Big] = 0\tag{68}
$$

where $\mathfrak{g}(X, X_{z_0}, \mathbf{W}, g) =$ $\Omega_{\boldsymbol{W}}$ Z $\int_{\Omega_X} {\mathbb{1}_{X \le x, \mathbf{W} = \mathbf{w}} - \mathbb{1}_{X_{z_0} \le x, \mathbf{W} = \mathbf{w}} g(X, \mathbf{W}) dx d\mathbf{w}}$. We denote residual function $\rho(Y, Y_{X_{z_0}}, X, X_{z_0}, \mathbf{W}, g) = (Y_{X_{z_0}} - Y) - \mathfrak{g}(X, \mathbf{W}, g)$. Then, the integral equation can be represented by $\mathbb{E}[\rho(Y, \tilde{Y}_{X_{z_0}}^{\circ}, X, X_{z_0}, \tilde{\bm{W}}, g)|Z] = 0.$

Consistency of Sieve CAPCE Estimator. First, we show consistency without compactness restriction. The Sieve CAPCE estimator reduces to the general form of the conditional moment restrictions method, which is well-studied in [\[Newey and](#page-10-8) [Powell, 2003\]](#page-10-8), as below:

$$
\hat{g} = \arg\min_{g \in \mathcal{G}} \sum_{i=1}^{N} \frac{1}{N} \hat{\rho}(z_i, g)^2,
$$
\n(69)

where $\hat{\rho}(z_i, g) = \hat{c}_i - \hat{d}_i \beta$, and $\hat{\rho}(z_i, g)$ can be considered as the estimators of $\mathbb{E}[\rho(Y, Y_{X_{z_0}}, X, X_{z_0}, \mathbf{W}, g)|Z = z_i]$.

ASSUMPTIONS

We make the following consistency assumptions introduced in [\[Newey and Powell, 2003\]](#page-10-8). We denote $\mathcal{G}_S = \{g \in \mathcal{G} :$ $\|\mathfrak{g}_{0}(x,\boldsymbol{w})\|_{\tilde{W}^{l,2}}^{2} \leq B_{S}\},$ and $\overline{\mathcal{G}_{S}}$ is a closure of \mathcal{G}_{S} .

Assumption B.1 (Uniqueness of g). $g_0 \in \mathcal{G}_S$ is the only $g \in \mathcal{G}_S$ satisfying $\mathbb{E}[\rho(Y, Y_{X_{z_0}}, X, X_{z_0}, \mathbf{W}, g)|Z = z] = 0$.

Assumption B.2 (Completeness of Stage 1.). *Taking limits* $P \to \infty$, $N \to \infty$ *with* $P/N \to 0$ *, there exists* π_P *with* $\mathbb{E}[\{b(z) - \boldsymbol{q}(z)^T\boldsymbol{\pi}_P\}^2] \to 0$ for any $b(z)$ with $\mathbb{E}[b(z)^2] < \infty$.

The above assumption is for the completeness of parameter space used in Stage 1.

Assumption B.3 (Boundedness of ρ). $\mathbb{E}[\|\rho(Y, Y_{X_{z_0}}, X, X_{z_0}, \mathbf{W}, g)\|^2 |Z]$ *is bounded and there exists* $M(Y,Y_{X_{z_0}},X,X_{z_0},\boldsymbol{W}),\,\nu>0$ such that for all $\tilde g,g\in\mathcal{G}_S,\,\|\rho(Y,Y_{X_{z_0}},X,X_{z_0},\boldsymbol{W},\tilde g)-\rho(Y,Y_{X_{z_0}},X,X_{z_0},\boldsymbol{W},g)\|\leq$ $M(Y,Y_{X_{z_0}},X,X_{z_0},\boldsymbol{W})\|\tilde g-g\|_{W^{l,2}}^{\nu}$ and $\mathbb{E}[M(Y,Y_{X_{z_0}},X,X_{z_0},\boldsymbol{W})^2|Z]$ is bounded.

The above assumption is for the boundness of the parameters used in stage 2.

Let W denote the domain of $g(x, w, g)$.

Assumption B.4 (Openness and Convexness of Restricted Parameter Space). W *is open and convex.*

The following lemma is shown in [\[Newey and Powell, 2003\]](#page-10-8):

Lemma B.1. *If (i)* Θ *is a compact subset of a space with norm* $\|\theta\|$ *: (ii)* $\hat{Q}(\theta) \to_p Q(\theta)$ *for all* $\theta \in \Theta$ *: (iii) there is* $v > 0$ and $B_nO_p(1)$ such that for all $\tilde{\theta},\theta\in\Theta$, $|\hat{Q}(\theta)-\hat{Q}(\tilde{(\theta)})|\leq B_n\Delta^v=B_n\epsilon/2M\leq\epsilon/2$ with a positive probability, then $Q(\theta)$ *is continuous and* $\sup_{\theta \in \Theta} |\hat{Q}(\theta) - Q(\theta)| \rightarrow_{p} 0$.

Theorem [4.1.](#page-4-3) Under SCM M_{IV} and Assumptions [3.1,](#page-2-1) [3.2,](#page-2-2) [4.1,](#page-2-6) [4.2,](#page-2-4) [4.3,](#page-3-3) [B.1,](#page-16-1) [B.2,](#page-16-2) [B.3,](#page-17-0) and [B.4,](#page-17-1) letting $P \to \infty$ and $J \to \infty$, *then* $\|\hat{g} - g_0\|_{W^{l,\infty}} \stackrel{p}{\to} 0$.

Proof. From the Assumption [B.2](#page-16-2) and [B.4,](#page-17-1) the parameter space is compact subset. From the Assumption [B.3,](#page-17-0) the following relation is satisfied:

$$
|\rho(Y, Y_{X_{z_0}}, X, X_{z_0}, \boldsymbol{W}, \tilde{g}) - \rho(Y, Y_{X_{z_0}}, X, X_{z_0}, \boldsymbol{W}, g)|
$$
\n(70)

$$
\leq M(Y, Y_{X_{z_0}}, X, X_{z_0}, \mathbf{W}) \|\tilde{g} - g\|_{W^{l,2}}^{\nu}
$$
\n(71)

From the Lemma [B.1,](#page-17-3)

$$
\|\tilde{g} - g\|_{W^{l,\infty}} \to_p 0. \tag{72}
$$

 \Box

From Assumption [B.1,](#page-16-1) the limits of \tilde{g} is g_0 .

From the definition of $W^{l,\infty}$, this theorem means uniform convergence.

C RATE OF CONVERGENCE OF SIEVE CAPCE ESTIMATOR

NOTATIONS

In this section, we explain the notations used in the assumptions for Theorem 4.2 and Theorem 4.4. Denote the estimation problem

$$
\inf_{g \in \mathcal{G}} \mathbb{E}\left[\mathfrak{g}(X, X_{z_0}, \boldsymbol{W}, g)^2\right]
$$
\n(73)

and introduce norm $\|\cdot\|_A$ as below:

$$
||g_1 - g_0||_A = \sqrt{\mathbb{E}\left[\left(\frac{d\mathfrak{g}(X, X_{z_0}, \mathbf{W}, g_0)}{dg}\right)^2\right]}
$$
(74)

where

$$
\frac{d\rho(Z, g_0)}{dg}[g - g_0] = \frac{d\rho(Z, (1 - \tau)g_0 + \tau g)}{d\tau} \text{ a.s. } Z
$$
\n(75)

$$
\frac{d\rho(Z,g_0)}{dg}[g_1 - g_2] = \frac{d\rho(Z,g_0)}{dg}[g_1 - g_0] - \frac{d\rho(Z,g_0)}{dg}[g_2 - g_0]
$$
\n(76)

$$
\frac{d\mathfrak{g}(X, X_{z_0}, \mathbf{W}, g_0)}{dg} = \mathbb{E}\left[\frac{d\rho(Z, g_0)}{dg}[g_1 - g_2]\Big| \{X, X_{z_0}, \mathbf{W}\}\right].
$$
\n(77)

These derivatives are called "pathwise derivatives." See [\[Ai and Chen, 2003\]](#page-8-3) for details.

To evaluate the rate of convergence, we denote the number of the basis functions depending on sample size be J_N and P_N . Note that $N \to \infty$ implies $J_N \to \infty$ and $P_N \to \infty$. We use more basis functions, $q^{P_N} = (q^1, \dots, q^{P_N})$, as the sample size grows for the stage 1.

ASSUMPTIONS

We make the following assumptions.

Assumption C.1 (Compactness of Domain). $\Omega_{(X,X_{z_0}, W)}$ is compact with non empty interior.

Assumption C.2 (Order of Convergence of Stage 1). *For any* $h \in \mathcal{G}_S$ *with* $\kappa > (1 + d)/2$ *, there exists* $q^{P_N}(X,X_{z_0},W)^T\pi_{P_N} \in \mathcal{G}_S$, where π_{P_N} is P_N vector, such that $\sup_{(X,X_{z_0},W)\in\Omega_{(X,X_{z_0},W)}}|h(X,X_{z_0},W)|$ $q^{P_N}(X, X_{z_0}, W)^T \pi_{P_N} = \mathcal{O}(P_N^{-\kappa/(1+d)})$ and $P_N^{-\kappa/(1+d)} = o(N^{-1/4})$.

The above assumption guarantees the order of convergence of regression (basis functions) used in Stage 1.

Assumption C.3 (Order of Convergence of Stage 2). *There is a constant* $\mu_1 > 0$ *such that for any* $g \in \mathcal{G}$ *, there is* $\Pi g \in \mathcal{G}$ *satisfying* $\|\Pi g - g\| = \mathcal{O}(J_N^{-\kappa/(1+d)})$ *and* $J_N^{-\kappa/(1+d)} = o(N^{-1/4})$. Π *is the projections to* \mathcal{G} *.*

The above assumption guarantees the order of convergence of regression (basis functions) used in Stage 2.

Assumption C.4 (Envelope condition). *Each element of* $\rho(Z, g)$ *satisfies the envelope condition in* $g \in \mathcal{G}$ *; and, each element of* $\rho(Z, g) \in \mathcal{G}_S$ *with* $\kappa > (1 + d)/2$.

The envelope condition is shown in [\[Milgrom and Segal, 2002\]](#page-10-25).

Denote $\xi_N = \sup_{(X, X_{z_0}, \mathbf{W})} ||\boldsymbol{q}^{P_N}(X, X_{z_0}, \mathbf{W})||.$

Assumption C.5 (Condition of J_N). $J_N \times ln(N) \times \xi_N \times N^{-1/2} = o(1)$

We denote $N(\epsilon^{1/k}, \mathcal{G}, \| \cdot \|_{W^{l,2}})$ as the minimal number of radius δ covering ball of \mathcal{G} .

Assumption C.6 (Condition of J_N). $ln[N(\epsilon^{1/k}, \mathcal{G}, || \cdot ||_{W^{l,2}})] \le const. \times J_N \times ln(J_N/\epsilon)$

These assumptions show how to make the models complex depending on sample size.

Assumption C.7 (Convexness of Parameter Space). G *is convex in* g*, and* ρ(Z, g) *is pathwise differentiable at* g*; and, for some* $c_1, c_2 > 0$ *,*

$$
c_1 \mathbb{E}[\hat{\rho}(Z,g)^2] \le ||\hat{g} - g||^2 \le c_2 \mathbb{E}[\hat{\rho}(Z,g)^2]
$$
\n(78)

holds for all $\hat{g} \in \mathcal{G}$ *with* $\|\hat{g} - g\|_{W^{l,2}}^2 = o(1)$

The following lemma holds [\[Ai and Chen, 2003\]](#page-8-3):

Lemma C.1. *Under Assumptions* [C.1,](#page-18-0) [C.2,](#page-18-1) [C.3,](#page-18-2) [C.4,](#page-18-3) [C.5,](#page-18-4) [C.6,](#page-18-5) and [C.7,](#page-18-6) (i) $\hat{L}_N(g) - L_N(g) = o_p(N^{-1/4})$ *uniformly over* $g \in \mathcal{G}$; and (ii) $\hat{L}_N(g) - \hat{L}_N(g_0) - \{L_N(g) - L_N(g_0)\} = o_p(\tau_N N^{-1/4})$ *uniformly over* $g \in \mathcal{G}$ *with* $||g - g_0|| \le o(\tau_N)$ *, where* $\tau_N = N^{-\tau}$ *with* $\tau \leq 1/4$ *.*

Theorem [4.2.](#page-4-4) Under SCM M_{IV} and Assumptions [3.1,](#page-2-1) [3.2,](#page-2-2) [4.1,](#page-2-6) [4.2,](#page-2-4) [4.3,](#page-3-3) [C.1,](#page-18-0) [C.2,](#page-18-1) [C.3,](#page-18-2) [C.4,](#page-18-3) [C.5,](#page-18-4) [C.6,](#page-18-5) and [C.7,](#page-18-6) setting $N = N_1 = N_2$, then $\|\hat{g} - g_0\|_A = o_p(N^{-1/4})$.

Proof. Let

$$
\hat{L}_N(g) = -\frac{1}{2N}\hat{\mathfrak{g}}(X, X_{z_0}, \mathbf{W}.g)^2, \quad L_N(g) = -\frac{1}{2N}\mathfrak{g}(X, X_{z_0}, \mathbf{W}, g)^2.
$$
\n⁽⁷⁹⁾

Then, Lemma [C.1](#page-18-7) implies

$$
\hat{L}_N(g) - \hat{L}_N(g_0) - \{L_N(g) - L_N(g_0)\} = o_p(N^{-1/4})
$$
\n(80)

and this proves

$$
\|\hat{g} - g_0\| = o_p(N^{-1/4}).\tag{81}
$$

 \Box

D CONSISTENCY OF PARAMETRIC CAPCE ESTIMATOR

In this section, we show the consistency property of parametric CAPCE estimator. We denote the functional space G be ${g \in \mathcal{G} : g(x, \mathbf{w}) = \sum_{k=1}^K \gamma_k \theta_k(x, \mathbf{w})}.$

Consistency of Parametric CAPCE Estimator. First, we show consistency without compactness restriction. The Parametric CAPCE estimator reduces to the general form of the conditional moment restrictions method, which is well-studied in [\[Newey and Powell, 2003\]](#page-10-8), as below:

$$
\hat{\gamma} = \arg\min_{\gamma} \sum_{i=1}^{N} \frac{1}{N} \hat{\rho}(z_i, \gamma)^2,
$$
\n(82)

where $\hat{\rho}(z_i, \gamma) = \hat{c}_i - \hat{\mathbf{e}}_i \gamma$. $\hat{\rho}(z_i, \gamma)$ can be considered as the estimators of $\mathbb{E}[\rho(Y, Y_{X_{z_0}}, X, X_{z_0}, \mathbf{W}, \gamma)|Z = z_i]$.

ASSUMPTIONS

We make the following assumptions introduced in [\[Newey and Powell, 2003\]](#page-10-8). We denote $\mathcal{G}_P = \{\gamma^T\gamma \leq B_P\}$, and $\overline{\mathcal{G}_P}$ is the closure of \mathcal{G}_P .

Assumption D.1 (Uniqueness of g). $\gamma \in \mathcal{G}_P$ is the only $\gamma \in \mathcal{G}_P$ satisfying $\mathbb{E}[\rho(Y, Y_{X_{z_0}}, X, X_{z_0}, \mathbf{W}, \gamma)|Z = z] = 0$.

Assumption D.2 (Completeness of q). Taking limits $P \to \infty$, $N \to \infty$ with $P/N \to 0$, there exists π_P with $\mathbb{E}[\{b(z)$ $q(z)^T \overline{\pi}_P \}^2] \rightarrow 0$ for any $b(z)$ with $\mathbb{E}[b(z)^2] < \infty$.

Assumption D.3 (Boundedness of ρ). $\mathbb{E}[\|\rho(Y, Y_{X_{z_0}}, X, X_{z_0}, W, \gamma)\|^2 |Z]$ *is bounded and there exists* $M(Y,Y_{X_{z_0}},X,X_{z_0},\boldsymbol{W}),\,\nu>0$ such that for all $\tilde\gamma,\boldsymbol{\gamma}\in\overline{\mathcal{G}_P},\,\|\rho(Y,Y_{X_{z_0}},X,X_{z_0},\boldsymbol{W},\tilde\gamma)-\rho(Y,Y_{X_{z_0}},X,X_{z_0},\boldsymbol{W},g)\|\leq$ $M(Y,Y_{X_{z_0}},X,X_{z_0},\boldsymbol{W})\|\tilde{\boldsymbol{\gamma}}-\boldsymbol{\gamma}\|^{\nu}$ and $\mathbb{E}[M(Y,Y_{X_{z_0}},X,X_{z_0},\boldsymbol{W})^2|Z]$ is bounded.

Let W denote the domain of $g(x, w, \gamma)$.

Assumption D.4 (Openness and Convexness of Restricted Parameter Space). W *is open and convex.*

Theorem [4.3.](#page-5-2) Under SCM M_{IV} and Assumptions [3.1,](#page-2-1) [3.2,](#page-2-2) [4.4,](#page-4-1) [D.1,](#page-19-0) [D.2,](#page-19-1) [D.3,](#page-19-2) and [D.4,](#page-19-3) letting $P \to \infty$, then $\|\hat{\gamma} - \gamma\| \stackrel{p}{\to} 0$.

Proof. From the Assumption [D.2](#page-19-1) and [D.4,](#page-19-3) the parameter space is compact subset. From the Assumption [D.3,](#page-19-2) the following relation is satisfied:

$$
|\rho(Y, Y_{X_{z_0}}, X, X_{z_0}, \mathbf{W}, \tilde{\boldsymbol{\gamma}}) - \rho(Y, Y_{X_{z_0}}, X, X_{z_0}, \mathbf{W}, \boldsymbol{\gamma})|
$$
\n(83)

$$
\leq M(Y, Y_{X_{z_0}}, X, X_{z_0}, \mathbf{W}) \|\tilde{\boldsymbol{\gamma}} - \boldsymbol{\gamma}\|^{ \nu}
$$
\n(84)

From Lemma [B.1,](#page-17-3)

$$
\|\tilde{\gamma} - \gamma\| \to_p 0. \tag{85}
$$

From Assumption [D.1,](#page-19-0) the limits is γ_0 .

 \Box

E RATE OF CONVERGENCE OF PARAMETRIC CAPCE ESTIMATOR

ASSUMPTIONS

We make the following assumptions.

Assumption E.1 (Compactness of Domain). $\Omega_{(X,X_{z_0}, W)}$ is compact with non empty interior.

Assumption E.2 (Order of Convergence of Stage 1). For any $h \in \mathcal{G}_P$ with $\kappa > (1 + d)/2$, there exists $q^{P_N}(X,X_{z_0},W)^T\pi_{P_N} \in \mathcal{G}_P$, where π_{P_N} is P_N vector, such that $\sup_{(X,X_{z_0},W)\in\Omega_{(X,X_{z_0},W)}}|h(X,X_{z_0},W)|$ $q^{P_N}(X, X_{z_0}, W)^T \pi_{P_N} = \mathcal{O}(P_N^{-\kappa/(1+d)})$ and $P_N^{-\kappa/(1+d)} = o(N^{-1/4})$.

Assumption E.3 (Order of Convergence of Stage 2). *There is a constant* $\mu_1 > 0$ *such that for any* $\gamma \in \mathcal{G}_P$ *, there is* $\Pi \gamma \in \mathcal{G}_P$ *satisfying* $\|\Pi \gamma - \gamma\| = \mathcal{O}(1)$ *.*

Assumption E.4 (Envelope condition). *Each element of* $\rho(Z, \gamma)$ *satisfies the envelope condition in* $\gamma \in \mathcal{G}_P$ *; and, each element of* $\rho(Z, \gamma) \in \mathcal{G}_P$ *with* $\kappa > (1 + d)/2$ *, for all* $\gamma \in \mathcal{G}_P$ *.*

The envelope condition is shown in [\[Milgrom and Segal, 2002\]](#page-10-25).

Assumption E.5 (Convexness of Parameter Space). \mathcal{G}_P *is convex in* γ *, and* $\rho(Z, \gamma)$ *is pathwise differentiable at* γ *; and, for some* $c_1, c_2 > 0$ *,*

$$
c_1 \mathbb{E}[\hat{\rho}(Z,\gamma)^2] \le ||\hat{\gamma} - \gamma||^2 \le c_2 \mathbb{E}[\hat{\rho}(Z,\gamma)^2]
$$
\n(86)

holds for all $\hat{\gamma} \in \mathcal{G}_P$ *with* $\|\hat{\gamma} - \gamma\|^2 = o(1)$

The following lemma holds [\[Ai and Chen, 2003\]](#page-8-3):

Lemma E.1. *Under Assumptions [E.1,](#page-20-0) [E.2,](#page-20-1) [E.3,](#page-20-2) [E.4,](#page-20-3) and [E.5,](#page-20-4) (i)* $\hat{L}_N(\gamma) - L_N(\gamma) = o_p(N^{-1/4})$ *uniformly over* γ *; and (ii)* $\hat{L}_N(\boldsymbol{\gamma}) - \hat{L}_N(\boldsymbol{\gamma}_0) - \{L_N(\boldsymbol{\gamma}) - L_N(\boldsymbol{\gamma}_0)\} = o_p(\tau_N N^{-1/4})$ *uniformly over* $\boldsymbol{\gamma}$ *with* $\|\boldsymbol{\gamma} - \boldsymbol{\gamma}_0\| \leq o(\tau_N)$ *, where* $\tau_N = N^{-\tau}$ *with* $\tau \leq 1/4$ *.*

Theorem [4.4.](#page-5-3) *Under SCM* M_{IV} *and Assumptions [3.1,](#page-2-1) [3.2,](#page-2-2) [4.4,](#page-4-1) [E.1,](#page-20-0) [E.2,](#page-20-1) [E.3,](#page-20-2) [E.4,](#page-20-3) and [E.5,](#page-20-4) setting* $N = N_1 = N_2$, then $\|\hat{\gamma} - \gamma\| = o_p(N^{-1/4}).$

Proof. Let

$$
\hat{L}_N(\gamma) = -\frac{1}{2N}\hat{\mathfrak{g}}(X, X_{z_0}, \mathbf{W}, \gamma)^2, \quad L_N(g) = -\frac{1}{2N}\mathfrak{g}(X, X_{z_0}, \mathbf{W}, \gamma)^2.
$$
 (87)

Then, Lemma [E.1](#page-20-7) implies

$$
\hat{L}_N(\gamma) - \hat{L}_N(\gamma_0) - \{L_N(\gamma) - L_N(\gamma_0)\} = o_p(N^{-1/4})
$$
\n(88)

and this proves

$$
\|\hat{\gamma} - \gamma_0\| = o_p(N^{-1/4}).\tag{89}
$$

 \Box

F PROPERTIES OF RKHS CAPCE ESTIMATOR

We show the consistency and rate of convergence of RKHS CAPCE estimator following [\[Singh et al., 2019\]](#page-10-9) when λ_3 is 0.

NOTATIONS

We use the integral operator notations from the kernel methods literature. $\mathcal{L}_2(\Omega_Z, \mathfrak{p}_Z)$ denotes a \mathcal{L}_2 integrable function from Ω_Z to Ω_Y with respect to measure \mathfrak{p}_Z .

Definition 2. *The stage 1 operators are*

$$
S_1^* : \mathcal{H}_Z \to \mathcal{L}_2(\Omega_Z, \mathfrak{p}_Z), l \mapsto \langle l, \psi(\cdot) \rangle_{\mathcal{H}_Z}
$$
\n
$$
(90)
$$

$$
S_1: \mathcal{L}_2(\Omega_Z, \mathfrak{p}_Z) \to \mathcal{H}_Z, \tilde{l} \mapsto \int \psi(z)\tilde{l}(z)\mathfrak{p}_Z(z)dz \tag{91}
$$

and $T_1 = S_1^* \circ S_1$ is the uncentered covariance operator. The details of the theory of vector-valued RKHS are shown in *[\[Singh et al., 2019\]](#page-10-9).*

In addition, we denote

Definition 3.

$$
G_{1\rho} = \arg\min \mathcal{E}_1(E), \mathcal{E}_1 = \mathbb{E}[\pi(X, \mathbf{W}) - G_1(\psi(Z))]^2_{\mathcal{H}_{X, \mathbf{W}}},\tag{92}
$$

$$
G_{1\lambda} = \arg\min \mathcal{E}_1(G_1), \mathcal{E}_1 = \mathbb{E}[\pi(X, \mathbf{W}) - G_1(\psi(Z))]_{\mathcal{H}_{X, \mathbf{W}}}^2 + \lambda \|G_1\|_{\mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_{X, \mathbf{W}})}^2,
$$
\n(93)

$$
\hat{G}_{1\lambda} = \arg\min \mathcal{E}_1(G_1), \mathcal{E}_1 = \hat{\mathbb{E}}[\pi(X, \mathbf{W}) - G_1(\psi(Z))]_{\mathcal{H}_{X,\mathbf{W}}}^2 + \lambda \|G_1\|_{\mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_{X,\mathbf{W}})}^2,
$$
\n(94)

$$
G_{2\rho} = \arg\min \mathcal{E}_1(E), \mathcal{E}_1 = \mathbb{E}[Y - G_2(\psi(Z))]^2,
$$
\n
$$
(95)
$$

$$
G_{2\lambda} = \arg\min \mathcal{E}_1(G_2), \mathcal{E}_1 = \mathbb{E}[Y - G_2(\psi(Z))]^2 + \lambda \|G_2\|_{\mathcal{L}_2(\mathcal{H}_Z, \Omega_Y)}^2,
$$
\n(96)

$$
\hat{G}_{2\lambda} = \arg\min \mathcal{E}_1(G_2), \mathcal{E}_1 = \hat{\mathbb{E}}[Y - G_2(\psi(Z))]^2 + \lambda \|G_2\|_{\mathcal{L}_2(\mathcal{H}_Z, \Omega_Y)}^2.
$$
\n
$$
(97)
$$

Definition 4. *The stage 2 operators are*

$$
S_2^* : \mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_{X,W}) \to \mathcal{L}_2(\mathcal{H}_{X,W}, \mathfrak{p}_{\mathcal{H}_{X,W}}), H \mapsto \Omega_{(\cdot)}^* H
$$
\n(98)

$$
S_2: \mathcal{L}_2(\mathcal{H}_{X,W}, \mathfrak{p}_{\mathcal{H}_{X,W}}) \to \mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_{X,W}),
$$
\n(99)

$$
\tilde{H} \mapsto \int \Omega_{\mu(z) - \mu(z_0)} \circ \tilde{H} \{ \mu(z) - \mu(z_0) \} \mathfrak{p}_{\mathcal{H}_{X,\mathbf{W}}}(\mu(z)) \tag{100}
$$

and $T_2 = S_2^* \circ S_2$ *is the uncentered covariance operator.*

Definition 5. *We denote*

$$
H_{\rho} = \arg \min \mathcal{E}(H), \mathcal{E}(H) = \mathbb{E}[Y - \mu_2(z_0) - H(\mu(Z) - \mu(z_0))]^2_{\mathcal{H}_{X,\mathbf{W}}},\tag{101}
$$

$$
H_{\xi} = \arg\min \mathcal{E}_{\xi}(H),\tag{102}
$$

$$
\mathcal{E}(H) = \mathbb{E}[Y - \mu_2(z_0) - H(\mu(Z) - \mu(z_0))]_{\mathcal{H}_{X,\mathbf{W}}}^2 + \xi \|H\|_{\mathcal{L}_2(\mathcal{H}_{X,\mathbf{W}},\Omega_Y)}^2,
$$
(103)

$$
\hat{H}_{\xi} = \arg\min \hat{\mathcal{E}}_{\xi}(H),\tag{104}
$$
\n
$$
\hat{\mathcal{E}}_{\xi}(H) = \hat{\mathcal{E}}_{\xi}(H) \quad (105)
$$

$$
\hat{\mathcal{E}}(H) = \hat{\mathbb{E}}[Y - \mu_2(z_0) - H(\mu(Z) - \mu(z_0))]_{\mathcal{H}_{X,\mathbf{W}}}^2 + \xi \|H\|_{\mathcal{L}_2(\mathcal{H}_{X,\mathbf{W}},\Omega_Y)}^2.
$$
\n(105)

ASSUMPTIONS

Next, we show assumptions for Theorem [4.5.](#page-6-1)

Assumption F.1 (Restriction for the domains). *Suppose that* Ω_X *w* and Ω_Z are Polish spaces, i.e., separable and completely *metrizable topological spaces.*

Assumption F.2 (Restriction for the feature functions). *Suppose that*

- *1.* $k_{X,W}$ and $k_{\mathbf{Z}}$ are continuous and bounded: $\sup_{x \in \Omega_{X,W}} ||\pi(x, \mathbf{w})||_{\mathcal{H}_{X,W}} \leq Q$ and $\sup_{z \in \Omega_{Z}} ||\psi(z)||_{\mathcal{H}_{\mathbf{Z}}} \leq \kappa$.
- *2.* π *and* ψ *are measurable.*
- *3.* kX,^W *is characteristic.*

Assumption F.3 (Uniqueness). Suppose that $G_{1\rho} \in \mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_Z)$, then $\mathcal{E}_1(G_{1\rho}) = \inf_{G_1 \in \mathcal{H}_Z} \mathcal{E}_1(G_1)$. Furthermore, *suppose that* $G_{2\rho} \in \mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_Z)$ *, then* $\mathcal{E}_1(G_{2\rho}) = \inf_{G_2 \in \mathcal{H}_Z} \mathcal{E}_1(G_2)$ *.*

Assumption F.4 (Boundness of stage 1). *Fix* $\zeta_1, \zeta_2 \leq \infty$ *. For given* $c_1, c_2 \in (1, 2]$ *, define the prior* $\mathcal{P}(\zeta_1, c_1)$ *and* $\mathcal{P}(\zeta_2,c_2)$ *as the set of the probability distributions on* $\Omega_{X,\mathbf{W}} \times \Omega_Z$ *such that a range space assumption is satisfied:* $\exists C_1 \in \mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_{X, W})$ such that $G_{1\rho} = T_1^{\frac{c_1-1}{2}} \circ C_1$ and $\|C_1\|^2_{\mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_{X, W})} \leq \zeta_1$, and $\exists C_2 \in \mathcal{L}_2(\mathcal{H}_Z, \Omega_Y)$ such that $G_{2\rho} = T_1^{\frac{c_2-1}{2}} \circ C_2$ and $||C_2||^2_{\mathcal{L}_2(\mathcal{H}_Z,\Omega_Y)} \leq \zeta_2$.

Lemma F.1 (Rate of convergence of stage 1 (A)). *Make Assumptions [F.1,](#page-22-0) [F.2,](#page-22-1) [F.3](#page-22-2) and [F.4.](#page-22-3) For all* $\delta \in (0,1)$ *, the following holds w.p.* $1 - \delta$ *:*

$$
\begin{split} \|\hat{G}_{1\lambda} - G_{1\rho}\|_{\mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_X, \mathbf{w})} \\ &\leq \frac{\sqrt{\zeta_1}(c_1 + 1)}{4^{\frac{1}{c_1 + 1}}} \left(\frac{4\kappa(Q + \kappa \|G_{1\rho}\|_{\mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_X, \mathbf{w})})ln(2/\delta)}{\sqrt{n\zeta_1}(c_1 - 1)} \right) \end{split} \tag{106}
$$

Lemma F.2 (Rate of convergence of stage 1 (B)). *Make Assumptions [F.1,](#page-22-0) [F.2,](#page-22-1) [F.3](#page-22-2) and [F.4.](#page-22-3) For all* $\delta \in (0,1)$ *, the following holds w.p.* $1 - \delta$ *:*

$$
\|\hat{G}_{2\lambda} - G_{2\rho}\|_{\mathcal{L}_2(\mathcal{H}_Z, \Omega_Z)}\n\leq \frac{\sqrt{\zeta_2}(c_2 + 1)}{4^{\frac{1}{c_2 + 1}}} \left(\frac{4\kappa (Q + \kappa \|G_{2\rho}\|_{\mathcal{L}_2(\mathcal{H}_Z, \Omega_Z)}) ln(2/\delta)}{\sqrt{n\zeta_2}(c_2 - 1)} \right)
$$
\n(107)

The proof is shown in [\[Singh et al., 2019\]](#page-10-9). The above lemma implies consistency of Stage 1 (A).

Assumption F.5 (Restriction of domain). *Suppose that* Ω_Y *is a Polish space, i.e., separable and completely metrizable topological spaces.*

Assumption F.6 (Boundness of stage 2). *Suppose that*

- *1. The* ${\Psi_{\mu(z) \mu(z_0)} }$ *operator family is uniformly bounded in Hilbert-Schmidt norm:* $\exists B$ *such that* $\forall \mu(z)$ *,* $\|\Psi_{\mu(z)-\mu(z_0)}\|_{\mathcal{L}_2(\Omega_Z, \mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_X, \mathbf{w}))}^2 = Tr(\Psi^*_{\mu(z)-\mu(z_0)} \circ \Psi_{\mu(z)-\mu(z_0)}) \leq B.$
- *2. The* $\{\Psi_{\mu(z)-\mu(z_0)}\}$ *operator family is Hölder continuous in operator norm:* $\exists L > 0, \iota \in (0,1]$ *such that* $\forall \mu(z), \mu(z')$, $\|\Psi_{\mu(z)-\mu(z_0)} - \Psi_{\mu(z')-\mu(z_0)}\|_{L(\Omega_Z, \mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_{X, W}))} \leq L \|\mu(z) - \mu(z')\|_{\mathcal{H}_{X, W}}^{\ell}.$

Assumption F.7 (Boundness of stage 2). *Suppose that*

- *1.* $\langle H_{\rho}, \cdot \rangle \in \mathcal{L}_2(\mathcal{H}_{X,W}, \Omega_Y)$ *. Then,* $\mathcal{E}(H_{\rho}) = \inf_{H \in \mathcal{H}_{X,W}} \mathcal{E}(H)$ *.*
- 2. *Y is bounded, i.e.* $\exists C < \infty$ *such that* $||Y|| \leq C$ *almost surely.*

Assumption F.8 (Boundness of stage 2). *Fix* $\zeta < \infty$ *. For given* $b \in (1, \infty]$ *and* $c \in (1, 2]$ *, define the prior* $\mathcal{P}(\zeta, b, c)$ *as the set of probability distributions* \mathfrak{p} *on* $\mathcal{H}_{X,\mathbf{W}} \times \Omega_Y$ *such that*

I. *A range space assumption is satisfied:* $\exists C \in \mathcal{L}_2(\mathcal{H}_{X,\mathbf{W}}, \Omega_Y)$ *such that* $H_\rho = T_2^{\frac{c-1}{2}} \circ C$ and $||C||^2_{\mathcal{L}_2(\mathcal{H}_{X,\mathbf{W}}, \Omega_Y)} \leq \zeta$.

2. In the spectral decomposition $T = \sum_{k=1}^{\infty} \lambda_k e_k \langle \cdot, e_k \rangle_{\mathcal{H}_{X,\mathbf{W}}}$, where $\{e_k\}_{k=1}^{\infty}$ is a basis of $Ker(T)^{\perp}$, the eigenvalues *satisfies* $\alpha \leq k^b \lambda_k \leq \beta$ *for some* $\alpha, \beta > 0$ *.*

These assumptions are for the boundness of Stage 2.

Lemma F.3. Make Assumptions [F.1,](#page-22-0) [F.2,](#page-22-1) [F.3,](#page-22-2) [F.4,](#page-22-3) [F.5,](#page-22-4) [F.6,](#page-22-5) [F.7](#page-22-6) and [F.8.](#page-22-7) Let $\lambda = N_1^{-\frac{1}{c_1+1}}$, $N_1 = N_2^{\frac{a(c_1+1)}{c(c_1-1)}}$, $a > 0$, and $\lambda_3 = 0$ *. We have*

1. if $a \leq \frac{b(c+1)}{bc+1}$ *then* $\mathcal{E}(\hat{H}_{\xi}) - \mathcal{E}(H_{\rho}) = \mathcal{O}_p(N_2^{-\frac{ac}{c+1}})$ *with* $\xi = N_2^{-\frac{a}{c+1}}$ *.* 2. *if* $a \ge \frac{b(c+1)}{bc+1}$ *then* $\mathcal{E}(\hat{H}_{\xi}) - \mathcal{E}(H_{\rho}) = \mathcal{O}_p(N_2^{-\frac{bc}{bc+1}})$ *with* $\xi = N_2^{-\frac{b}{bc+1}}$.

Lemma [F.3](#page-23-1) can be proved from the proof of Theorem 4 in [\[Singh et al., 2019\]](#page-10-9) by subsituting $\mu(z)$ with $\mu(z) - \mu(z_0)$.

Theorem [4.5.](#page-6-1) *Under SCM* MIV *and Assumptions [3.1,](#page-2-1) [3.2,](#page-2-2) [F.1,](#page-22-0) [F.2,](#page-22-1) [F.3,](#page-22-2) [F.4,](#page-22-3) [F.5,](#page-22-4) [F.6,](#page-22-5) [F.7](#page-22-6) and [F.8,](#page-22-7) the RKHS CAPCE estimator in (25) converges pointwise to CAPCE when* $\lambda_3 = 0$ *.*

Proof. Lemma [F.3](#page-23-1) implies consistency of RKHS CAPCE estimator by taking limit $N_2 \to \infty$.

\Box

G ADDITIONAL INFORMATION ON EXPERIMENTS AND THE APPLICATION

In this section, we give detailed information about the settings of the experiments and additional experimental results.

We note that the choice of the reference point z_0 does not affect the consistency results or rate of convergence, but it may affect the variance of the estimator. In our experiments, we take the minimum value of Z as a standard reference point z_0 . The choice of the reference point z_0 did not affect the standard deviation of the estimators much in our experiments.

G.1 DETAILED SETTINGS OF EXPERIMENTS

We present detailed settings of numerical experiments in the following.

Setting of P-CAPCE and PTSLS. We learn the conditional expectations of basis functions $\mathbb{E}[Y|Z=z]$, $\mathbb{E}[X|Z=z]$, $\mathbb{E}[WX|Z=z]$ and $\mathbb{E}[X^2|Z=z]$ by the nonlinear model, $b_0 + b_1Z + b_2Z^2$. We used the basis terms $\{1, W, X\}$ for P-CAPCE and $\{1, W, X, W X, X^2\}$ for PTSLS, which match setting (A), and let $z_0 = -1$. Regularize value is determined by test error from $\{1, 10^{-1}, 10^{-2}, 10^{-3}\}.$

Setting of NTSLS and sieve CAPCE. We learn the conditional expectations by the nonlinear model, $b_0+b_1Z+b_2Z^2+b_3Z^3$, We consider the basis terms $h_p(X)h_q(W)$ for $p = 0, 1, 2$ and $q = 0, 1, 2$, where h_p is Hermite polynomial functions $(h_0(t) = 1, h_1(t) = t, h_2(t) = t^2 - 1$ and $h_3(t) = t^3 - 3t$, and let $z_0 = -1$. Let $\kappa = 2$ and $l = 1$, and we calculate $\hat{\Lambda}$ by Monte Carlo integration using uniform distribution $(x, w) = (U(-4, 4), U(-2, 2))$, where $\Omega_X \subseteq [-4, 4]$ and $\Omega_X \subseteq [-2, 2]$. Regularize value is determined by test error from $\{1, 10^{-1}, 10^{-2}, 10^{-3}\}$. We estimate CAPCE via differentiating estimated $\mathbb{E}[Y_x|W=w].$

Setting of kernel IV and RKHS CAPCE estimator. We use polynomial kernel function $k_Z(z, z') = (z^T z' + C_1)^{C_2}$ and $k_{X,W}((x,w)(x,w)^T + C_3)^{C_4}$. We select the kernel parameters (C_1, C_2) and (C_3, C_4) from $\{1, 2, 3, 4, 5\} \times \{1, 2, 3, 4, 5\}$, respectively. We select the regularize values λ_1 and λ_2 from $\{1, 10^{-1}, 10^{-2}, 10^{-3}\}$, respectively, and (λ_3, ξ) is from Cartesian product set $\{100, 10, 1\} \times \{100, 10, 1\}.$

G.2 ADDITIONAL INFORMATION ON EXPERIMENTAL RESULTS IN THE BODY OF PAPER

Results: Parametric setting (A). The basic statistics of estimated coefficients by 100 time simulations of PTSLS and P-CAPCE are shown in Tables [3](#page-24-0) and [4.](#page-24-1) These tables supplement Table 1 in the paper. The true and estimated CAPCE surfaces over (X, W) are shown in Fig. [4.](#page-24-2)

Results: Nonparametric setting (B). The true and estimated CAPCE surfaces over (X, W) are shown in Fig. [5.](#page-25-0)

Figure 4: Parametric estimated surfaces in setting (A) (Mean, $N = 10000$). X-axis is the value of treatment variable $(X = x)$, Y-axis is the value of covariate $(W = w)$, and Z-axis is the value of CAPCE.

$N = 1000$		W	X
True Coeff.			20
Min.	-51.515	-18.715	-116.480
1st Qu.	-10.044	0.160	-10.809
Median	-1.849	3.035	17.691
3rd Qu.	7.926	12.239	50.007
Max.	40.458	109.791	213.306
Mean	-1.651	10.383	19.293
SD	14.707	22.309	50.957

Table 3: Basic statistics of the P-CAPCE estimator over 1000 runs when $N = 1000$ and $N = 10000$ in setting (A).

Table 4: Basic statistics of the PTSLS over 1000 runs when $N = 1000$ and $N = 10000$ in setting (A).

$N = 1000$		W	\boldsymbol{X}		$N = 10000$			W
True Coeff.			20		True Coeff.			
Min.	-33.368	2.971	-113.509	Min.		-12.117	30.794	
1st Ou.	-4.258	28.662	0.518	1st Ou.		-2.336	45.907	
Median	2.785	45.497	28.629	Median		1.704	50.716	
3rd Ou.	7.617	62.155	61.569	3rd Ou.		4.494	57.017	
Max.	26.799	161.738	138.283	Max.		8.952	78.573	
Mean	1.248	50.032	27.862	Mean		1.101	51.181	
SD	11.374	29.523	46.388	SD		4.638	8.814	

G.3 ADDITIONAL EXPERIMENTS: NO INTERACTION BETWEEN COVARIATES AND UNOBSERVED **CONFOUNDERS**

In this section, we give additional experiments with no interaction between covariates and unobserved confounders. **SCM Settings.** We consider the following two SCMs: $W := H + E_1, X := Z + W + H + E_2$, and

$$
\begin{cases}\nY := 10X^2 + WX + X + W + 50H + E_3 & \cdots \text{ (C)} \\
Y := \exp(X)\exp(W) + 50H + E_3 & \cdots \text{ (D)}\n\end{cases} (108)
$$

Figure 5: Nonparametric estimated surfaces in setting (B) (Mean, $N = 10000$). X-axis is the value of treatment variable $(X = x)$, Y-axis is the value of covariate $(W = w)$, and Z-axis is the value of CAPCE.

The other settings of each estimator are the same as in setting (A) and (B).

Results. The basic statistics of estimated coefficients by 100 time simulations of PTSLS and P-CAPCE in setting (C) are shown in Tables [5](#page-26-0) and [6.](#page-26-1) The MSE of each estimator in settings (C) and (D) are shown in Table [7.](#page-26-2) The results show that the performance of the previous works PTSLS, NTSLS, Kernel IV is comparable with our proposed methods under the settings where the interaction between the covariates W and unobserved confounders H is absent.

$N = 1000$		W	\boldsymbol{X}
True Coeff.			20
Min.	-4.419	-38.895	-21.176
1st Qu.	0.896	0.351	19.614
Median	0.983	1.361	19.919
3rd Qu.	1.065	2.620	20.246
Max.	6.066	19.864	41.021
Mean	0.944	1.151	19.642
SD	0.811	5.535	4.884

Table 5: Basic statistics of the P-CAPCE estimator over 1000 runs when $N = 1000$ and $N = 10000$ in setting (C).

Table 6: Basic statistics of the PTSLS over 1000 runs when $N = 1000$ and $N = 10000$ in setting (C).

$N = 1000$	1	W	\boldsymbol{X}
True Coeff.	1		20
Min.	0.350	-2.045	15.831
1st Qu.	0.957	-0.199	19.303
Median	1.021	1.009	19.731
3rd Qu.	1.101	1.921	19.953
Max.	1.456	5.165	20.260
Mean	1.029	0.997	19.474
SD	0.155	1.609	0.782

$N = 10000$	$\mathbf{1}$	W	\boldsymbol{X}
True Coeff.	1	1	20
Min.	0.904	-1.251	19.501
1st Qu.	0.986	0.515	19.905
Median	1.003	0.962	19.963
3rd Qu.	1.021	1.407	20.019
Max.	1.074	3.148	20.120
Mean	1.003	0.939	19.939
SD	0.028	0.814	0.118

Table 7: MSE of estimators in settings (C) and (D).

G.4 ADDITIONAL EXPERIMENTS: WEAKER INTERACTION BETWEEN COVARIATES AND UNOBSERVED CONFOUNDERS

In this section, we give additional experiments with weak interaction between covariates and unobserved confounders.

SCM Settings. We consider the following two SCMs: $W := H + E_1, X := Z + W + H + E_2$, and

$$
\begin{cases}\nY := 10X^2 + WX + X + W + 10(W^5 + W^4 + W^3 + W^2)H + E_3 \cdots (E) \\
Y := \exp(X)\exp(W) + 5(W^5 + W^4 + W^3 + W^2)H + E_3 \cdots (F)\n\end{cases} (109)
$$

The other settings of each estimator are the same as in setting (A) and (B).

Results. The basic statistics of estimated coefficients by 100 time simulations of PTSLS and P-CAPCE in setting (E) are shown in Tables [8](#page-27-1) and [9.](#page-27-2) The MSE of estimators in settings (E) and (F) are shown in Table [10.](#page-27-3) The results show that our methods are superior to the previous works PTSLS, NTSLS, Kernel IV while the performance differences are less than that in the settings (A) and (B) where the interaction between covariates and unobserved confounders are stronger.

$N = 1000$		W	X
True Coeff.			20
Min.	-2.056	-9.914	-6.174
1st Qu.	-0.103	-0.589	11.002
Median	0.848	1.996	15.528
3rd Ou.	1.898	6.510	29.150
Max.	2.047	3.502	25.181
Mean	1.185	1.765	18.248
SD	2.416	5.991	14.165

Table 8: Basic statistics of the P-CAPCE estimator over 1000 runs when $N = 1000$ and $N = 10000$ in setting (E).

Table 9: Basic statistics of the PTSLS over 1000 runs when $N = 1000$ and $N = 10000$ in setting (E).

Min. -1.072 7.402 11.514 0.394 9.613 17.370 Median 0.957 10.748 19.355 1.446 11.977 21.967 2.684 15.641 26.645 0.934 10.883 19.459 SD 0.778 1.687 3.478

X W $N = 1000$ $N = 10000$ 20 True Coeff. True Coeff. Min. -3.732 Min. -5.345 -1.064 14.958 -0.074 9.187 1st Qu. 1st Qu. Median Median 1.195 10.862 20.450 13.322 24.988 3rd Qu. 3rd Qu. 2.667 Max. Max. 37.757 5.766 34.620 Mean Mean 1.195 10.862 20.450 SD 8.597 SD 2.161 5.437		
-1.072		
0.394		
0.957		
1.446 2.684 0.934 0.778		

Table 10: MSE of estimators in settings (E) and (F).

G.5 ADDITIONAL EXPERIMENTS: ESTIMATION BASED ON THEOREM 3.1'.

In this section, we give additional experiments about estimating CAPCE in the settings (A) and (B) in Eq. [\(29\)](#page-6-0) based on Theorem 3.1' in Appendix [A.2.](#page-13-0) P-CAPCE', S-CAPCE', and RKHS CAPCE' estimate CAPCE based on Theorem 3.1'. We present detailed settings of numerical experiments in the following.

Setting of P-CAPCE'. We learn the conditional expectations of basis functions $\mathbb{E}[Y|Z=z, W=w], \mathbb{E}[X|Z=z, W=w]$, $\mathbb{E}[WX|Z=z, W=w]$ and $\mathbb{E}[X^2|Z=z, W=w]$ by the nonlinear model, $b_0 + b_1Z + b_2Z^2$. We used the basis terms $\{1, X, X^2\}$ for P-CAPCE' and $\{1, X\}$ for PTSLS, which match setting (A), and let $z_0 = -1$ and $w = 1$. Regularize value is determined by test error from $\{1, 10^{-1}, 10^{-2}, 10^{-3}\}.$

Setting of S-CAPCE'. We learn the conditional expectations by the nonlinear model, $b_0 + b_1 Z + b_2 Z^2 + b_3 Z^3 + b_4 W +$ $b_5W^2 + b_6W^3$, We consider the basis terms $h_p(X)$ for $p = 0, 1, 2$, where h_p is Hermite polynomial functions $(h_0(t) = 1, 1)$

 $h_1(t) = t$, $h_2(t) = t^2 - 1$ and $h_3(t) = t^3 - 3t$), and let $z_0 = -1$ and $w = 1$. Let $\kappa = 2$ and $l = 1$, and we calculate $\hat{\Lambda}$ by Monte Carlo integration using uniform distribution $x \sim U(-4, 4)$, where $\Omega_X \subseteq [-4, 4]$. Regularize value is determined by test error from $\{1, 10^{-1}, 10^{-2}, 10^{-3}\}$. We estimate CAPCE via differentiating estimated $\mathbb{E}[Y_x|W=w]$.

Setting of RKHS CAPCE' estimator. We use polynomial kernel function $k_{Z,W}((z,w)(z,w)^T + C_1)^{C_2}$ and $k_X(x,x') =$ $(xx' + C_3)^{C_4}$. We select the kernel parameters (C_1, C_2) and (C_3, C_4) from $\{1, 2, 3, 4, 5\} \times \{1, 2, 3, 4, 5\}$, respectively. We select the regularize values λ_1 and λ_2 from $\{1, 10^{-1}, 10^{-2}, 10^{-3}\}$, respectively, and (λ_3, ξ) is from Cartesian product set $\{100, 10, 1\} \times \{100, 10, 1\}.$

Results. The MSEs of P-CAPCE, S-CAPCE, RKHS CAPCE, P-CAPCE', S-CAPCE', and RKHS CAPCE' in settings (A) and (B) for $w = 1$ are shown in Table [11.](#page-28-0) The results show that estimators based on Theorem 3.1 and 3.1' have very similar performance.

MSE	P-CAPCE		S-CAPCE RKHS CAPCE P-CAPCE'		S-CAPCE'	RKHS CAPCE'
(A) $N = 1000$	453.233	225.301	339.091	132.167	399.446	193.306
(A) $N = 10000$	98.885	220.358	164.798	91.5647	275.907	153.689
(B) $N = 1000$	284.598	14.398	30.562	129.721	11.780	28.266
(B) $N = 10000$	52.217	5.189	3.475	63.302	5.726	3.194

Table 11: MSE of each estimator based on Theorem 3.1 and 3.1' in settings (A) and (B) for $w = 1$.

G.6 ADDITIONAL INFORMATION ON THE APPLICATION

We present detailed settings of the application in Section 6. We applied P-CAPCE and PTSLS. We learn the expected values of basis functions by the nonlinear model, $\beta_0 + \beta_1 Z + \beta_2 Z^2$. We use terms $\{1, W, W^2, X, XW, XW^2\}$ for P-CAPCE and $\{1, W, W^2, X, XW, XW^2, X^2, X^2W, X^2W^2\}$ for PTSLS, and let $z_0 = 8$. We estimate CAPCE via differentiating estimated $\mathbb{E}[Y_x|w]$ for PTSLS. Regularize parameter is determined by test error from $\{1, 10^{-1}, 10^{-2}, 10^{-3}, \ldots\}$.

Results. The basic bootstrapping statistical properties of the P-CAPCE and PTSLS estimators are shown in Tables [12](#page-28-1) and [13.](#page-28-2) The predicted CAPCE values are shown in Tables [14](#page-30-0) and [15.](#page-30-1) The estimated CAPCE surfaces are shown in Fig. [6.](#page-29-0)

Table 12: Basic statistics of the P-CAPCE estimator over 1000 bootstrapping.

Terms		W	W^2	X	WX	$W^2 X$
Min.	-0.00267	-0.00003	-0.00126	-0.00006	-0.00084	-0.00237
1st Ou.	-0.00061	0.00002	0.00510	-0.00001	-0.00029	-0.00099
Median	-0.00006	0.00004	0.00904	-0.00001	-0.00016	-0.00053
3rd Qu.	0.00058	0.00007	0.01331	0.00000	-0.00008	-0.00017
Max.	0.00226	0.00018	0.02786	0.00004	0.00059	0.00068
Mean	-0.00003	0.00005	0.00949	-0.00001	-0.00018	-0.00056
SD	0.00090	0.00004	0.00602	0.00001	0.00018	0.00062

Table 13: Basic statistics of the PTSLS estimator over 1000 bootstrapping.

Figure 6: Bootstrap mean surface of each estimator. X-axis is years of education, Y-axis is IQ, and Z-axis is CAPCE.

			99.079 86.350 86.3623 73.435 9.978 9.751 2.751					15.480
	7.384		86.294 75.204 64.114 64.114 53.024 41.934 90.844 90.845				-2.425	-13.515
130	3.955		74.391 64.827 55.263 56.572 36.572 36.572 7.444				2.120	11.684
$\overline{20}$			$\begin{array}{l} 63.372\\ 55.221\\ 55.271\\ 47.070\\ 38.919\\ 30.768\\ 22.618\\ 14.467\\ 16.316 \end{array}$				1.835	9.986
	980°C		53.235 46.384 46.334 32.683 35.832 5.380 1.570					8.421
\approx			$\begin{array}{l} 43.981 \\ 38.318 \\ 38.54 \\ 26.991 \\ 21.328 \\ 15.664 \\ 10.001 \\ 4.338 \\ \end{array}$					6.989
			35.610 31.021 26.432 20.843 17.254 12.665 8.076 3.487				1.102	5.691
			28.122 24.495 20.867 17.239 13.612 9.984 6.357				0.898	4.526
			21.517 18.738 18.959 15.959 15.004 1.622 4.843				0.715	3.494
			15.794 13.751 11.708 1.765 7.621 5.578 3.535				0.552	2.595
		0.955			9.534 8.114 5.693 5.273 5.432 1.011		0.409	1.829

Table 15: Predicted CAPCE values by PTSLS estimator Table 15: Predicted CAPCE values by PTSLS estimator

