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

Yuta Kawakami^{1,2}

Manabu Kuroki¹

Jin Tian²

¹Department of Mathematics, Physics, Electrical Engineering and Computer Science, Yokohama National University, Yokohama, Kanagawa, JAPAN

²Department of Computer Science, Iowa State University, Ames, Iowa, USA

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, Angrist and Krueger, 2001]. Traditionally, there are a large number of works focusing on binary or categorical treatment variables [Imbens and Angrist, 1994, Balke and Pearl, 1997]; recently, there has been a growing interest in continuous treatment variables [Hirano and Imbens, 2005, Kennedy et al., 2017, Bahadori et al., 2022]. There is also considerable recent interest in estimating heterogeneous causal effects across subsets of the population [Athey and Imbens, 2016, Ding et al., 2016, Athey and Imbens, 2019, Künzel et al., 2019, Wager and Athey, 2018, Zhang et al., 2022, Singh et al., 2023], including IV-based methods [Angrist, 2004, Syrgkanis et al., 2019, Huntington-Klein, 2020, Bargagli-Stoffi et al., 2022]. Most of the works focus on *conditional average causal effect (CACE)* $\mathbb{E}[Y_1 - Y_0 | \mathbf{w}]$, 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 \mathbf{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 $\mathbb{E}[Y_x | \mathbf{w}]$. The most widely used methods include parametric two-stage least squared (PTSLs) [Wright, 1928, Angrist and Pischke, 2009, Wooldridge, 2010], sieve nonparametric two-stage least squared (sieve NTSLS) [Newey and Powell, 2003, Chen and Christensen, 2018], and Kernel IV [Singh et al., 2019]. The line of works in [Syrgkanis et al., 2019, Dikkala et al., 2020, Muandet et al., 2020, Bennett et al., 2023] focus on the efficiency of estimators assuming simple additive errors. All these methods rely on a *separability* assumption for identifying $\mathbb{E}[Y_x | \mathbf{w}]$ [Newey and Powell, 2003].

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, Wooldridge, 2005, Graham and Powell, 2012]. Wong [2022] provided a condition for identifying $\mathbb{E}[\partial_x Y_x]$ and Kawakami et al. [2023] presented APCE estimators.

In this paper, we consider $\mathbb{E}[\partial_x Y_x | \mathbf{w}]$, 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, 2016]). Still existing works have focused on $\mathbb{E}[Y_x | \mathbf{w}]$. 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, PTSLs, Kernel IV) for identifying $\mathbb{E}[Y_x | \mathbf{w}]$. Thus, computing CAPCE allows scientists to estimate causal effects in a larger class of models. Granted, given an estimated $\mathbb{E}[Y_x | \mathbf{w}]$, 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-

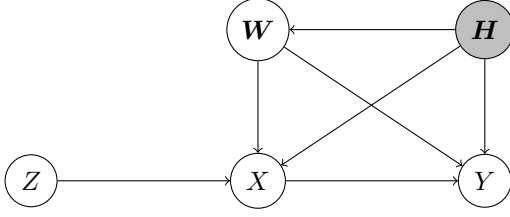


Figure 1: A causal graph representing the IV model.

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

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

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, Leoni, 2009]. Let λ be a $d + 1$ dimensional vector of non-negative integer, $|\lambda| = \sum_{l=1}^{d+1} \lambda_l$, and

$D^\lambda f(x, \mathbf{w}) = \partial^{|\lambda|} f(x, \mathbf{w}) / \partial x^{\lambda_1} \partial w_1^{\lambda_2} \dots \partial w_d^{\lambda_{d+1}}$. Sobolev norm is defined as follows: $\|f\|_{W^{l,p}} =$

$$\left\{ \sum_{|\lambda| \leq l} \int \{D^\lambda f(x, \mathbf{w})\}^p dx d\mathbf{w} \right\}^{1/p} \quad \text{for } 1 \leq p < \infty,$$

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

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

over \mathbf{V} , and a causal graph $G(\mathcal{M})$ over \mathbf{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 \mathbf{X} to constants \mathbf{x} replaces the functions of \mathbf{X} by the constants \mathbf{x} and induces a *sub-model* \mathcal{M}_x . We denote the potential outcome Y under intervention $do(x)$ by $Y_x(\mathbf{u})$, which is the solution of Y in the sub-model \mathcal{M}_x given $\mathbf{U} = \mathbf{u}$.

Instrumental Variable (IV) Model with Covariates. We consider the IV model represented by the causal graph in Fig 1, with the following SCM \mathcal{M}_{IV} over $\mathbf{V} = \{Z, X, Y, \mathbf{W}\}$ and $\mathbf{U} = \{\mathbf{H}, \mathbf{u}_X, \mathbf{u}_Y, \mathbf{u}_Z, \mathbf{u}_W\}$:

$$\begin{aligned} Y &:= f_Y(X, \mathbf{W}, \mathbf{H}, \mathbf{u}_Y), \quad X := f_X(Z, \mathbf{W}, \mathbf{H}, \mathbf{u}_X), \\ \mathbf{W} &:= f_W(\mathbf{H}, \mathbf{u}_W), \quad Z := f_Z(\mathbf{u}_Z), \end{aligned} \quad (1)$$

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

Related work. Under the IV model, Newey and Powell [2003] introduced sieve NTSLS for identifying and estimating $\mathbb{E}[Y_x | \mathbf{w}]$ via an integral equation, $\mathbb{E}[Y | Z = z] = \int_{\Omega_W} \int_{\Omega_X} p(X = x, \mathbf{W} = \mathbf{w} | Z = z) \mathbb{E}[Y_x | \mathbf{w}] dx d\mathbf{w}$, under the following assumption called *separability*:

$$\begin{aligned} f_Y(X, \mathbf{W}, \mathbf{H}, \mathbf{u}_Y) &= f_Y^1(X, \mathbf{W}, \mathbf{u}_Y) + f_Y^2(\mathbf{H}, \mathbf{u}_Y), \\ \mathbb{E}[f_Y^2(\mathbf{H}, \mathbf{u}_Y) | \mathbf{W}] &= 0, \end{aligned} \quad (2)$$

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

Recently, Wong [2022] introduced an integral equation for identifying APCE $\mathbb{E}[\partial_x Y_x] := \mathbb{E}_U[\partial_x Y_x(\mathbf{U})]$ under the IV model with no covariates \mathbf{W} : $\mathbb{E}[Y | Z = z] - \mathbb{E}[Y | Z = z_0] = - \int_{\Omega_X} \{\mathbb{P}(X \leq x | Z = z) - \mathbb{P}(X \leq x | Z = z_0)\} \mathbb{E}[\partial_x Y_x] dx$. Kawakami et al. [2023] 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 \mathbf{W} is empty. The sieve and RKHS estimators in this paper were not provided in [Kawakami et al., 2023]. We note that Picard-iteration estimator in [Kawakami et al., 2023] is not suitable here because equation (3) 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). $\mathbb{E}[\partial_x Y_x | \mathbf{w}] := \mathbb{E}_U \left[\frac{\partial}{\partial x} Y_x(\mathbf{U}) \mid \mathbf{W} = \mathbf{w} \right].$

CAPCE is a real-valued function from $x \in \Omega_X$ and $\mathbf{w} \in \Omega_{\mathbf{W}}$ to \mathbb{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 \mathcal{M}_{IV} , given $\mathbf{W} = \mathbf{w}$,

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_x is differentiable and bounded in $x \in \Omega_X$.
3. $\sup_{x, z, \mathbf{w}} \mathbb{P}(X_z = x | \mathbf{W} = \mathbf{w}) < \infty$.
4. The set of distributions $\mathbb{P}(X | Z = z, \mathbf{W} = \mathbf{w})$ 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 $\mathbf{w} \in \Omega_{\mathbf{W}}$. The third assumption means the density function of $X_{z, \mathbf{w}}$ is bounded. The fourth assumption implies that h is a zero function if $\mathbb{E}[h(X) | Z = z, \mathbf{W} = \mathbf{w}]$ does not depend on z for all $\mathbf{w} \in \Omega_{\mathbf{W}}$, which is also assumed in [Newey and Powell, 2003] for identifying $\mathbb{E}[Y_x | \mathbf{w}]$.

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 \mathbf{H} separately, i.e., $f_Y(X, \mathbf{W}, \mathbf{H}, \mathbf{u}_Y) = f_Y^1(X, \mathbf{W}, \mathbf{u}_Y) + f_Y^2(\mathbf{W}, \mathbf{H}, \mathbf{u}_Y)$.

We obtain the following result.

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

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

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

Remark: Assumption 3.2 is weaker than the assumption (2) needed by existing work sieve NTSLS [Newey and Powell,

2003], PTSLS [Wooldridge, 2010], and Kernel IV [Singh et al., 2019] for identifying $\mathbb{E}[Y_x | \mathbf{w}]$, which require both covariates \mathbf{W} and the treatment X to be separable from the unmeasured confounders \mathbf{H} . Assumption 3.2 is particularly less restrictive when there are many covariates. Theorem 3.1 states that CAPCE $\mathbb{E}[\partial_x Y_x | \mathbf{w}]$ is identifiable under a weaker assumption than required by $\mathbb{E}[Y_x | \mathbf{w}]$. The result enables us to compute causal effects in IV models where Assumption 3.2 holds but assumption (2) does not such that existing methods are not applicable. Theorem 3.1 extends the results in [Wong, 2022, Kawakami et al., 2023] 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 [2022] and Kawakami et al. [2023] because they study the setting with no covariates \mathbf{W} .

4 ESTIMATION OF CAPCE

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

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 and Hwang, 1982].

Approximation by Orthonormal Basis Functions. We approximate the CAPCE $\mathbb{E}[\partial_x Y_x | \mathbf{w}]$ by a set of orthonormal basis functions, such as Hermite polynomial functions [Hermite, 2009]. Specifically,

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

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 ($0 \leq l \leq \infty$) is used:

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

Assumption 4.2. $\sum_{j=1}^J \beta_j \phi_j(x, \mathbf{w})$ convergences uniformly to $g_0(x, \mathbf{w})$ if $J \rightarrow \infty$.

We note that Hermite polynomial functions satisfy Assumption 4.2 for any bounded and continuous function g_0 [Damelin et al., 2001].

Compactness Restriction. The integral equation (3), known as a ‘‘Fredholm Integral Equation of the First Kind’’ [Bôcher, 1926], is ill-posed since the integral operator \mathcal{K} , where $\mathcal{K}(f)(z) = \int_{\Omega_W} \int_{\Omega_X} k(z, x, \mathbf{w}) f(x, \mathbf{w}) dx d\mathbf{w}$, 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] and lead to severe estimation difficulties. To relieve the issue, we put restrictions on the functional space of $g_0(x, \mathbf{w})$. Let $\mathbf{g}(X, \mathbf{W}) = \int_{\Omega_W} \int_{\Omega_X} \{\mathbb{1}_{X \leq x, \mathbf{W}=\mathbf{w}} - \mathbb{E}[\mathbb{1}_{X \leq x, \mathbf{W}=\mathbf{w}} | Z = z_0]\} g(X, \mathbf{W}) dx d\mathbf{w}$, and define regularized Sobolev norm $\bar{W}^{l,2}$, which is called ‘‘consistency norm’’ in [Gallant and Nychka, 1987], as follows

$$\|\mathbf{g}(x, \mathbf{w})\|_{\bar{W}^{l,2}}^2 = \sum_{|\lambda| \leq l} \int \{D^\lambda \mathbf{g}(x, \mathbf{w})\}^2 \times \{1 + (x, \mathbf{w}^T)(x, \mathbf{w}^T)^T\}^\kappa dx d\mathbf{w}, \quad (5)$$

where $l \geq 1$ is an integer and κ is a constant satisfying $\kappa > (1 + d)/2$ where d is the dimension of \mathbf{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 $\mathcal{G}_{B_S} = \{g : \|\mathbf{g}(x, \mathbf{w})\|_{\bar{W}^{l,2}}^2 \leq B_S\}$.

Using the approximation in (4), equation (3) reduces to

$$\mu(z) = \sum_{j=1}^J \beta_j \int_{\Omega_W} \int_{\Omega_X} k(z, x, \mathbf{w}) \phi_j(x, \mathbf{w}) dx d\mathbf{w}. \quad (6)$$

Letting the anti-derivative of the basis functions be $\varphi_j(x, \mathbf{w}) = \int \phi_j(x, \mathbf{w}) dx$.¹ Then, the equation becomes

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

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

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

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

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

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

$$\begin{aligned} Q_1(\nu^j; \mathcal{D}^{(1)}) \\ = \frac{1}{N_1} \sum_{i=1}^{N_1} (\varphi_j(x_i^{(1)}, \mathbf{w}_i^{(1)}) - \mathbf{q}(z_i^{(1)})^T \nu^j)^2, \end{aligned} \quad (8)$$

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

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

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

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

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

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

Under Assumption 4.3, our estimator $\hat{\beta}$ is given by the optimization problem below:

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

where

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

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 $\hat{\mathbf{\Lambda}}$ [Kroese et al., 2011]. The optimization problem (12) can be solved by a ridge regression method with the following solution [Hilt et al.]:

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

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

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

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) as a performance metric of the trained model in Stage 2 with parameters $\hat{\beta}$ if given separate test datasets $\mathcal{D}^{(1)'} = \{x_i^{(1)'}, z_i^{(1)'}, \mathbf{w}_i^{(1)'}\}_{i=1}^{N'_1}$ and $\mathcal{D}^{(2)'} = \{y_i^{(2)'}, z_i^{(2)'}, \mathbf{w}_i^{(2)'}\}_{i=1}^{N'_2}$. Let $N' = N'_1 + N'_2$. Assume \hat{c}'_i and $\hat{\mathbf{d}}'_i$ for $i = 1, \dots, N'$ are computed using $\mathcal{D}^{(1)'}$ and $\mathcal{D}^{(2)'}$. Then, we can evaluate the trained model by the test error $\hat{Q}_3(\hat{\beta}; \mathcal{D}^{(1)'}, \mathcal{D}^{(2)'}) = \frac{1}{N'} \sum_{i=1}^{N'} (\hat{c}'_i - \hat{\mathbf{d}}'^T_i \hat{\beta})^2$. 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]. Assumptions B.1 - 4 are shown in Appendix B.

Theorem 4.1 (Consistency). *Under SCM \mathcal{M}_{IV} and Assumptions 3.1, 3.2, 4.1, 4.2, 4.3, B.1, B.2, B.3, and B.4, letting $P \rightarrow \infty$ and $J \rightarrow \infty$, then $\|\hat{g} - g_0\|_{W^1, \infty} \xrightarrow{P} 0$.*

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

Assumpts. C.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:

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

where $\{\theta_k(x, \mathbf{w})\}_{k=1}^K$ are a set of known functions, and $\gamma = (\gamma_1, \dots, \gamma_K)^T$ 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 $k = 1, \dots, K$. Let $c = \mathbb{E}[Y|Z = z] - \mathbb{E}[Y|Z = z_0]$, and $\mathbf{e} = (e^1, \dots, e^K)^T$ where $e^k = \mathbb{E}[\vartheta_k(X, \mathbf{W})|Z = z] - \mathbb{E}[\vartheta_k(X, \mathbf{W})|Z = z_0]$. Then, equation (3) reduces to a linear equation $c = \gamma^T \mathbf{e}$.

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

Stage 1. Let basis functions be $\mathbf{q}(z) = (q_1(z), q_2(z), \dots, q_P(z))^T$. Denote $\hat{c}_i = \hat{\mathbb{E}}[Y|Z = z_i] - \hat{\mathbb{E}}[Y|Z = z_0]$ and $\hat{e}_i^k = \hat{\mathbb{E}}[\vartheta_k(X, \mathbf{W})|Z = z_i] - \hat{\mathbb{E}}[\vartheta_k(X, \mathbf{W})|Z = z_0]$. 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

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

for $k = 1, \dots, K$. Let $N = N_1 + N_2$ and $(z_1, \dots, z_N) = (z_1^{(1)}, \dots, z_{N_1}^{(1)}, z_1^{(2)}, \dots, z_{N_2}^{(2)})$. We will compute predicted values in (16) for all $i = 1, \dots, N$.

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

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

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, our estimator $\hat{\gamma}$ is given by the optimization problem below:

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

This problem can be solved by the ridge regression method with the following solution [Hilt et al.]:

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

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

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

Model Selection. We presume the models in Stage 1 have been selected appropriately. We can use the empirical risk in equation (17) as a performance metric of the

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

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

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 \mathcal{M}_{IV} and Assumptions 3.1, 3.2, 4.4, D.1, D.2, D.3, and D.4, letting $P \rightarrow \infty$, then $\|\hat{\gamma} - \gamma\| \xrightarrow{P} 0$.*

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

Assumptions D.1 - 4 are shown in Appendix D. Assumptions E.1 - 5 are in Appendix E.

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 Koutroumbas, 2006, Schölkopf et al., 2013].

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

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

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 $H \circ \pi : \Omega_{X, \mathbf{W}} \rightarrow$

Ω_Y . Our RKHS CAPCE estimator consists of two stages (a detailed derivation is provided in Appendix A.2).

Stage 1. We learn an operator $G_1 \in \mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_{X, \mathbf{W}})$ 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 $\hat{\mathbb{E}}[Y | Z = z] - \hat{\mathbb{E}}[Y | Z = z_0] = H(\hat{\mathbb{E}}[\pi(X, \mathbf{W}) | Z = z] - \hat{\mathbb{E}}[\pi(X, \mathbf{W}) | Z = z_0]) \Leftrightarrow \hat{G}_1(\psi(z) - \psi(z_0)) = H(\hat{G}_2(\psi(z) - \psi(z_0)))$, 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 $\mathcal{D}^{(2)}$:

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

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

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

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

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

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

where

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

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

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]. 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

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

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

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

where $\mathbf{P}_2 = (\mathbf{K}_{Z^{(1)}Z^{(1)}} + N_1 \lambda_2 \mathbf{I}_{N_1})^{-1} \mathbf{K}_{Z^{(1)}Z^{(2)}}$. Finally, we determine the optimal ξ^* and λ_3^* by minimizing test error $L(\lambda_3, \xi) = \frac{1}{N'_2} \sum_{i=1}^{N'_2} \|\mathbf{y}^{(2)'}{}^T (\mathbf{K}_{Z^{(2)'Z^{(2)'}}} + N'_2 \lambda_2^* \mathbf{I}_{N'_2})^{-1} (\mathbf{K}_{Z^{(2)'Z^{(2)'}}} - \hat{H}_{\lambda_3, \xi}(x_i^{(1)'}, \mathbf{w}_i^{(1)'})\|^2$ 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 [Saunders et al., 1998]. We show that RKHS CAPCE is consistent under assumptions similar to Kernel IV [Singh et al., 2019]. Assumptions F.1 - 8 are shown in Appendix F.

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

When $\lambda_3 = 0$, the inverse of the matrix $\hat{\mathbf{O}}\hat{\mathbf{O}}^T + N_2 \xi \mathbf{K}_{(X, \mathbf{W})^{(1)}(X, \mathbf{W})^{(1)}}$ in Eq. (25) 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. 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

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

where $f(W) = W^5 + W^4 + W^3 + W^2$. The SCMs satisfy separability Assumption 3.2 but not (2). 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 $\{1, W, X, WX, X^2\}$ for PTSLS, 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. We observe that, when $N = 1000$, both P-CAPCE and PTSLS estimates have large standard deviations (SD) (shown in Appendix G) 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(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.

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

where MSE is computed as $\frac{1}{N'_1} \sum_{i=1}^{N'_1} \{\hat{g}(x_i^{(1)'}, w_i^{(1)'}) - g(x_i^{(1)'}, w_i^{(1)'})\}^2$ with test dataset $\mathcal{D}^{(1)'}$, and the results are shown in Table 2. 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

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

Estimated coefficients	$N = 1000$			$N = 10000$		
Terms	1	W	X	1	W	X
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	1	1	20	1	1	20

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(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.

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) 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)) is absent, and the results (presented in Appendix G) 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

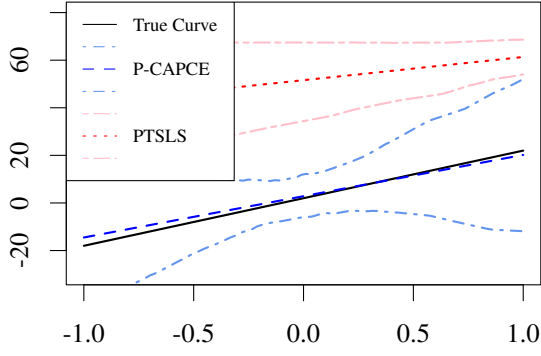
In this section, we present an application of our CAPCE estimators to a real-world dataset in economics.

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/package=wooldridge>), which has been analyzed by

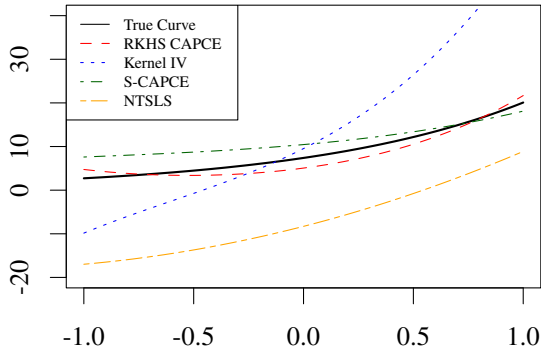
many works, e.g., in [Griliches, 1977, Blackburn and Neumark, 1992]. The sample size is 935 with 857 left after excluding missing values. We evaluate the heterogeneity of the effect of years of education on monthly wages, which is of great interest in economics [Angrist and Krueger, 1991, Card, 1999]. We followed Blackburn and Neumark [1992] 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, Kling, 2001, Wooldridge, 2010]). 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 PTSLS. Detailed settings are in Appendix G.

Results. The estimated CAPCE values are shown in Appendix G. 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, Wooldridge, 2010]. 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, Caplan, 2018]. 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, Card, 1999, Kling, 2001, Wooldridge, 2010, Kawakami et al., 2023] using this dataset have focused on the effects of education on wages over the whole population. Card [1999] and Wooldridge [2010] 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]. 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].

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 $\mathbb{E}[\partial_x Y_x | w]$ is identifiable under a weaker assumption than required by $\mathbb{E}[Y_x | w]$, showing the merit of studying CAPCE instead of $\mathbb{E}[Y_x | w]$, 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 PTSLS [Angrist and Pischke, 2009, Wooldridge, 2010], sieve NTSLS [Newey and Powell, 2003], and Kernel IV [Singh et al., 2019] in settings where the standard separability assumption (2) 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 $W \rightarrow Z$. An identification theorem similar to Theorem 3.1 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.

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

Yuta Kawakami^{1,2}

Manabu Kuroki¹

Jin Tian²

¹Department of Mathematics, Physics, Electrical Engineering and Computer Science, Yokohama National University,
Yokohama, Kanagawa, JAPAN

²Department of Computer Science, Iowa State University, Ames, Iowa, USA

A PROOFS OF THEOREM 3.1 AND RKHS CAPCE ESTIMATOR

A.1 PROOF OF THEOREM 3.1

We give proof of Theorem 3.1.

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

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

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

Proof. First, we show the following integral equation holds under Assumptions 3.1 and 3.2 following the idea in [Wong, 2022]:

$$\begin{aligned} & \mathbb{E}[Y | Z = z, \mathbf{W} = \mathbf{w}] - \mathbb{E}[Y | Z = z_0, \mathbf{W} = \mathbf{w}] \\ &= - \int_{\Omega_X} \{ \mathbb{P}(X \leq x | Z = z, \mathbf{W} = \mathbf{w}) - \mathbb{P}(X \leq x | Z = z_0, \mathbf{W} = \mathbf{w}) \} \mathbb{E}[\partial_x Y_x | \mathbf{w}] dx. \end{aligned} \quad (31)$$

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

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

given $\mathbf{W} = \mathbf{w}$ for each subject, where $\mathbb{1}_{\cdot}$ 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 $Y_{X_z} = \int_{\Omega_X} \mathbb{1}_{X_z=x} Y_x dx$ and $Y_{X_{z_0}} = \int_{\Omega_X} \mathbb{1}_{X_{z_0}=x} Y_x dx$, then

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

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

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

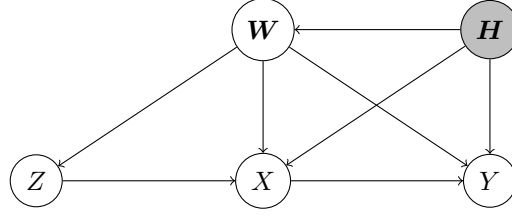


Figure 3: A causal graph representing the IV setting with covariates when there is an edge $\mathbf{W} \rightarrow Z$.

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

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

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 $\partial_x Y_x$ are independent given $\mathbf{W} = \mathbf{w}$. Thus, we take expectations on both sides:

$$\mathbb{E}[Y_{X_z} | \mathbf{W} = \mathbf{w}] - \mathbb{E}[Y_{X_{z_0}} | \mathbf{W} = \mathbf{w}] \quad (36)$$

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

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

Then, the integral equation becomes

$$\mathbb{E}[Y | Z = z, \mathbf{W} = \mathbf{w}] - \mathbb{E}[Y | Z = z_0, \mathbf{W} = \mathbf{w}] \quad (39)$$

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

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

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

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

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

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 $\mathbb{E}[\delta(X) | Z = z, \mathbf{W} = \mathbf{w}] = \mathbb{E}[\delta(X), \mathbf{W} = \mathbf{w} | Z = z] \mathbb{P}(\mathbf{W} = \mathbf{w})$, there exists a function which satisfies $\mathbb{E}[\delta(X), \mathbf{W} = \mathbf{w} | Z = z] = 0$ for any $z \in \Omega_Z$ and $\mathbf{w} \in \Omega_{\mathbf{W}}$ if there exists a function which satisfies $\mathbb{E}[\delta(X) | Z = z] = 0$ for any $z \in \Omega_Z$ and $\mathbf{w} \in \Omega_{\mathbf{W}}$. 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 $\mathbf{w} \in \Omega_{\mathbf{W}}$. \square

A.2 IDENTIFICATION THEOREM UNDER IV MODEL IN FIG 3

We consider the IV model with covariates represented by the causal graph in Fig 3, with the following SCM \mathcal{M}'_{IV} over $V = \{Z, X, Y, \mathbf{W}\}$ and $U = \{\mathbf{H}, \mathbf{u}_X, \mathbf{u}_Y, \mathbf{u}_Z, \mathbf{u}_{\mathbf{W}}\}$:

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

where $f_{\mathbf{W}}$ is a vector function. We assume all variables are continuous, \mathbf{W} are d -dimensional pre-treatment covariates, and \mathbf{H} stands for unmeasured confounders. We show a similar identification result to Theorem 3.1.

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

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

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

Proof. Eq. (44) is guaranteed by Eq. (39), which appears in the proof of Theorem 3.1. \square

Based on Theorem 3.1', we have to learn $\mathbb{E}[\partial_x Y_x | \mathbf{w}]$ as a function of x for each $\mathbf{w} \in \Omega_{\mathbf{W}}$ respectively. In contrast, based on Theorem 3.1, we can learn $\mathbb{E}[\partial_x Y_x | \mathbf{w}]$ directly as a function of x and \mathbf{w} .

We perform experiments about estimating CAPCE based on Theorem 3.1' in Appendix G.5.

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

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

$(\lambda_1, \lambda_2, \lambda_3, \xi)$ 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 $\pi(x, \mathbf{w})$, where $\pi(x, \mathbf{w}) = -\int_{-\infty}^x \eta(x', \mathbf{w}) dx'$ for some feature function $\eta(x', \mathbf{w})$. The optimization problem in **Stage 1 (A)** becomes

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

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

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

where $\mathbf{K}_{Z^{(1)}Z^{(1)}}$ and $\mathbf{K}_{X^{(1)}X^{(1)}}$ are the empirical kernel matrices, the i -th column of $\pi_{X^{(1)}, \mathbf{W}^{(1)}}$ is $-\int_{-\infty}^{x_i^{(1)}} \eta(x, \mathbf{w}) dx$, and the i -th column of $\psi_{X^{(1)}}$ is $\psi(z_i^{(1)})$. The prediction values are

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

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

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

and $\gamma(z) - \gamma_i(z_0) = (\mathbf{K}_{Z^{(1)}Z^{(1)}} + N_1\lambda_1\mathbf{I})^{-1}\psi_Z^{(1)T}\{\psi(z) - \psi(z_0)\} = (\mathbf{K}_{Z^{(1)}Z^{(1)}} + N_1\lambda_1\mathbf{I})^{-1}(\mathbf{K}_{Z^{(1)}z} - \mathbf{K}_{Z^{(1)}z_0})$ 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 $\text{span}(\{\eta(x_j^{(1)}, \mathbf{w}_j^{(1)})\}_{j=1}^{N_1})$ from the representer theorem [Schölkopf et al., 2001]. Then the functional form of $d(z)$ is restricted by

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

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

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

From the kernel trick, it becomes

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

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

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

Stage 1 (B). The optimization problem in **Stage 1 (B)** is

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

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

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

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

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

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

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

and, the difference of the predication values are

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

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

$$\begin{aligned} \min_{H \in \mathcal{L}_2(\mathcal{H}_{X, \mathbf{w}}, \Omega_Y)} N_2^{-1} \sum_{i=1}^{N_2} \left\| \hat{G}_2(\psi(z_i^{(2)}) - \psi(z_0)) - H(\hat{G}_1(\psi(z_i^{(2)}) - \psi(z_0))) \right\|^2 \\ + \xi \|H\|_{\mathcal{L}_2(\mathcal{H}_{X, \mathbf{w}}, \Omega_Y)}^2 + \lambda_3 \|H \circ \hat{G}_1\|_{\mathcal{L}_2(\mathcal{H}_Z, \Omega_Y)}^2. \end{aligned} \quad (60)$$

Then, the estimation problem reduces to

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

$$= \frac{1}{N_2} \|\mathbf{y}^{(2)} - \mathbf{y}^{(2)T}(\mathbf{K}_{Z^{(2)}Z^{(2)}} + N_2\lambda_2\mathbf{I})^{-1}\mathbf{K}_{Z^{(2)}z_0} - (\mathbf{K}_{X^{(1)}X^{(1)}}(\mathbf{K}_{Z^{(1)}Z^{(1)}} + N_1\lambda_1\mathbf{I})^{-1}(\mathbf{K}_{Z^{(1)}Z^{(2)}} - \mathbf{K}_{Z^{(1)}z_0}))^T\boldsymbol{\alpha}\|^2 \quad (62)$$

$$+ \xi \boldsymbol{\alpha}^T \mathbf{K}_{(X,\mathbf{W})^{(1)}(X,\mathbf{W})^{(1)}} \boldsymbol{\alpha} + \lambda_3 \boldsymbol{\alpha}^T \boldsymbol{\alpha}, \quad (63)$$

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

and the solution to this optimization problem can be represented as

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

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

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

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

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].

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, Ai and Chen, 2003], and it is widely used in machine learning fields [Kato et al., 2022]. Since $\mathbb{E}[Y|Z = z_0] - \mathbb{E}[Y|Z] = \mathbb{E}[\mathbb{E}[Y|Z = z_0] - Y|Z]$ and $\mathbb{E}[\mathbb{1}_{X \leq x, \mathbf{W}=\mathbf{w}}|Z = z] - \mathbb{E}[\mathbb{1}_{X \leq x, \mathbf{W}=\mathbf{w}}|Z = z_0] = \mathbb{E}[\mathbb{1}_{X \leq x, \mathbf{W}=\mathbf{w}} - \mathbb{E}[\mathbb{1}_{X \leq x, \mathbf{W}=\mathbf{w}}|Z = z_0]|Z = z]$, Theorem 3.1 reduces to

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

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

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 Powell, 2003], as below:

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

where $\hat{\rho}(z_i, g) = \hat{c}_i - \hat{\mathbf{d}}_i^T \mathbf{g}$, 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]. We denote $\mathcal{G}_S = \{g \in \mathcal{G} : \|\mathbf{g}_0(x, \mathbf{w})\|_{\tilde{W}^{1,2}}^2 \leq B_S\}$, 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 $P \rightarrow \infty$, $N \rightarrow \infty$ with $P/N \rightarrow 0$, there exists $\boldsymbol{\pi}_P$ with $\mathbb{E}[\{b(z) - \mathbf{q}(z)^T \boldsymbol{\pi}_P\}^2] \rightarrow 0$ 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 $M(Y, Y_{X_{z_0}}, X, X_{z_0}, \mathbf{W})$, $\nu > 0$ such that for all $\tilde{g}, g \in \overline{\mathcal{G}_S}$, $\|\rho(Y, Y_{X_{z_0}}, X, X_{z_0}, \mathbf{W}, \tilde{g}) - \rho(Y, Y_{X_{z_0}}, X, X_{z_0}, \mathbf{W}, g)\| \leq M(Y, Y_{X_{z_0}}, X, X_{z_0}, \mathbf{W})\|\tilde{g} - g\|_{W^{l,2}}^\nu$ and $\mathbb{E}[M(Y, Y_{X_{z_0}}, X, X_{z_0}, \mathbf{W})^2 | Z]$ is bounded.

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

Let \mathcal{W} denote the domain of $\mathbf{g}(x, \mathbf{w}, g)$.

Assumption B.4 (Openness and Convexness of Restricted Parameter Space). \mathcal{W} is open and convex.

The following lemma is shown in [Newey and Powell, 2003]:

Lemma B.1. If (i) Θ is a compact subset of a space with norm $\|\theta\|$; (ii) $\hat{Q}(\theta) \rightarrow_p Q(\theta)$ for all $\theta \in \Theta$; (iii) there is $v > 0$ and $B_n O_p(1)$ such that for all $\tilde{\theta}, \theta \in \Theta$, $|\hat{Q}(\tilde{\theta}) - \hat{Q}(\theta)| \leq B_n \Delta^v = B_n \epsilon / 2M \leq \epsilon / 2$ 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. Under SCM \mathcal{M}_{IV} and Assumptions 3.1, 3.2, 4.1, 4.2, 4.3, B.1, B.2, B.3, and B.4, letting $P \rightarrow \infty$ and $J \rightarrow \infty$, then $\|\hat{g} - g_0\|_{W^{l,\infty}} \xrightarrow{p} 0$.

Proof. From the Assumption B.2 and B.4, the parameter space is compact subset. From the Assumption B.3, the following relation is satisfied:

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

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

From the Lemma B.1,

$$\|\tilde{g} - g\|_{W^{l,\infty}} \rightarrow_p 0. \quad (72)$$

From Assumption B.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

$$\inf_{g \in \mathcal{G}} \mathbb{E} [\mathbf{g}(X, X_{z_0}, \mathbf{W}, g)^2] \quad (73)$$

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

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

where

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

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

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

These derivatives are called “pathwise derivatives.” See [Ai and Chen, 2003] 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 $N \rightarrow \infty$ implies $J_N \rightarrow \infty$ and $P_N \rightarrow \infty$. We use more basis functions, $\mathbf{q}^{P_N} = (q^1, \dots, q^{P_N})$, as the sample size grows for the stage 1.

ASSUMPTIONS

We make the following assumptions.

Assumption C.1 (Compactness of Domain). $\Omega_{(X, X_{z_0}, \mathbf{W})}$ 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 $\mathbf{q}^{P_N}(X, X_{z_0}, \mathbf{W})^T \boldsymbol{\pi}_{P_N} \in \mathcal{G}_S$, where $\boldsymbol{\pi}_{P_N}$ is P_N vector, such that $\sup_{(X, X_{z_0}, \mathbf{W}) \in \Omega_{(X, X_{z_0}, \mathbf{W})}} |h(X, X_{z_0}, \mathbf{W}) - \mathbf{q}^{P_N}(X, X_{z_0}, \mathbf{W})^T \boldsymbol{\pi}_{P_N}| = \mathcal{O}(P_N^{-\kappa/(1+d)})$ 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].

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

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). $\ln[N(\epsilon^{1/k}, \mathcal{G}, \|\cdot\|_{W^{l,2}})] \leq \text{const.} \times J_N \times \ln(J_N/\epsilon)$

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

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

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

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]:

Lemma C.1. Under Assumptions C.1, C.2, C.3, C.4, C.5, C.6, and C.7, (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 $\|g - g_0\| \leq o(\tau_N)$, where $\tau_N = N^{-\tau}$ with $\tau \leq 1/4$.

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

Proof. Let

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

Then, Lemma C.1 implies

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

and this proves

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

□

D CONSISTENCY OF PARAMETRIC CAPCE ESTIMATOR

In this section, we show the consistency property of parametric CAPCE estimator. We denote the functional space \mathcal{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], as below:

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

where $\hat{\rho}(z_i, \gamma) = \hat{c}_i - \hat{e}_i \gamma$. $\hat{\rho}(z_i, \gamma)$ 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]. 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 $\mathbb{E}[\rho(Y, Y_{X_{z_0}}, X, X_{z_0}, \mathbf{W}, \gamma) | Z = z] = \mathbf{0}$.

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

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

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

Assumption D.4 (Openness and Convexness of Restricted Parameter Space). \mathcal{W} is open and convex.

Theorem 4.3. Under SCM \mathcal{M}_{IV} and Assumptions 3.1, 3.2, 4.4, D.1, D.2, D.3, and D.4, letting $P \rightarrow \infty$, then $\|\hat{\gamma} - \gamma\| \xrightarrow{p} 0$.

Proof. From the Assumption D.2 and D.4, the parameter space is compact subset. From the Assumption D.3, the following relation is satisfied:

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

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

From Lemma B.1,

$$\|\tilde{\gamma} - \gamma\| \rightarrow_p 0. \quad (85)$$

From Assumption D.1, the limits is γ_0 . □

E RATE OF CONVERGENCE OF PARAMETRIC CAPCE ESTIMATOR

ASSUMPTIONS

We make the following assumptions.

Assumption E.1 (Compactness of Domain). $\Omega_{(X, X_{z_0}, \mathbf{W})}$ 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 $\mathbf{q}^{P_N}(X, X_{z_0}, \mathbf{W})^T \boldsymbol{\pi}_{P_N} \in \mathcal{G}_P$, where $\boldsymbol{\pi}_{P_N}$ is P_N vector, such that $\sup_{(X, X_{z_0}, \mathbf{W}) \in \Omega_{(X, X_{z_0}, \mathbf{W})}} |h(X, X_{z_0}, \mathbf{W}) - \mathbf{q}^{P_N}(X, X_{z_0}, \mathbf{W})^T \boldsymbol{\pi}_{P_N}| = \mathcal{O}(P_N^{-\kappa/(1+d)})$ 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].

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 $c_1, c_2 > 0$,

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

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

The following lemma holds [Ai and Chen, 2003]:

Lemma E.1. Under Assumptions E.1, E.2, E.3, E.4, and E.5, (i) $\hat{L}_N(\gamma) - L_N(\gamma) = o_p(N^{-1/4})$ uniformly over γ ; and (ii) $\hat{L}_N(\gamma) - \hat{L}_N(\gamma_0) - \{L_N(\gamma) - L_N(\gamma_0)\} = o_p(\tau_N N^{-1/4})$ uniformly over γ with $\|\gamma - \gamma_0\| \leq o(\tau_N)$, where $\tau_N = N^{-\tau}$ with $\tau \leq 1/4$.

Theorem 4.4. Under SCM \mathcal{M}_{IV} and Assumptions 3.1, 3.2, 4.4, E.1, E.2, E.3, E.4, and E.5, setting $N = N_1 = N_2$, then $\|\hat{\gamma} - \gamma\| = o_p(N^{-1/4})$.

Proof. Let

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

Then, Lemma E.1 implies

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

and this proves

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

□

F PROPERTIES OF RKHS CAPCE ESTIMATOR

We show the consistency and rate of convergence of RKHS CAPCE estimator following [Singh et al., 2019] when λ_3 is 0.

NOTATIONS

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

Definition 2. *The stage 1 operators are*

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

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

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].

In addition, we denote

Definition 3.

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

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

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

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

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

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

Definition 4. *The stage 2 operators are*

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

$$S_2 : \mathcal{L}_2(\mathcal{H}_{X, \mathbf{W}}, \mathbf{p}_{\mathcal{H}_{X, \mathbf{W}}}) \rightarrow \mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_{X, \mathbf{W}}), \quad (99)$$

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

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

Definition 5. *We denote*

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

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

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

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

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

ASSUMPTIONS

Next, we show assumptions for Theorem 4.5.

Assumption F.1 (Restriction for the domains). *Suppose that $\Omega_{X,W}$ 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_Z are continuous and bounded: $\sup_{x \in \Omega_{X,W}} \|\pi(x, w)\|_{\mathcal{H}_{X,W}} \leq Q$ and $\sup_{z \in \Omega_Z} \|\psi(z)\|_{\mathcal{H}_Z} \leq \kappa$.
2. π and ψ are measurable.
3. $k_{X,W}$ 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 $\Omega_{X,W} \times \Omega_Z$ 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 $\|C_1\|_{\mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_{X,W})}^2 \leq \zeta_1$, 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 $\|C_2\|_{\mathcal{L}_2(\mathcal{H}_Z, \Omega_Y)}^2 \leq \zeta_2$.*

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

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

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

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

The proof is shown in [Singh et al., 2019]. 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 $\forall \mu(z), \|\Psi_{\mu(z)-\mu(z_0)}\|_{\mathcal{L}_2(\Omega_Z, \mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_{X,W}))}^2 = \text{Tr}(\Psi_{\mu(z)-\mu(z_0)}^* \circ \Psi_{\mu(z)-\mu(z_0)}) \leq B$.
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 $\forall \mu(z), \mu(z'), \|\Psi_{\mu(z)-\mu(z_0)} - \Psi_{\mu(z')-\mu(z_0)}\|_{L(\Omega_Z, \mathcal{L}_2(\mathcal{H}_Z, \mathcal{H}_{X,W}))} \leq L\|\mu(z) - \mu(z')\|_{\mathcal{H}_{X,W}}^\iota$.

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 \mathbf{p} on $\mathcal{H}_{X,W} \times \Omega_Y$ such that*

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

2. In the spectral decomposition $T = \sum_{k=1}^{\infty} \lambda_k e_k \langle \cdot, e_k \rangle_{\mathcal{H}_{X,W}}$, where $\{e_k\}_{k=1}^{\infty}$ is a basis of $\text{Ker}(T)^\perp$, 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, F.2, F.3, F.4, F.5, F.6, F.7 and F.8. Let $\lambda = N_1^{-\frac{1}{c_1+1}}$, $N_1 = N_2^{\frac{a(c_1+1)}{c_1-1}}$, $a > 0$, 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 $a \geq \frac{b(c+1)}{bc+1}$ 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 can be proved from the proof of Theorem 4 in [Singh et al., 2019] by substituting $\mu(z)$ with $\mu(z) - \mu(z_0)$.

Theorem 4.5. Under SCM \mathcal{M}_{IV} and Assumptions 3.1, 3.2, F.1, F.2, F.3, F.4, F.5, F.6, F.7 and F.8, the RKHS CAPCE estimator in (25) converges pointwise to CAPCE when $\lambda_3 = 0$.

Proof. Lemma F.3 implies consistency of RKHS CAPCE estimator by taking limit $N_2 \rightarrow \infty$. □

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 $\{1, W, X, WX, X^2\}$ 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 and 4. These tables supplement Table 1 in the paper. The true and estimated CAPCE surfaces over (X, W) are shown in Fig. 4.

Results: Nonparametric setting (B). The true and estimated CAPCE surfaces over (X, W) are shown in Fig. 5.

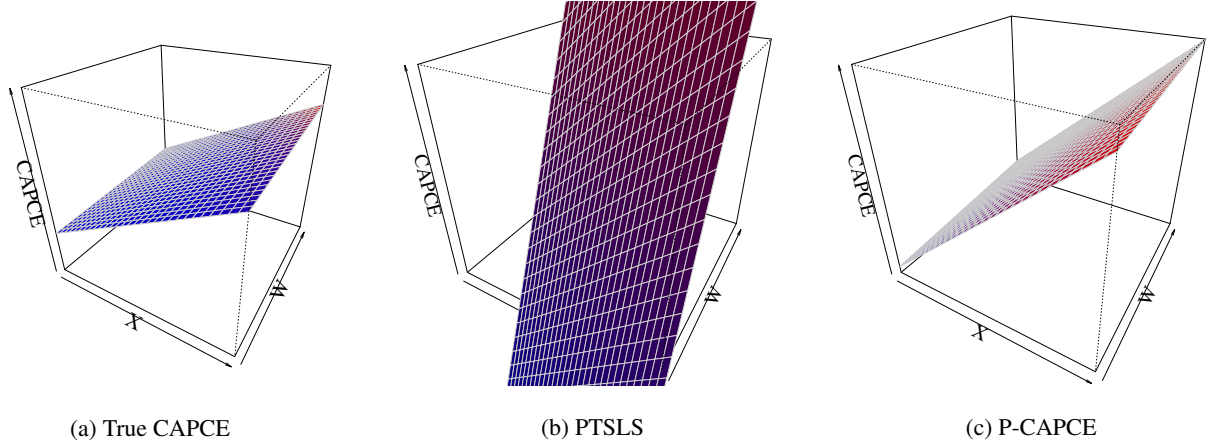


Figure 4: Parametric estimated surfaces in setting (A) (Mean, $N = 10000$). X-axis is the value of treatment variable ($X = x$), Y-axis is the value of covariate ($W = w$), and Z-axis is the value of CAPCE.

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

$N = 1000$	1	W	X	$N = 10000$	1	W	X
True Coeff.	1	1	20	True Coeff.	1	1	20
Min.	-51.515	-18.715	-116.480	Min.	-13.466	-2.302	-23.863
1st Qu.	-10.044	0.160	-10.809	1st Qu.	-2.324	-0.157	10.908
Median	-1.849	3.035	17.691	Median	1.138	0.543	22.075
3rd Qu.	7.926	12.239	50.007	3rd Qu.	4.643	1.568	29.509
Max.	40.458	109.791	213.306	Max.	14.988	11.017	59.559
Mean	-1.651	10.383	19.293	Mean	1.226	0.963	19.971
SD	14.707	22.309	50.957	SD	5.380	2.124	15.487

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

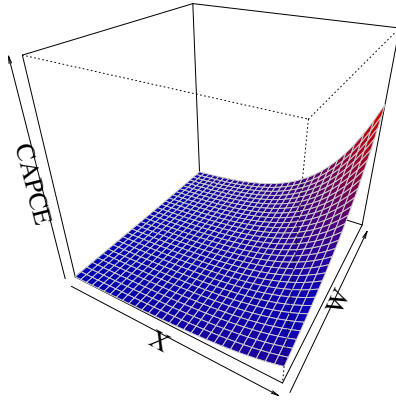
$N = 1000$	1	W	X	$N = 10000$	1	W	X
True Coeff.	1	1	20	True Coeff.	1	1	20
Min.	-33.368	2.971	-113.509	Min.	-12.117	30.794	-20.407
1st Qu.	-4.258	28.662	0.518	1st Qu.	-2.336	45.907	9.404
Median	2.785	45.497	28.629	Median	1.704	50.716	19.347
3rd Qu.	7.617	62.155	61.569	3rd Qu.	4.494	57.017	30.498
Max.	26.799	161.738	138.283	Max.	8.952	78.573	54.494
Mean	1.248	50.032	27.862	Mean	1.101	51.181	19.763
SD	11.374	29.523	46.388	SD	4.638	8.814	15.171

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

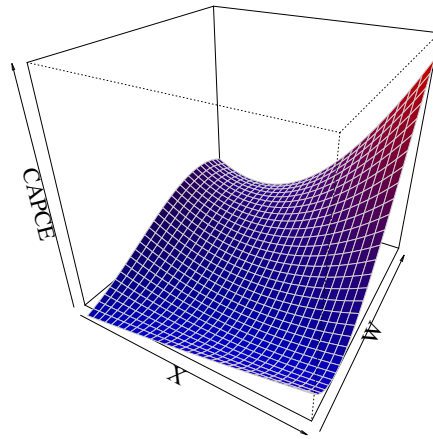
In this section, we give additional experiments with no interaction between covariates and unobserved confounders.

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

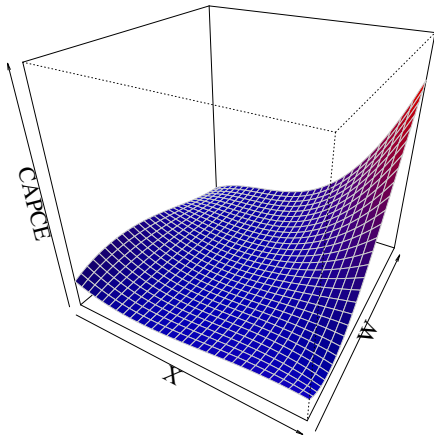
$$\begin{cases} Y := 10X^2 + WX + X + W + 50H + E_3 & \cdots \text{ (C)} \\ Y := \exp(X) \exp(W) + 50H + E_3 & \cdots \text{ (D)} \end{cases} \quad (108)$$



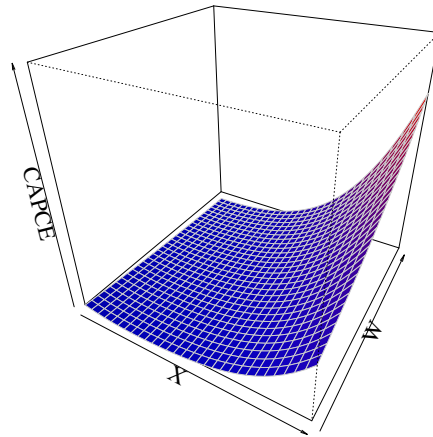
(a) True CAPCE



(b) Sieve NTSLs



(c) Sieve CAPCE



(d) RKHS CAPCE

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 and 6. The MSE of each estimator in settings (C) and (D) are shown in Table 7. 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.

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

$N = 1000$	1	W	X	$N = 10000$	1	W	X
True Coeff.	1	1	20	True Coeff.	1	1	20
Min.	-4.419	-38.895	-21.176	Min.	0.522	-21.630	18.680
1st Qu.	0.896	0.351	19.614	1st Qu.	0.976	0.158	19.901
Median	0.983	1.361	19.919	Median	1.000	0.830	20.006
3rd Qu.	1.065	2.620	20.246	3rd Qu.	1.021	1.989	20.101
Max.	6.066	19.864	41.021	Max.	1.724	24.138	21.684
Mean	0.944	1.151	19.642	Mean	0.999	0.966	19.998
SD	0.811	5.535	4.884	SD	0.106	4.851	0.305

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

$N = 1000$	1	W	X	$N = 10000$	1	W	X
True Coeff.	1	1	20	True Coeff.	1	1	20
Min.	0.350	-2.045	15.831	Min.	0.904	-1.251	19.501
1st Qu.	0.957	-0.199	19.303	1st Qu.	0.986	0.515	19.905
Median	1.021	1.009	19.731	Median	1.003	0.962	19.963
3rd Qu.	1.101	1.921	19.953	3rd Qu.	1.021	1.407	20.019
Max.	1.456	5.165	20.260	Max.	1.074	3.148	20.120
Mean	1.029	0.997	19.474	Mean	1.003	0.939	19.939
SD	0.155	1.609	0.782	SD	0.028	0.814	0.118

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

MSE	PTSLS	NTSLS	Kernel IV	P-CAPCE	S-CAPCE	RKHS CAPCE
(C) $N = 1000$	3.004	4.124	8.165	8.316	11.827	3.572
(C) $N = 10000$	0.254	0.367	0.614	0.774	1.324	0.567
(D) $N = 1000$	139.713	4.224	4.438	52.861	4.254	2.943
(D) $N = 10000$	57.006	0.334	1.026	40.062	0.477	0.696

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

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

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 and 9. The MSE of estimators in settings (E) and (F) are shown in Table 10. 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.

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

$N = 1000$	1	W	X
True Coeff.	1	1	20
Min.	-2.056	-9.914	-6.174
1st Qu.	-0.103	-0.589	11.002
Median	0.848	1.996	15.528
3rd Qu.	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

$N = 10000$	1	W	X
True Coeff.	1	1	20
Min.	0.057	-1.633	10.648
1st Qu.	0.635	-0.286	17.381
Median	1.193	1.187	22.993
3rd Qu.	1.743	2.306	23.704
Max.	2.047	3.502	25.181
Mean	1.160	0.979	20.531
SD	0.662	1.713	4.798

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

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

$N = 10000$	1	W	X
True Coeff.	1	1	20
Min.	-1.072	7.402	11.514
1st Qu.	0.394	9.613	17.370
Median	0.957	10.748	19.355
3rd Qu.	1.446	11.977	21.967
Max.	2.684	15.641	26.645
Mean	0.934	10.883	19.459
SD	0.778	1.687	3.478

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

MSE	PTSLS	NTSLS	Kernel IV	P-CAPCE	S-CAPCE	RKHS CAPCE
(E) $N = 1000$	170.152	129.132	113.733	29.408	17.181	31.267
(E) $N = 10000$	64.645	55.104	65.055	3.592	4.527	3.171
(F) $N = 1000$	141.678	28.73	24.125	101.902	13.84	14.806
(F) $N = 10000$	61.569	4.323	3.197	42.422	1.788	1.731

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) based on Theorem 3.1’ in Appendix A.2. 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, $b_0 + b_1Z + b_2Z^2 + b_3Z^3 + b_4W + b_5W^2 + b_6W^3$. We consider the basis terms $h_p(X)$ for $p = 0, 1, 2$, where h_p is Hermite polynomial functions ($h_0(t) = 1$,

$h_1(t) = t$, $h_2(t) = t^2 - 1$ 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. The results show that estimators based on Theorem 3.1 and 3.1' have very similar performance.

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

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

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 $\{1, 10^{-1}, 10^{-2}, 10^{-3}, \dots\}$.

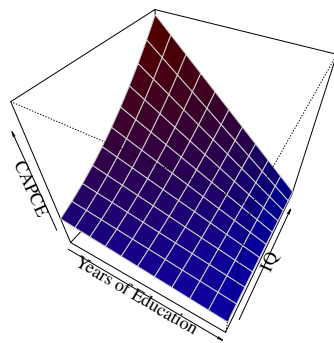
Results. The basic bootstrapping statistical properties of the P-CAPCE and PTSLS estimators are shown in Tables 12 and 13. The predicted CAPCE values are shown in Tables 14 and 15. The estimated CAPCE surfaces are shown in Fig. 6.

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

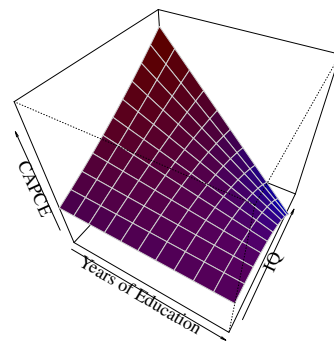
Terms	1	W	W^2	X	WX	W^2X
Min.	-0.00267	-0.00003	-0.00126	-0.00006	-0.00084	-0.00237
1st Qu.	-0.00061	0.00002	0.00510	-0.00001	-0.00029	-0.00099
Median	-0.00006	0.00004	0.00904	-0.00001	-0.00016	-0.00053
3rd Qu.	0.00058	0.00007	0.01331	0.00000	-0.00008	-0.00017
Max.	0.00226	0.00018	0.02786	0.00004	0.00059	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.

Terms	1	W	W^2	X	WX	W^2X
Min.	-0.00082	-0.03024	-0.00319	-0.01294	-0.47307	-0.00180
1st Qu.	0.00000	0.00023	0.00729	0.00005	0.00238	-0.00126
Median	0.00007	0.00259	0.00996	0.00134	0.06028	-0.00108
3rd Qu.	0.00012	0.00499	0.01341	0.00260	0.10789	-0.00089
Max.	0.00051	0.01539	0.04302	0.00773	0.30066	0.00046
Mean	0.00004	0.00191	0.01083	0.00102	0.04417	-0.00103
SD	0.00017	0.00617	0.00660	0.00299	0.11830	0.00039



(a) P-CAPCE



(b) PTSLS

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

Table 14: Predicted CAPCE values by P-CAPCE estimator

$\begin{array}{c} W \\ \backslash \\ X \end{array}$	50	60	70	80	90	100	110	120	130	140	150
8	12.375	17.838	24.296	31.750	40.199	49.645	60.086	71.523	83.955	97.384	111.808
9	10.955	15.794	21.517	28.122	35.610	43.981	53.235	63.372	74.391	86.294	99.079
10	9.534	13.751	18.738	24.495	31.021	38.318	46.384	55.221	64.827	75.204	86.350
11	8.114	11.708	15.959	20.867	26.432	32.654	39.534	47.070	55.263	64.114	73.622
12	6.693	9.665	13.180	17.239	21.843	26.991	32.683	38.919	45.700	53.024	60.893
13	5.273	7.621	10.401	13.612	17.254	21.328	25.832	30.768	36.136	41.934	48.164
14	3.852	5.578	7.622	9.984	12.665	15.664	18.982	22.618	26.572	30.844	35.435
15	2.432	3.535	4.843	6.357	8.076	10.001	12.131	14.467	17.008	19.755	22.707
16	1.011	1.492	2.064	2.729	3.487	4.338	5.280	6.316	7.444	8.665	9.978
17	-0.409	-0.552	-0.715	-0.898	-1.102	-1.326	-1.570	-1.835	-2.120	-2.425	-2.751
18	-1.829	-2.595	-3.494	-4.526	-5.691	-6.989	-8.421	-9.986	-11.684	-13.515	-15.480

Table 15: Predicted CAPCE values by PTSLS estimator

$\begin{array}{c} W \\ \backslash \\ X \end{array}$	50	60	70	80	90	100	110	120	130	140	150
8	24.192	30.570	37.461	44.866	52.785	61.218	70.164	79.625	89.598	100.086	111.087
9	23.820	29.504	35.495	41.793	48.399	55.312	62.532	70.059	77.894	86.035	94.484
10	23.449	28.438	33.529	38.721	44.013	49.406	54.899	60.494	66.189	71.985	77.881
11	23.077	27.373	31.563	35.648	39.626	43.499	47.267	50.928	54.484	57.934	61.279
12	22.705	26.307	29.597	32.575	35.240	37.593	39.634	41.363	42.779	43.884	44.676
13	22.334	25.242	27.631	29.502	30.854	31.687	32.001	31.797	31.075	29.833	28.073
14	21.962	24.176	25.665	26.429	26.467	25.781	24.369	22.232	19.370	15.782	11.470
15	21.590	23.110	23.699	23.356	22.081	19.874	16.736	12.666	7.665	1.732	-5.133
16	21.219	22.045	21.733	20.283	17.694	13.968	9.104	3.101	-4.040	-12.319	-21.736
17	20.847	20.979	19.767	17.210	13.308	8.062	1.471	-6.465	-15.745	-26.369	-38.339
18	20.476	19.914	17.801	14.137	8.922	2.156	-6.162	-16.030	-27.449	-40.420	-54.941