Kernel Methods for Causal Functions: 
Dose Response Curves and 
Heterogeneous Treatment Effects

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Abstract

We propose a family of estimators based on kernel ridge regression for nonparametric causal functions such as the dose response curve, heterogeneous treatment effect, and incremental response curve. We assume selection on observable covariates. Treatment and covariates may be discrete or continuous and may take values in general spaces. We reduce causal estimation to combinations of kernel ridge regressions, which have closed form solutions and are easily computed by matrix operations, unlike other machine learning paradigms. We prove uniform consistency of the causal function estimators, with finite sample convergence rates that are the sums of minimax optimal rates for kernel ridge regression. In nonlinear simulations with many covariates, we demonstrate state-of-the-art performance despite the relative simplicity of our proposed approach. We estimate the dose response curve, heterogeneous treatment effect, and incremental response curve of the US Jobs Corps training program. As extensions, we generalize our main results to counterfactual distributions and to causal functions identified by Pearl’s front and back door criteria.

Keywords: potential outcome, reproducing kernel Hilbert space, program evaluation, uniform consistency, counterfactual distribution

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1 Introduction

1.1 Motivation

The goal of program evaluation is to determine the counterfactual relationship between treatment $D$ and outcome $Y$: if we intervened on treatment, what would be the expected counterfactual outcome $Y^{(d)}$? When treatment is binary, the causal parameter is a scalar $\theta_0 = \mathbb{E}[Y^{(1)} - Y^{(0)}]$ called the treatment effect; when treatment is continuous, it is a function $\theta_0(d) = \mathbb{E}[Y^{(d)}]$ called the dose response curve or average structural function [Imbens, 2000]. Under the assumption of selection on observable covariates $X$, the causal function $\theta_0(d)$ can be recovered by appropriately reweighting the regression function $\gamma_0(d, x) = \mathbb{E}[Y|D = d, X = x]$: $\theta_0(d) = \int \gamma_0(d, x) d\mathbb{P}(x)$ [Rosenbaum and Rubin, 1983] [Robins, 1986]. The same is true for other causal functions such as the heterogeneous treatment effect and incremental response curve, and even counterfactual distributions, albeit with different regressions and different reweightings. Therefore nonparametric estimation of a causal function involves three steps: estimating a nonlinear regression, with possibly many covariates; estimating the distribution for reweighting; and using the nonparametric distribution to reweight the nonparametric regression. For this reason, flexible estimation of nonparametric causal functions is often deemed too computationally demanding to be practical for program evaluation. See Section 2 for a discussion of related work.

We adapt kernel ridge regression, a classic machine learning algorithm that generalizes splines [Wahba, 1990], to address the computational challenges of estimating causal functions such as the dose response curve, heterogeneous treatment effect, and incremental response curve. Nonparametric estimation with kernels is considerably simpler: the nonlinear regres-
sion with many covariates can be estimated by simple matrix operations; the reweighting
distribution can be expressed as a regression problem and estimated by simple matrix
operations as well; and the step of reweighting can be performed by taking the product of
the results. The final nonparametric estimator for the causal function has a one line, closed
form solution, unlike previous work. This simplicity makes the family of estimators highly
practical. The proposed estimators are substantially simpler yet outperform some leading
alternatives in nonlinear simulations with many covariates. As extensions, we generalize
our new algorithmic techniques to counterfactual distributions and to graphical models.

Theoretically, our statistical guarantees rely on smoothness of the causal function and
spectral decay of the covariance operator rather than the explicit dimension of treatment,
covariates, or sparse approximations thereof. Such analysis aligns with economic modelling,
where many variables may matter for labor market decisions, yet economic theory suggests
that the effect of different intensities of job training should be smooth. These smoothness
and spectral decay approximation assumptions differ from the sparsity approximation
assumption that underpins Lasso type estimators. Under our assumptions, we prove that
our causal function estimators are uniformly consistent with rates that are the sums of
minimax optimal rates for nonparametric regressions. Our main results are nonasymptotic
and imply asymptotic uniform validity over large classes of models.

1.2 Contribution

We provide computational, statistical, and conceptual contributions to nonparametric causal
inference under the assumption of selection on observables. Through a case study, we
provide empirical contributions to the labor economics toolkit.
Computational. We demonstrate state-of-the-art performance in nonlinear simulations with many covariates, despite the relative simplicity of our proposed approach compared to existing machine learning approaches. In order to simplify the causal estimation problem, we assume that underlying conditional expectation functions are elements in a reproducing kernel Hilbert space (RKHS), a popular nonparametric setting in machine learning. With this additional structure, we propose a family of global estimators with closed form solutions. Throughout, the only hyperparameters are kernel hyperparameters and ridge regression penalties. The former have well known heuristics, and the latter are easily tuned using the closed form solution for generalized cross validation (which is asymptotically optimal) or leave-one-out cross validation (which we derive).

Statistical. We prove uniform consistency: our estimators converge to the true causal functions in sup norm, which encodes caution about worst case scenarios when informing policy decisions. Moreover, we provide finite sample rates of convergence, which help to evaluate the data requirements by explicitly accounting for each source of error at any finite sample size. Our rates do not directly depend on the data dimension, but rather the smoothness of the causal estimand and spectral decay of the covariance operator.\footnote{The rates may indirectly depend on dimension; see Section 5 for discussion in the context of the Sobolev space, which is a special case of an RKHS.} We generalize our main results to prove convergence in distribution for counterfactual distributions. At this point, the analysis of uniform confidence bands for our causal function estimators remains an open question that we pose for future research.\footnote{Uniform inference for kernel ridge regression remains an open question in statistics. For this reason, uniform confidence bands for our nonparametric estimators, which are inner products of kernel ridge regressions, remain an open question for future work.}

Conceptual. We provide a template for researchers to develop simple kernel estimators for complex causal estimands. We clarify five assumptions under which we derive our various
results: (i) identification, from the social scientific problem at hand; (ii) basic regularity conditions on the kernels, which are satisfied by all of the kernels typically used in practice; (iii) basic regularity on the outcome, treatment, and covariates, allowing them to be discrete or continuous variables that take values in general spaces (even texts, images, or graphs); (iv) smoothness of the causal estimand; and (v) spectral decay of the covariance operator. We combine these five assumptions to estimate causal functions.

**Empirical.** Our kernel ridge regression approach allows for simple yet flexible estimation of nuanced causal estimands. Such estimands provide meaningful insights about the Job Corps, the largest job training program for disadvantaged youth in the US. Our key statistical assumption is that different intensities of job training have smooth effects on counterfactual employment, and those effects are smoothly modified by age—an assumption motivated by labor market theory. In our program evaluation, we find that the effect of job training on employment substantially varies by class hours and by age; a targeted policy will be more effective. Our program evaluation confirms earlier findings while also uncovering meaningful heterogeneity. In this case study, we demonstrate how kernel methods for causal functions are a practical addition to the empirical economic toolkit.

The structure of the paper is as follows. Section 2 describes related work. Section 3 defines our class of causal functions. Section 4 proposes kernel methods for this class. Section 5 presents our theoretical guarantees of uniform consistency. Section 6 conducts nonlinear simulations as well as a real world program evaluation of the US Job Corps. Section 7 concludes. We extend our analysis to counterfactual distributions in Appendix A and to causal functions identified by Pearl’s front and back door criteria in Appendix B.
2 Related work

**Nonparametric causal functions.** We view nonparametric causal functions as reweightings of an underlying regression, synthesizing the $g$-formula [Robins, 1986] and partial means [Newey, 1994] frameworks. To express causal functions in this way, we build on canonical identification theorems under the assumption of selection on observables [Rosenbaum and Rubin, 1983, Robins, 1986, Altonji and Matzkin, 2005]. We propose simple, global estimators that combine kernel ridge regressions. Previous works that take a global view include [van der Laan and Dudoit, 2003, Luedtke and van der Laan, 2016b, Díaz and van der Laan, 2013, Kennedy, 2020], and references therein. A broad literature instead views causal functions as collections of localized treatment effects and proposes local estimators with Nadaraya-Watson smoothing, e.g. [Imai and Van Dyk, 2004, Rubin and van der Laan, 2005, Rubin and van der Laan, 2006, Galvao and Wang, 2015, Luedtke and van Kennedy et al., 2017, Semenova and Chernozhukov, 2021, Kallus and Zhou, 2018, Fan et al., 2019, Zimmert and Lechner, 2019, Colangelo and Lee, 2020], and references therein. By taking a global view rather than a local view, we propose simple estimators that can be computed once and evaluated at any value of a continuous treatment, rather than a computationally intensive procedure that must be reimplemented at any treatment value.

Our work appears to be the first to reduce estimation of the dose response curve, heterogeneous treatment effect, and incremental response curve to kernel ridge regressions. Previous works incorporating the RKHS into nonparametric estimation focus on different causal functions: nonparametric instrumental variable regression [Carrasco et al., 2007, Darolles et al., 2011, Singh et al., 2019], and heterogeneous treatment effect conditional on the full vector of covariates [Nie and Wager, 2021]. [Nie and Wager, 2021] propose the $R$
learner to estimate the heterogeneous treatment effect of binary treatment conditional on the entire covariate vector: \( \theta_0(x) = \mathbb{E}[Y^{(1)} - Y^{(0)} | X = x] \). See [Nie and Wager, 2021] Section 3 for a review of the extensive literature that considers this estimand. The R learner minimizes a loss that contains inverse propensities and different regularization [Nie and Wager, 2021] eq. A24, and it does not appear to have a closed form solution. The authors prove oracle mean square error rates. By contrast, we pursue a more general definition of heterogeneous treatment effect with discrete or continuous treatment, conditional on some interpretable subvector \( V \subseteq X \) [Abrevaya et al., 2015]: \( \theta_0(d, v) = \mathbb{E}[Y^{(d)} | V = v] \). Unlike previous work on nonparametric causal functions in the RKHS, we (i) consider dose and incremental response curves; (ii) propose estimators with closed form solutions; and (iii) prove uniform consistency, which is an important norm for policy evaluation.

**Counterfactual distributions.** We extend the framework from causal functions to counterfactual distributions. Existing work focuses on distributional generalizations of average treatment effect (ATE) or average treatment on the treated (ATT) for binary treatment [Firpo, 2007, Cattaneo, 2010, Chernozhukov et al., 2013], e.g. \( \theta_0 = \mathbb{P}(Y^{(1)}) - \mathbb{P}(Y^{(0)}) \). [Muandet et al., 2021] propose an RKHS approach for distributional ATE and ATT with binary treatment using inverse propensity scores and an assumption on the smoothness of a ratio of densities, which differs from our approach. Unlike previous work, we (i) allow treatment to be continuous; (ii) avoid inversion of propensity scores and densities; and (iii) study a broad class of counterfactual distributions for the full population, subpopulations, and alternative populations, e.g. \( \theta_0(d, v) = \mathbb{P}(Y^{(d)} | V = v) \).

This paper subsumes our previous draft [Singh et al., 2020] Section 2.
3 Causal functions

3.1 Definition

A causal function summarizes the expected counterfactual outcome $Y^{(d)}$ given a hypothetical intervention on continuous treatment $D = d$. The causal inference literature aims to measure a rich variety of causal functions with nuanced interpretation. We define these causal functions below. Unless otherwise noted, expectations are with respect to the population distribution $\mathbb{P}$. The operator $\nabla_d$ means $\partial/\partial d$.

**Definition 1** (Causal functions). We define

1. **Dose response**: $\theta_0^{ATE}(d) := \mathbb{E}[Y^{(d)}]$ is the counterfactual mean outcome given intervention $D = d$ for the entire population.

2. **Dose response with distribution shift**: $\theta_0^{DS}(d, \tilde{\mathbb{P}}) := \mathbb{E}_{\tilde{\mathbb{P}}}[Y^{(d)}]$ is the counterfactual mean outcome given intervention $D = d$ for an alternative population with data distribution $\tilde{\mathbb{P}}$ (elaborated in Assumption 2).

3. **Conditional dose response**: $\theta_0^{ATT}(d, d') := \mathbb{E}[Y^{(d')}|D = d]$ is the counterfactual mean outcome given intervention $D = d'$ for the subpopulation who actually received treatment $D = d$.

4. **Heterogeneous treatment effect**: $\theta_0^{CATE}(d, v) := \mathbb{E}[Y^{(d)}|V = v]$ is the counterfactual mean outcome given intervention $D = d$ for the subpopulation with covariate value $V = v$.

Likewise we define incremental functions, e.g. $\theta_0^{\nabla,ATE}(d) := \mathbb{E}[\nabla_d Y^{(d)}]$ and $\theta_0^{\nabla,ATT}(d, d') := \mathbb{E}[\nabla_d Y^{(d')}|D = d]$. 
The superscript of each nonparametric causal function corresponds to its familiar parametric analogue. Our results for means of potential outcomes immediately imply results for differences thereof. See Appendix A for counterfactual distributions and Appendix B for causal functions defined in graphical models.

The dose response curves $\theta_0^{ATE}(d)$ and $\theta_0^{DS}(d, \bar{P})$ are causal functions for entire populations. They are also called average structural functions in econometrics. The second argument of $\theta_0^{DS}(d, \bar{P})$ gets to the heart of external validity: though our data were drawn from population $P$, what would be the dose response curve for a different population $\bar{P}$? For example, a job training study may be conducted in Virginia, yet we may wish to inform policy in Arkansas, a state with different demographics [Hotz et al., 2005]. Predictive questions of this nature are widely studied in machine learning under the names of transfer learning, distribution shift, and covariate shift [Quiñonero-Candela et al., 2009].

$\theta_0^{ATE}(d)$ and $\theta_0^{DS}(d, \bar{P})$ are dose response curves for entire populations, but causal functions may vary for different subpopulations. Towards the goal of personalized or targeted interventions, an analyst may ask another nuanced counterfactual question: what would have been the effect of treatment $D = d'$ for the subpopulation who actually received treatment $D = d$? When treatment is continuous, we may define the conditional dose response $\theta_0^{ATT}(d, d') := \mathbb{E}[Y^{(d')} | D = d]$. This quantity is also called the conditional average structural function in econometrics [Altonji and Matzkin, 2005].

In $\theta_0^{ATT}(d, d')$, heterogeneity is indexed by treatment $D$. Heterogeneity may instead be indexed by some interpretable covariate subvector $V$, e.g. age, race, or gender [Abrevaya et al., 2015]. An analyst may therefore prefer to measure heterogeneous treatment effects for subpopulations characterized by different values of $V$. For simplicity, we will write covariates as $(V, X)$ for this setting, where $X$ are additional identifying covariates besides the interpretable
covariates of interest $V$. While many works focus on the special case where treatment is binary, our definition of heterogeneous treatment effect $\theta_{CATE}^{0}(d, v) := \mathbb{E}[Y(d) | V = v]$ allows for treatment $D$ that may be continuous.

### 3.2 Identification

In seminal work, [Rosenbaum and Rubin, 1983] state sufficient conditions under which causal functions—philosophical quantities defined in terms of potential outcomes $\{Y(d)\}$—can be measured from empirical quantities such as outcomes $Y$, treatments $D$, and covariates $(V, X)$. Colloquially, this collection of sufficient conditions is known as selection on observables. We assume selection on observables in the main text, and Pearl’s front and back door criteria in Appendix B.

**Assumption 1** (Selection on observables). Assume

1. No interference: if $D = d$ then $Y = Y^{(d)}$.

2. Conditional exchangeability: $\{Y^{(d)}\} \perp D | X$.

3. Overlap: if $f(x) > 0$ then $f(d|x) > 0$, where $f(x)$ and $f(d|x)$ are densities.

For $\theta_{CATE}^{0}$, replace $X$ with $(V, X)$.

No interference is also called the stable unit treatment value assumption. It rules out network effects, also called spillovers. Conditional exchangeability states that conditional on covariates $X$, treatment assignment is as good as random. Overlap ensures that there is no covariate stratum $X = x$ such that treatment has a restricted support. To handle $\theta_{DS}^{0}$, we place a standard assumption in transfer learning.

**Assumption 2** (Distribution shift). Assume
1. \[ \hat{P}(Y, D, X) = P(Y|D, X)\hat{P}(D, X); \]

2. \[ \hat{P}(D, X) \text{ is absolutely continuous with respect to } P(D, X). \]

The difference in population distributions \( P \) and \( \hat{P} \) is only in the distribution of treatments and covariates. Moreover, the support of \( P \) contains the support of \( \hat{P} \). An immediate consequence is that the regression \( \gamma_0(d, x) := \mathbb{E}[Y|D = d, X = x] \) remains the same across the different populations \( P \) and \( \hat{P} \).

**Lemma 1** (Identification of causal functions \([\text{Rosenbaum and Rubin, 1983} \text{ Robins, 1986}]\)). If Assumption [1] holds then

1. \[ \theta_0^{ATE}(d) = \int \gamma_0(d, x) dP(x). \]

2. If in addition Assumption [2] holds, then \[ \theta_0^{DS}(d, \hat{P}) = \int \gamma_0(d, x) d\hat{P}(x). \]

3. \[ \theta_0^{ATT}(d, d') = \int \gamma_0(d', x) dP(x|d). \]

4. \[ \theta_0^{CATE}(d, v) = \int \gamma_0(d, v, x) dP(x|v). \]

For \( \theta_0^{CATE} \), we use \( \gamma_0(d, v, x) := \mathbb{E}[Y|D = d, V = v, X = x] \). Likewise we identify incremental functions, e.g. \( \theta_0^{V:ATE}(d) = \int \nabla_d \gamma_0(d, x) dP(x) \) \([\text{Altonji and Matzkin, 2005}]\).

Lemma [1] clarifies the data requirements for estimating each causal function. The dose response \( \theta_0^{ATE}(d) \) requires observations of outcome \( Y \), treatment \( D \), and covariates \( X \) drawn from the population \( P \). The dose response with distribution shift \( \theta_0^{DS}(d, \hat{P}) \) additionally requires observations of covariates \( \hat{X} \) drawn from the alternative population \( \hat{P} \). The conditional dose response \( \theta_0^{ATT}(d, d') \) has the same data requirements as the dose response \( \theta_0^{ATE}(d) \). For the heterogeneous treatment effect \( \theta_0^{CATE}(d, v) \), we abuse notation by denoting the covariates by \( (V, X) \), where \( V \) is the subcovariate of interest and \( X \) are
other covariates such that selection on observables holds with respect to the union \((V, X)\).

An analyst requires observations of \((Y, D, V, X)\) drawn from the population \(\mathbb{P}\).

In particular, Lemma 1 expresses each causal function as a reweighting of the regression function \(\gamma_0\) according to a marginal or conditional distribution. As previewed in Section 1, nonparametric estimation of \(\theta_0^{CATE}(d, v)\) involves three steps: estimating a nonlinear regression \(\gamma_0(d, v, x)\), which may involve many covariates \(X\); estimating the distribution \(\mathbb{P}(x|v)\) for reweighting; and using the latter to reweight the former. In the next section, we propose original estimators that achieve all three steps in a one line, closed form solution.

4 Algorithm

To present the algorithm, we provide background on the RKHS. The essential property of a function \(\gamma\) in an RKHS \(\mathcal{H}\) is the eponymous reproducing property: \(\gamma(w) = \langle \gamma, \phi(w) \rangle_{\mathcal{H}}\) where \(\phi(w)\) are features, formally defined below, that can be interpreted as the dictionary of basis functions for \(\mathcal{H}\). Our key algorithmic insight is to interpret the reproducing property as a way to separate the function \(\gamma\) from the features \(\phi(w)\). We use this property to decouple the three steps of nonparametric causal estimation. The RKHS is precisely the class of functions for which the steps of nonparametric causal estimation can be separated. After providing RKHS background material, we prove an inner product representation that formalizes the decoupling, and then we introduce the causal estimators.

4.1 RKHS background

**Basic notation.** A *scalar-valued* RKHS \(\mathcal{H}\) is a Hilbert space with elements that are functions \(\gamma : \mathcal{W} \rightarrow \mathbb{R}\), on which the operator of evaluation is continuous. Polynomial, spline, and Sobolev spaces are widely used examples of RKHSs. \(\mathcal{W}\) can be
any Polish space, so a value \( w \in \mathcal{W} \) can be discrete or continuous. An RKHS is fully characterized by its feature map, which takes a point \( w \) in the original space \( \mathcal{W} \) and maps it to a feature \( \phi(w) \) in the RKHS \( \mathcal{H} \). The closure of \( \text{span}\{\phi(w)\}_{w \in \mathcal{W}} \) is the RKHS \( \mathcal{H} \).

In other words, \( \{\phi(w)\}_{w \in \mathcal{W}} \) can be viewed as the dictionary of basis functions for the RKHS \( \mathcal{H} \). The kernel \( k : \mathcal{W} \times \mathcal{W} \to \mathbb{R} \) is the inner product of features \( \phi(w) \) and \( \phi(w') \):

\[
k(w, w') = \langle \phi(w), \phi(w') \rangle_{\mathcal{H}}.
\]

A real-valued kernel \( k \) is continuous, symmetric, and positive definite. Though we have constructed the kernel from the feature map, the Moore-Aronszajn Theorem states that, for any positive definite kernel \( k \), there exists a unique RKHS \( \mathcal{H} \) with feature map \( \phi : w \mapsto k(w, \cdot) \). We have already seen that if \( \gamma \in \mathcal{H} \), then \( \gamma : \mathcal{W} \to \mathbb{R} \). With the additional notation of the feature map, we write \( \gamma(w) = \langle \gamma, \phi(w) \rangle_{\mathcal{H}} \). If \( \mathcal{W} \) is separable and \( \phi \) is continuous, then \( \mathcal{H} \) is separable and may be infinite dimensional.

**Kernel ridge regression.** The RKHS is a practical hypothesis space for nonparametric regression. Consider output \( Y \in \mathbb{R} \), input \( W \in \mathcal{W} \), and the goal of estimating the conditional expectation function \( \gamma_0(w) := \mathbb{E}[Y|W = w] \). A kernel ridge regression estimator of \( \gamma_0 \) is

\[
\hat{\gamma} := \arg\min_{\gamma \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \left[ Y_i - \langle \gamma, \phi(W_i) \rangle_{\mathcal{H}} \right]^2 + \lambda \|\gamma\|_{\mathcal{H}}^2.
\]

\( \lambda > 0 \) is a hyperparameter on the ridge penalty \( \|\gamma\|_{\mathcal{H}}^2 \), which imposes smoothness in estimation. The solution to the optimization problem has a well known closed form \[\text{Kimeldorf and Wahba, 1971}\], which we exploit and generalize throughout this work:

\[
\hat{\gamma}(w) = Y^T(K_{WW} + n\lambda I)^{-1}K_{Ww}.
\]

The closed form solution involves the kernel matrix \( K_{WW} \in \mathbb{R}^{n \times n} \) with \( (i,j) \)-th entry \( k(W_i, W_j) \), and the kernel vector \( K_{Ww} \in \mathbb{R}^n \) with \( i \)-th entry \( k(W_i, w) \). To tune the ridge penalty hyperparameter \( \lambda \), both generalized cross validation and leave-one-out cross validation have closed form solutions, and the former is asymptotically optimal \[\text{Li, 1986}\].
Kernel mean embedding. We have seen that the feature map takes a value in the original space \( w \in W \) and maps it to a feature in the RKHS \( \phi(w) \in \mathcal{H} \). Now we generalize this idea, from the embedding of a value \( w \) to the embedding of a distribution \( Q \). Just as a value \( w \) in the original space is embedded as an element \( \phi(w) \) in the RKHS, so too the distribution \( Q \) over the original space can be embedded as an element \( \mu := \mathbb{E}_Q[\phi(W)] \) in the RKHS \cite{Smola07, Berlinet11}. Boundedness of the kernel implies existence of the mean embedding as well as Bochner integrability, which permits us to exchange the expectation and inner product. Mean embeddings facilitate the evaluation of expectations of RKHS functions: for \( \gamma \in \mathcal{H} \), \( \mathbb{E}_Q[\gamma(W)] = \mathbb{E}_Q[\langle \gamma, \phi(W) \rangle_\mathcal{H}] = \langle \gamma, \mu \rangle_\mathcal{H} \). The final expression foreshadows how we will use the technique of mean embeddings to decouple the nonparametric regression step from the nonparametric reweighting step in the estimation of causal functions. A natural question is whether the embedding \( Q \mapsto \mathbb{E}_Q[\phi(W)] \) is injective, i.e. whether the RKHS element representation is unique. This property is called the characteristic property of the kernel \( k \), and it holds for commonly used RKHSs e.g. the exponentiated quadratic kernel \cite{Sriperumbudur10}.

Tensor product RKHS. The tensor product RKHS is one way to construct an RKHS for functions with multiple arguments. Suppose we define the RKHSs \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \) with positive definite kernels \( k_1 : \mathcal{W}_1 \times \mathcal{W}_1 \to \mathbb{R} \) and \( k_2 : \mathcal{W}_2 \times \mathcal{W}_2 \to \mathbb{R} \), respectively. By construction, an element \( \gamma_1 \in \mathcal{H}_1 \) is a function \( \gamma_1 : \mathcal{W}_1 \to \mathbb{R} \) and an element \( \gamma_2 \in \mathcal{H}_2 \) is a function \( \gamma_2 : \mathcal{W}_2 \to \mathbb{R} \). The tensor product RKHS \( \mathcal{H} := \mathcal{H}_1 \otimes \mathcal{H}_2 \) is the RKHS with the product kernel \( k : (\mathcal{W}_1 \times \mathcal{W}_2) \times (\mathcal{W}_1 \times \mathcal{W}_2) \to \mathbb{R}, \{(w_1, w_2), (w_1', w_2')\} \mapsto k_1(w_1, w_1') \cdot k_2(w_2, w_2'). \) Equivalently, the tensor product RKHS \( \mathcal{H} \) has feature map \( \phi(w_1) \otimes \phi(w_2) \). Formally, tensor product notation means that \( [a \otimes b]c = a\langle b, c \rangle \). An element of the tensor product RKHS \( \gamma \in \mathcal{H} \) is a function \( \gamma : \mathcal{W}_1 \times \mathcal{W}_2 \to \mathbb{R} \). In the present work, we will assume
that the regression function \( \gamma_0(w_1,w_2) := \mathbb{E}[Y|W = w_1, w_2 = w_2] \) is an element of a tensor product RKHS, i.e. \( \gamma_0 \in \mathcal{H} \). As such, the different arguments of \( \gamma_0 \) will be decoupled, which we will exploit when calculating partial means.

**RKHS for conditional expectation operators.** Finally, we introduce the RKHS \( \mathcal{L}_2(\mathcal{H}_1, \mathcal{H}_2) \) that we will employ for conditional expectation operators. Rather than being a space of real-valued functions, it is a space of Hilbert-Schmidt operators from one RKHS to another. If the operator \( E \) is an element of \( \mathcal{L}_2(\mathcal{H}_1, \mathcal{H}_2) \), then \( E : \mathcal{H}_1 \to \mathcal{H}_2 \). Formally, it can be shown that \( \mathcal{L}_2(\mathcal{H}_1, \mathcal{H}_2) \) is an RKHS in its own right with an appropriately defined kernel and feature map. \( \mathcal{L}_2(\mathcal{H}_1, \mathcal{H}_2) \) is an example of a *vector-valued* RKHS; see [Micchelli and Pontil, 2005](#) for a more general discussion. In the present work, we assume the conditional expectation operator \( E : \gamma_1(\cdot) \mapsto \mathbb{E}[\gamma_1(W_1)|W_2 = \cdot] \) is an element of this RKHS, i.e. \( E \in \mathcal{L}_2(\mathcal{H}_1, \mathcal{H}_2) \). We estimate \( E \) by a kernel ridge regression in \( \mathcal{L}_2(\mathcal{H}_1, \mathcal{H}_2) \), which coincides with estimating the conditional mean embedding \( \mu_{w_1}(w_2) := \mathbb{E}[\phi(W_1)|W_2 = w_2] \) via the kernel ridge regression of \( \phi(W_1) \) on \( \phi(W_2) \); see the derivation of Algorithm 1 below.

### 4.2 Inner product representation

Lemma 1 makes precise how each causal function is identified as a partial mean of the form \( \int \gamma_0(d,x)dQ \) for some distribution \( Q \). To facilitate estimation, we now assume that \( \gamma_0 \) is an element of an RKHS. In our construction, we define scalar valued RKHSs for treatment \( D \) and covariates \((V,X)\), then assume that the regression is an element of the tensor product space. Let \( k_D : \mathcal{D} \times \mathcal{D} \to \mathbb{R} \), \( k_V : \mathcal{V} \times \mathcal{V} \to \mathbb{R} \), and \( k_X : \mathcal{X} \times \mathcal{X} \to \mathbb{R} \) be measurable positive definite kernels corresponding to scalar valued RKHSs \( \mathcal{H}_D \), \( \mathcal{H}_V \), and \( \mathcal{H}_X \). Denote the feature maps \( \phi_D : \mathcal{D} \to \mathcal{H}_D, d \mapsto k_D(d,\cdot); \phi_V : \mathcal{V} \to \mathcal{H}_V, v \mapsto k_V(v,\cdot); \phi_X : \mathcal{X} \to \mathcal{H}_X, x \mapsto k_X(x,\cdot) \). To lighten notation, we suppress subscripts when arguments are provided, e.g. \( \phi(d) = \phi_D(d) \).
For $\theta_0^{ATE}$, $\theta_0^{DS}$, and $\theta_0^{ATT}$, we assume the regression $\gamma_0$ is an element of the RKHS $\mathcal{H}$ with the kernel $k(d, x; d', x') = k_D(d, d')k_X(x, x')$. In this construction, we appeal to the fact that the product of positive definite kernels corresponding to $\mathcal{H}_D$ and $\mathcal{H}_X$ defines a new positive definite kernel corresponding to $\mathcal{H}$. The product construction provides a rich composite basis; $\mathcal{H}$ has the tensor product feature map $\phi(d) \otimes \phi(x)$ and $\mathcal{H} = \mathcal{H}_D \otimes \mathcal{H}_X$. In this RKHS, $\gamma_0(d, x) = \langle \gamma_0, \phi(d) \otimes \phi(x) \rangle_{\mathcal{H}}$. Likewise for $\theta_0^{CATE}$ we assume $\gamma_0 \in \mathcal{H} := \mathcal{H}_D \otimes \mathcal{H}_V \otimes \mathcal{H}_X$. We place regularity conditions on this RKHS construction in order to represent causal functions as inner products in $\mathcal{H}$. In anticipation of counterfactual distributions in Appendix A, we also include conditions for an outcome RKHS in parentheses.

**Assumption 3** (RKHS regularity conditions). Assume

1. $k_D$, $k_V$, $k_X$ (and $k_Y$) are continuous and bounded. Formally, $\sup_{d \in D} \| \phi(d) \|_{\mathcal{H}_D} \leq \kappa_d$, $\sup_{v \in V} \| \phi(v) \|_{\mathcal{H}_V} \leq \kappa_v$, $\sup_{x \in X} \| \phi(x) \|_{\mathcal{H}_X} \leq \kappa_x$ (and $\sup_{y \in Y} \| \phi(y) \|_{\mathcal{H}_Y} \leq \kappa_y$).

2. $\phi(d)$, $\phi(v)$, $\phi(x)$ (and $\phi(y)$) are measurable.

3. $k_X$ (and $k_Y$) are characteristic.

For incremental functions, further assume $D \subset \mathbb{R}$ is an open set and $\nabla_d \nabla_d' k_D(d, d')$ exists and is continuous, hence $\sup_{d \in D} \| \nabla_d \phi(d) \|_{\mathcal{H}} \leq \kappa'_d$.

Commonly used kernels are continuous and bounded. Measurability is a similarly weak condition. The characteristic property ensures injectivity of the mean embeddings.

**Theorem 1** (Representation via kernel mean embeddings). Suppose the conditions of Lemma 1, Assumption 3, and $\gamma_0 \in \mathcal{H}$ hold. Then

1. $\theta_0^{ATE}(d) = \langle \gamma_0, \phi(d) \otimes \mu_x \rangle_{\mathcal{H}}$ where $\mu_x := \int \phi(x) d\mathbb{P}(x)$.

2. $\theta_0^{DS}(d, \tilde{P}) = \langle \gamma_0, \phi(d) \otimes \nu_x \rangle_{\mathcal{H}}$ where $\nu_x := \int \phi(x) d\tilde{\mathbb{P}}(x)$.
3. \( \theta_{0}^{ATT}(d, d') = \langle \gamma_0, \phi(d') \otimes \mu_x(d) \rangle_{\mathcal{H}} \) where \( \mu_x(d) := \int \phi(x)d\mathbb{P}(x|d) \).

4. \( \theta_{0}^{CATE}(d, v) = \langle \gamma_0, \phi(d) \otimes \phi(v) \otimes \mu_x(v) \rangle_{\mathcal{H}} \) where \( \mu_x(v) := \int \phi(x)d\mathbb{P}(x|v) \).

Likewise for incremental functions, e.g. \( \theta_{0}^{\nabla:ATE}(d) = \langle \gamma_0, \nabla \phi(d) \otimes \mu_x \rangle_{\mathcal{H}} \).

Proof sketch. Consider \( \theta_{0}^{CATE}(d, v) \). Boundedness of the kernel implies Bochner integrability, which allows us to exchange the integral and inner product:

\[
\int \gamma_0(d, v, x)d\mathbb{P}(x|v) = \int \langle \gamma_0, \phi(d) \otimes \phi(v) \otimes \phi(x) \rangle_{\mathcal{H}}d\mathbb{P}(x|v) = \langle \gamma_0, \phi(d) \otimes \mu_x \rangle_{\mathcal{H}}.
\]

See Appendix C for the full proof. \( \mu_x(v) := \int \phi(x)d\mathbb{P}(x|v) \) is the mean embedding of the conditional distribution \( \mathbb{P}(x|v) \). It encodes the distribution \( \mathbb{P}(x|v) \) as a vector \( \mu_x(v) \in \mathcal{H}_X \) such that the causal function \( \theta_{0}^{CATE}(d, v) \) can be expressed as an inner product in \( \mathcal{H} \).

4.3 Closed form solution

While the representation in Theorem 1 may appear abstract, it is essential to the algorithm derivation. In particular, the representation cleanly separates the three steps necessary to estimate a causal function: estimating a nonlinear regression, which may involve many covariates; estimating the distribution for reweighting; and using the nonparametric distribution to reweight the nonparametric regression. For example, for \( \theta_{0}^{CATE}(d, v) \), our estimator will be \( \hat{\theta}^{CATE}(d, v) = \langle \hat{\gamma}, \phi(d) \otimes \phi(v) \otimes \hat{\mu}_x \rangle_{\mathcal{H}} \). The nonlinear regression estimator \( \hat{\gamma} \) is a standard kernel ridge regression of \( Y \) on \( \phi(D) \otimes \phi(V) \otimes \phi(X) \); the reweighting distribution estimator \( \hat{\mu}_x \) is a generalized kernel ridge regression of \( \phi(X) \) on \( \phi(V) \); and the latter can be used to reweight the former by simply multiplying the two. This algorithmic insight is a key innovation of the present work, and the reason why our estimators have simple closed form solutions despite complicated causal reweighting.
Algorithm 1 (Estimation of causal functions). Denote the empirical kernel matrices $K_{DD}, K_{VV}, K_{XX} \in \mathbb{R}^{n \times n}$ calculated from observations drawn from population $P$. Let $\{\tilde{X}_i\}_{i \in [n]}$ be observations drawn from population $\tilde{P}$. Denote by $\odot$ the elementwise product.

Causal function estimators have the closed form solutions

1. $\hat{\theta}_{ATE}(d) = n^{-1} \sum_{i=1}^{n} Y^\top (K_{DD} \odot K_{XX} + n\lambda I)^{-1}(K_{Dd} \odot K_{Xx_i})$;

2. $\hat{\theta}_{DS}(d, \tilde{P}) = \tilde{n}^{-1} \sum_{i=1}^{\tilde{n}} Y^\top (K_{DD} \odot K_{XX} + n\lambda I)^{-1}(K_{Dd} \odot K_{X\tilde{x}_i})$;

3. $\hat{\theta}_{ATT}(d, d') = Y^\top (K_{DD} \odot K_{XX} + n\lambda I)^{-1}(K_{Dd'} \odot [K_{XX}(K_{DD} + n\lambda I)^{-1}K_{Dd}])$;

4. $\hat{\theta}_{CATE}(d, v) = Y^\top (K_{DD} \odot K_{VV} \odot K_{XX} + n\lambda I)^{-1}(K_{Dd} \odot K_{Vv} \odot K_{XX}(K_{VV} + n\lambda_2 I)^{-1}K_{Vv})$;

where $(\lambda, \lambda_1, \lambda_2)$ are ridge regression penalty hyperparameters. Likewise for incremental functions, e.g. $\hat{\theta}^{\nabla:ATE}(d) = n^{-1} \sum_{i=1}^{n} Y^\top (K_{DD} \odot K_{XX} + n\lambda I)^{-1}(\nabla_d K_{Dd} \odot K_{Xx_i})$ where $[\nabla_d K_{Dd}]_i = \nabla_d k(D_i, d)$.

Derivation sketch. Consider $\theta^*_{CATE}(d, v)$. Analogously to (1), the kernel ridge regression estimators of the regression $\gamma_0$ and the conditional mean embedding $\mu_x(v)$ are given by

\[
\hat{\gamma} = \arg\min_{\gamma \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \left[ Y_i - \langle \gamma, \phi(D_i) \otimes \phi(V_i) \otimes \phi(X_i) \rangle_{\mathcal{H}} \right]^2 + \lambda \| \gamma \|_{\mathcal{H}}^2,
\]

\[
\hat{E} = \arg\min_{E \in L_2(\mathcal{H}_x, \mathcal{H}_v)} \frac{1}{n} \sum_{i=1}^{n} \left[ \phi(X_i) - E^* \phi(V_i) \right]^2 + \lambda_2 \| E \|_{L_2(\mathcal{H}_x, \mathcal{H}_v)}^2,
\]

where $\hat{\mu}_x(v) = \hat{E}^* \phi(v)$ and $E^*$ is the adjoint of $E$. Analogously to (2), the closed forms are

\[
\hat{\gamma}(d, v, \cdot) = Y^\top (K_{DD} \odot K_{VV} \odot K_{XX} + n\lambda I)^{-1}(K_{Dd} \odot K_{Vv} \odot K_{X\cdot}),
\]

\[
[\hat{\mu}_x(v)](\cdot) = K_{X}(K_{VV} + n\lambda_2 I)^{-1}K_{V\cdot}.
\]

To arrive at the main result, match the empty arguments ($\cdot$) of the kernel ridge regressions. \(\square\)
See Appendix C for the full derivation. We give theoretical values for \((\lambda, \lambda_1, \lambda_2)\) that balance bias and variance in Theorem 2 below. Appendix D gives practical tuning procedures based on generalized cross validation and leave-one-out cross validation to empirically balance bias and variance. Note that \(\hat{\theta}^{DS}\) requires observations of covariates from \(\tilde{P}\).

For intuition, consider \(\hat{\theta}^{ATE}(d)\) with linear kernels \(k(d, d') = d \cdot d'\) and \(k(x, x') = x^\top x'\). Then by singular value decomposition,

\[
\hat{\theta}^{ATE}(d) = \left\{d \cdot \frac{1}{n} \sum_{i=1}^{n} X_i\right\}^\top \left\{\frac{1}{n} \sum_{i=1}^{n} D_i^2 X_i X_i^\top + \lambda I\right\}^{-1} \left\{\frac{1}{n} \sum_{i=1}^{n} D_i X_i \cdot Y_i\right\}.
\]

This formulation is interpretable as a regularized partial mean with basis function \(\phi(d, x) = dx\). However, it requires scalar treatment, finite dimensional covariate, linear ridge regression, and computation \(O(dim(X)^3)\). By contrast, the formulation in Algorithm 1 allows for generic treatment, generic covariate, nonlinear ridge regression, and computation \(O(n^3)\).

5 Consistency

In Section 3, we defined the causal functions of interest, and identified them as partial means. In Section 4 we introduced the tensor product RKHS as the function space in which the three steps of nonparametric causal estimation may be decoupled. We then proposed estimators based on kernel ridge regression with closed form solutions. In this section, we prove uniform consistency of the estimators, with finite sample rates that are the sums of minimax optimal rates. To do so, we define our key approximation assumptions, which are standard in RKHS learning theory: smoothness and spectral decay.
5.1 RKHS background

**Spectral view.** To state our key approximation assumptions, we must introduce a certain eigendecomposition. Recall the example of a generic RKHS $\mathcal{H}$ with kernel $k : \mathcal{W} \times \mathcal{W} \to \mathbb{R}$ consisting of functions $\gamma : \mathcal{W} \to \mathbb{R}$. Let $\nu$ be any Borel measure on $\mathcal{W}$. We denote by $L^2_\nu(\mathcal{W})$ the space of square integrable functions with respect to measure $\nu$. Given the kernel, define the integral operator $L : L^2_\nu(\mathcal{W}) \to L^2_\nu(\mathcal{W})$, $\gamma \mapsto \int k(\cdot, w)\gamma(w)d\nu(w)$. If the kernel $k$ is defined on $\mathcal{W} \subset \mathbb{R}^d$ and shift invariant, then $L$ is a convolution of $k$ and $\gamma$. If $k$ is smooth, then $L\gamma$ is a smoothed version of $\gamma$. $L$ is a self adjoint, positive, compact operator, so by the spectral theorem we can denote its countable eigenvalues by $\{\eta_j\}$ and its countable eigenfunctions, which are equivalence classes, by $\{[\varphi_j]\nu\}$:

$$L\gamma = \sum_{j=1}^{\infty} \eta_j \langle [\varphi_j]\nu, \gamma \rangle_{L^2_\nu(\mathcal{W})} \cdot [\varphi_j]\nu, \quad [\varphi_j]\nu := \{f : \nu(\{f \neq \varphi_j\}) = 0\}.$$

Without loss of generality, $\eta_j \geq \eta_{j+1}$, and these are also the eigenvalues of the feature covariance operator $T := \mathbb{E}[\phi(W) \otimes \phi(W)]$. For simplicity, we assume $\{\eta_j\} > 0$ in this discussion; see [Cucker and Smale, 2002] Remark 3 for the more general case. $\{[\varphi_j]\nu\}$ form an orthonormal basis of $L^2_\nu(\mathcal{W})$. By the generalized Mercer’s Theorem for Polish spaces [Steinwart and Scovel, 2012] Corollary 3.5], we can express the kernel as $k(w, w') = \sum_{j=1}^{\infty} \eta_j \varphi_j(w)\varphi_j(w')$, where $(w, w')$ are in the support of $\nu$, $\varphi_j$ is a continuous element in the equivalence class $[\varphi_j]\nu$, and the convergence is absolute and uniform.

With this notation, we express $L^2_\nu(\mathcal{W})$ and the RKHS $\mathcal{H}$ in terms of the series $\{[\varphi_j]\nu\}$. If $\gamma \in L^2_\nu(\mathcal{W})$, then $\gamma$ can be uniquely expressed as $\gamma = \sum_{j=1}^{\infty} \gamma_j [\varphi_j]\nu$ and the partial sums $\sum_{j=1}^{J} \gamma_j [\varphi_j]\nu$ converge to $\gamma$ in $L^2_\nu(\mathcal{W})$. Indeed,

$$L^2_\nu(\mathcal{W}) = \left\{ \gamma = \sum_{j=1}^{\infty} \gamma_j [\varphi_j]\nu : \sum_{j=1}^{\infty} \gamma_j^2 < \infty \right\}, \quad \langle \gamma, \gamma' \rangle_{L^2_\nu(\mathcal{W})} = \sum_{j=1}^{\infty} \gamma_j \gamma_j'.$$
for $\gamma = \sum_{j=1}^{\infty} \gamma_j \varphi_j$ and $\gamma' = \sum_{j=1}^{\infty} \gamma'_j \varphi_j$. By [Cucker and Smale, 2002, Theorem 4], the RKHS $\mathcal{H}$ corresponding to the kernel $k$ can be explicitly represented as

$$\mathcal{H} = \left\{ \gamma = \sum_{j=1}^{\infty} \gamma_j \varphi_j : \sum_{j=1}^{\infty} \frac{\gamma_j^2}{\eta_j} < \infty \right\}, \quad \langle \gamma, \gamma' \rangle_{\mathcal{H}} = \sum_{j=1}^{\infty} \frac{\gamma_j \gamma'_j}{\eta_j}.$$

Let us interpret this result, known as Picard’s criterion. Recall that $\{\eta_j\}$ is a weakly decreasing sequence. The RKHS $\mathcal{H}$ is the subset of functions in $L^2_\nu(\mathcal{W})$ which are continuous and for which higher order terms in the series $\{[\varphi_j]_{\nu}\}$ have a smaller contribution. The RKHS inner product is a penalized inner product; the penalty is on higher order coefficients, and the magnitude of the penalty corresponds to how small the eigenvalue is.

**Source condition.** We have seen how to conduct kernel ridge regression with the RKHS $\mathcal{H}$. To analyze the bias from ridge regularization, we place a smoothness assumption called the source condition on the regression function $\gamma_0(w) = \mathbb{E}[Y|W = w]$ [Smale and Zhou, 2007, Caponnetto and De Vito, 2007, Carrasco et al., 2007]. Formally, we place assumptions of the form

$$\gamma_0 \in \mathcal{H}^c := \left\{ f = \sum_{j=1}^{\infty} \gamma_j \varphi_j : \sum_{j=1}^{\infty} \frac{\gamma_j^2}{\eta_j^c} < \infty \right\} \subset \mathcal{H}, \quad c \in (1, 2]. \quad (3)$$

While $c = 1$ recovers correct specification $\gamma_0 \in \mathcal{H}$, $c \in (1, 2]$ is a stronger condition: $\gamma_0$ is a particularly smooth element of $\mathcal{H}$, well approximated by the leading terms in the series $\{[\varphi_j]_{\nu}\}$. Smoothness delivers uniform consistency. A larger value of $c$ corresponds to a smoother target $\gamma_0$ and a faster rate.

**Effective dimension.** To analyze the variance of kernel ridge regression, we place a spectral decay assumption called the effective dimension of the RKHS $\mathcal{H}$. To obtain faster rates, we place a direct assumption on the rate at which the eigenvalues $\{\eta_j\}$ decay: we

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\[4\]The fact that rates do not further improve for $c > 2$ is known as the saturation effect for ridge regularization.
assume there exists some constant $C$ such that for all $j$

$$\eta_j \leq Cj^{-b}, \quad b \geq 1.$$  (4)

A bounded kernel, which we have already assumed, implies $b = 1$  [Fischer and Steinwart, 2020] Lemma 10]. The limit $b \to \infty$ may be interpreted as a finite dimensional RKHS  [Caponnetto and De Vito, 2007]. For intermediate values of $b$, the polynomial rate of spectral decay quantifies the effective dimension of the RKHS $\mathcal{H}$ in light of the measure $\nu$. Intuitively, a higher value of $b$ corresponds to a lower effective dimension and a faster rate.

**Special case: Sobolev space.** For intuition, we relate the source condition and effective dimension to a familiar notion of smoothness in the Sobolev space. The restriction that defines an RKHS generalizes the restriction of higher order smoothness in a Sobolev space. Indeed, certain Sobolev spaces are RKHSs. Let $\mathcal{W} \subset \mathbb{R}^p$. Denote by $\mathbb{H}^s_2$ the Sobolev space with $s > p/2$ derivatives that are square integrable. This space can be generated by the Matèrn kernel. Suppose $\mathcal{H} = \mathbb{H}^s_2$ is chosen as the RKHS for estimation. Suppose the measure $\nu$ supported on $\mathcal{W}$ is absolutely continuous with respect to the uniform distribution and bounded away from zero. If $\gamma_0 \in \mathbb{H}^{s_0}_2$, then $c = s_0/s$  [Pillaud-Vivien et al., 2018]. Written another way, $[\mathbb{H}^s_2]^c = \mathbb{H}^{s_0}_2$. In this sense, $c$ precisely quantifies the additional smoothness of $\gamma_0$ relative to $\mathcal{H}$. Moreover, in this Sobolev space, $b = 2s/p > 1$  [Fischer and Steinwart, 2020]. The effective dimension is increasing in the input dimension $p$ and decreasing in the degree of smoothness $s$. We emphasize that our analysis applies to Sobolev spaces over $\mathbb{R}^p$ as a special case; our results are much more general, allowing treatment and covariates to take values in Polish spaces.

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5As $s \to \infty$, the Matèrn kernel converges to the popular exponentiated quadratic kernel.
5.2 Uniform consistency

Towards a guarantee of uniform consistency, we place regularity conditions on the original spaces. In anticipation of counterfactual distributions in Appendix A we also include conditions for the outcome space in parentheses.

**Assumption 4** (Original space regularity conditions). Assume

1. $\mathcal{D}$, $\mathcal{V}$, $\mathcal{X}$ (and $\mathcal{Y}$) are Polish spaces.

2. $\mathcal{Y} \subset \mathbb{R}$, $\int y^2 d\mathbb{P}(y) < \infty$, and a moment condition holds: there exist constants $\sigma, \tau$ such that for all $m \geq 2$, $\int |y - \gamma_0(D, X)|^m d\mathbb{P}(y|D, X) \leq m!\sigma^2\tau^{m-2}/2$ almost surely.

For $\theta_{0}^{CATE}$, replace $X$ with $(V, X)$.

A Polish space is a separable and completely metrizable topological space. Random variables with support in a Polish space may be discrete or continuous and may even be infinite dimensional. Bounded $Y$ implies the moment condition.

Next, we assume the regression $\gamma_0$ is smooth in the sense of (3), and $\mathcal{H}$ has low effective dimension in the sense of (4). Denote the $j$-th eigenvalue of the convolution operator for $\mathcal{H}$ by $\eta_j(\mathcal{H})$. Recall that $\eta_j(\mathcal{H})$ is also the $j$-th eigenvalue of the feature covariance operator.

**Assumption 5** (Smoothness and spectral decay for regression). Assume $\gamma_0 \in \mathcal{H}^c$ with $c \in (1, 2]$, and $\eta_j(\mathcal{H}) \leq Cj^{-b}$ with $b \geq 1$.

We place similar smoothness and spectral decay conditions on the conditional mean embeddings $\mu_x(d)$ and $\mu_x(v)$, which are generalized conditional expectation functions. We articulate this assumption abstractly for the conditional mean embedding $\mu_a(b) := \int \phi(a)d\mathbb{P}(a|b)$ where $a \in \mathcal{A}_\ell$ and $b \in \mathcal{B}_\ell$. In this way, all one has to do is specify $\mathcal{A}_\ell$ and
B_ℓ to specialize the assumption. For \(\mu_x(d), A_1 = \mathcal{X} \) and \(B_1 = \mathcal{D}\); for \(\mu_x(v), A_2 = \mathcal{X} \) and \(B_2 = \mathcal{V}\). For fixed \(A_\ell \) and \(B_\ell \), we parametrize smoothness by \(c_\ell \) and spectral decay by \(b_\ell \).

Formally, define the conditional expectation operator \(E_\ell : \mathcal{H}_{A_\ell} \to \mathcal{H}_{B_\ell}, f(\cdot) \mapsto \mathbb{E}[f(A_\ell)|B_\ell = \cdot]\). By construction, \(E_\ell \) encodes the same information as \(\mu_a(b)\) since

\[
[\mu_a(b)](\cdot) = \int \phi(a) d\mathbb{P}(a|b) = [E_\ell \phi(\cdot)](b) = [E_\ell^* \phi(b)](\cdot), \quad a \in A_\ell, \quad b \in B_\ell,
\]

where \(E_\ell^* \) is the adjoint of \(E_\ell \). We denote the space of Hilbert-Schmidt operators between \(\mathcal{H}_{A_\ell} \) and \(\mathcal{H}_{B_\ell} \) by \(L_2(\mathcal{H}_{A_\ell}, \mathcal{H}_{B_\ell})\). Grünewälder et al., 2013, Singh et al., 2019 prove that \(L_2(\mathcal{H}_{A_\ell}, \mathcal{H}_{B_\ell})\) is an RKHS in its own right, for which we can assume smoothness in the sense of (3) and spectral decay in the sense of (4).

**Assumption 6** (Smoothness and spectral decay for mean embedding). Assume \(E_\ell \in L_2(\mathcal{H}_{A_\ell}, \mathcal{H}_{B_\ell})\) with \(c_\ell \in (1, 2]\), and \(\eta_\ell(\mathcal{H}_{B_\ell}) \leq C j^{-b_\ell} \) with \(b_\ell \geq 1\).

Under these conditions, we arrive at our main theoretical guarantee.

**Theorem 2** (Uniform consistency of causal functions). Suppose Assumptions [1, 3, 4 and 5] hold. Set \((\lambda, \lambda_1, \lambda_2) = (n^{-1/(c+1/b)}, n^{-1/(c_1+1/b_1)}, n^{-1/(c_2+1/b_2)})\).

1. Then with high probability

\[
\|\hat{\theta}_{ATE} - \theta_{ATE}^0\|_\infty = O\left(n^{-\frac{1}{2} \frac{c-1}{c+1/b}}\right).
\]

2. If in addition Assumption [2] holds, then with high probability

\[
\|\hat{\theta}_{DS}(\cdot, \bar{P}) - \theta_{DS}^0(\cdot, \bar{P})\|_\infty = O\left(n^{-\frac{1}{2} \frac{c_1-1}{c+1/b}} + \tilde{n}^{-\frac{1}{2}}\right).
\]

3. If in addition Assumption [6] holds with \(A_1 = \mathcal{X} \) and \(B_1 = \mathcal{D}\), then with high probability

\[
\|\hat{\theta}_{ATT} - \theta_{ATT}^0\|_\infty = O\left(n^{-\frac{1}{2} \frac{c-1}{c+1/b}} + n^{-\frac{1}{2} \frac{c_1-1}{c_1+1/b_1}}\right).
\]
4. If in addition Assumption 6 holds with $A_2 = \mathcal{X}$ and $B_2 = \mathcal{V}$, then with high probability

$$\|\hat{\theta}_{CATE} - \theta_{0 CATE}\|_{\infty} = O \left( n^{-\frac{1}{2}} \varepsilon^{c_2} + n^{-\frac{1}{2}} \varepsilon^{c_2+1/b_2} \right).$$

Likewise for incremental functions, e.g. with high probability

$$\|\hat{\theta}_{\nabla ATE} - \theta_{0 \nabla ATE}\|_{\infty} = O \left( n^{-\frac{1}{2}} \varepsilon^{c_2} \right).$$

Explicit constants hidden by the $O(\cdot)$ notation are indicated in Appendices E and F, as well as explicit specializations of Assumption 6. These rates approach $n^{-1/4}$ when $(c, c_1, c_2) = 2$ and $(b, b_1, b_2) \to \infty$, i.e. when the regressions are smooth and when the effective dimensions are finite. Interestingly, each rate is the sum of minimax optimal rates in RKHS norm, which is stronger than sup norm: $n^{-\frac{1}{2}} \varepsilon^{c_2}$ is the minimax rate for standard kernel ridge regression [Fischer and Steinwart, 2020, Theorem 2]; $n^{-\frac{1}{2}} \varepsilon^{c_2}$ is the minimax rate for unconditional mean embeddings [Tolstikhin et al., 2017, Theorem 1]; and we conjecture that $n^{-\frac{1}{2}} \varepsilon^{c_2}$ is the minimax rate for conditional mean embeddings, though a lower bound analysis is a direction for future work. Overall, slow rates reflect the challenge of a sup norm guarantee, which is much stronger than a mean square error guarantee. The sup norm guarantee encodes caution about worst case scenarios when informing policy decisions.

6 Simulations and program evaluation

6.1 Simulations

We demonstrate that our nonparametric causal function estimators outperform some leading alternatives in nonlinear simulations with many covariates, despite the relative simplicity of our proposed approach. For each causal function design and sample size, we implement 100 simulations and calculate MSE with respect to the true causal function. Figure 1 visualizes
Figure 1: Nonparametric causal function simulations

The dose response curve design [Colangelo and Lee, 2020] involves learning the causal function $\theta_{0}^{ATE}(d) = 1.2d + d^2$. A single observation consists of the triple $(Y, D, X)$ for outcome, treatment, and high dimensional covariates where $Y, D \in \mathbb{R}$ and $X \in \mathbb{R}^{100}$. In addition to our one-line nonparametric estimator (RKHS), we implement the estimators of [Kennedy et al., 2017] (DR1), [Colangelo and Lee, 2020] (DR2), and [Semenova and Chernozhukov, 2021] (DR-series). DR1 and DR2 are local estimators that involve Nadaraya-Watson smoothing around doubly robust estimating equations. DR-series uses series regression with debiased pseudo outcomes, and we give it the advantage of correct specification as a quadratic function. By the Wilcoxon rank sum test, RKHS significantly outperforms alternatives at sample size 10,000, with p-value less than $10^{-3}$, despite its relative simplicity.

Though our approach allows for heterogeneous treatment effect of a continuous treatment, we implement a design for heterogeneous treatment effect of a binary treatment in order to facilitate comparison with existing methods. The heterogeneous treatment effect
design [Abrevaya et al., 2015] involves learning the causal functions $\theta_0^{CATE}(0, v) = 0$ and $\theta_0^{CATE}(1, v) = v(1 + 2v)^2(v - 1)^2$. A single observation consists of the tuple $(Y, D, V, X)$ for outcome, treatment, covariate of interest, and other covariates. In this design, $Y, D, V \in \mathbb{R}$ and $X \in \mathbb{R}^3$. In addition to our one-line nonparametric estimator (RKHS), we implement the estimators of [Abrevaya et al., 2015] (IPW) and [Semenova and Chernozhukov, 2021] (DR-series). The former involves Nadaraya-Watson smoothing around an inverse propensity estimator, and the latter involves (correctly specified) series regression with a debiased pseudo outcome. The R learner [Nie and Wager, 2021] cannot be implemented since $V \neq X$.

The simple RKHS approach significantly outperforms alternatives at sample sizes 500 and 1,000 by the Wilcoxon rank sum test, with p-values less than $10^{-5}$.

### 6.2 Program evaluation: US Job Corps

To demonstrate how kernel methods for causal functions are a practical addition to the empirical economic toolkit, we conduct a real-world program evaluation. Specifically, we estimate the dose response curve, heterogeneous treatment effect, and incremental response curve of the Jobs Corps, the largest job training program for disadvantaged youth in the US. The Job Corps is financed by the US Department of Labor, and it serves about 50,000 participants annually. Participation is free for individuals who meet low income requirements. Access to the program was randomized from November 1994 to February 1996; see [Schochet et al., 2008] for details. Many studies focus on data from this period to evaluate the effect of job training on employment [Flores et al., 2012, Colangelo and Lee, 2020]. Though access to the program was randomized, individuals could decide whether to participate and for how many hours. From a causal perspective, we assume selection on observables: conditional on observed covariates, participation was
Figure 2: Effect of job training on employment

exogenous on the extensive and intensive margins. From a statistical perspective, we assume that different intensities of job training have smooth effects on counterfactual employment, and that those effects are smoothly modified by age—assumptions motivated by labor market theory.

In this setting, the continuous treatment $D \in \mathbb{R}$ is total hours spent in academic or vocational classes in the first year after randomization, and the continuous outcome $Y \in \mathbb{R}$ is the proportion of weeks employed in the second year after randomization. The covariates $X \in \mathbb{R}^{40}$ include age, gender, ethnicity, language competency, education, marital status, household size, household income, previous receipt of social aid, family background, health,
and health related behavior at base line. As in [Colangelo and Lee, 2020], we focus on the
$n = 3,906$ observations for which $D \geq 40$, i.e. individuals who completed at least one week
of training. We implement various causal parameters in Figure 2: the dose response curve;
the incremental response curve; the discrete treatment effects with confidence intervals of
[Singh, 2021] (DR3); and the heterogeneous treatment effect with respect to age. For the
discrete effects, we discretize treatment into roughly equiprobable bins: $[40, 250], (250, 500],$
$(500, 750], (750, 1000], (1000, 1250], (1250, 1500], (1500, 1750], and (1750, 2000] class hours.
As far as we know, the heterogeneous treatment effect of class hours, a continuous treatment,
has not been previously studied in this empirical setting. In Appendix H, we provide
implementation details and verify that our results are robust to the choice of sample.

The dose response curve plateaus and achieves its maximum around $d = 500$, corre-
responding to 12.5 weeks of classes. Our global estimate (RKHS) has the same overall
shape but is smoother and slightly lower than the collection of local estimates from
[Colangelo and Lee, 2020] (DR2). The smoothness of our estimator is a consequence of
the RKHS assumptions, and we see how it is a virtue for empirical economic research; a
smooth dose response curve is more economically plausible in this setting. The first 12.5
weeks of classes confer most of the gain in employment: from 35% employment to more
than 47% employment for the average participant. The incremental response curve is the
derivative of the dose response curve, and it visualizes where the greatest gain happens. The
discrete treatment effects of [Singh, 2021] (DR3) corroborate our dose response curve, and
the 95% confidence intervals contain the dose response curve of [Colangelo and Lee, 2020]
(DR2) as well as our own (RKHS). Finally, the heterogeneous treatment effect shows that age
plays a substantial role in the effectiveness of the intervention. For the youngest participants,
the intervention has a small effect: employment only increases from 28% to at most 36%.
For older participants, the intervention has a large effect: employment increases from 40% to 56%. Our policy recommendation is therefore 12-14 weeks of classes targeting individuals 21-23 years old.

7 Conclusion

We propose a family of novel estimators for nonparametric causal functions. Our estimators are easily implemented with closed form solutions, yet outperform some of the more complicated machine learning alternatives, in nonlinear simulations with many covariates. The smoothness assumptions of the RKHS framework are economically plausible: different intensities of job training have smooth effects on counterfactual employment, and those effects are smoothly modified by age. As a contribution to the causal estimation literature, we propose flexible and practical estimators for causal functions identified by selection on observables. As a contribution to the RKHS literature, we demonstrate how kernel methods can decouple and simplify nonparametric causal estimation. We pose as a question for future work how to extend these methods to partially identified estimands, i.e. causal sets.

References

[Abrevaya et al., 2015] Abrevaya, J., Hsu, Y.-C., and Lieli, R. P. (2015). Estimating conditional average treatment effects. *Journal of Business & Economic Statistics*, 33(4):485–505.

[Altonji and Matzkin, 2005] Altonji, J. G. and Matzkin, R. L. (2005). Cross section and panel data estimators for nonseparable models with endogenous regressors. *Econometrica*, 73(4):1053–1102.
[Altun and Smola, 2006] Altun, Y. and Smola, A. (2006). Unifying divergence minimization and statistical inference via convex duality. In Conference on Computational Learning Theory, pages 139–153. Springer.

[Bach et al., 2012] Bach, F., Lacoste-Julien, S., and Obozinski, G. (2012). On the equivalence between herding and conditional gradient algorithms. In International Conference on Machine Learning, pages 1355–1362.

[Berlinet and Thomas-Agnan, 2011] Berlinet, A. and Thomas-Agnan, C. (2011). Reproducing Kernel Hilbert Spaces in Probability and Statistics. Springer Science & Business Media.

[Caponnetto and De Vito, 2007] Caponnetto, A. and De Vito, E. (2007). Optimal rates for the regularized least-squares algorithm. Foundations of Computational Mathematics, 7(3):331–368.

[Carrasco et al., 2007] Carrasco, M., Florens, J.-P., and Renault, E. (2007). Linear inverse problems in structural econometrics estimation based on spectral decomposition and regularization. Handbook of Econometrics, 6:5633–5751.

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

[Chernozhukov et al., 2013] Chernozhukov, V., Fernández-Val, I., and Melly, B. (2013). Inference on counterfactual distributions. Econometrica, 81(6):2205–2268.

[Colangelo and Lee, 2020] Colangelo, K. and Lee, Y.-Y. (2020). Double debiased machine learning nonparametric inference with continuous treatments. arXiv:2004.03036.
[Craven and Wahba, 1978] Craven, P. and Wahba, G. (1978). Smoothing noisy data with spline functions: Estimating the correct degree of smoothing by the method of generalized cross-validation. *Numerische Mathematik*, 31(4):377–403.

[Cucker and Smale, 2002] Cucker, F. and Smale, S. (2002). On the mathematical foundations of learning. *Bulletin of the American Mathematical Society*, 39(1):1–49.

[Darolles et al., 2011] Darolles, S., Fan, Y., Florens, J.-P., and Renault, E. (2011). Nonparametric instrumental regression. *Econometrica*, 79(5):1541–1565.

[Díaz and van der Laan, 2013] Díaz, I. and van der Laan, M. J. (2013). Targeted data adaptive estimation of the causal dose–response curve. *Journal of Causal Inference*, 1(2):171–192.

[Fan et al., 2019] Fan, Q., Hsu, Y.-C., Lieli, R. P., and Zhang, Y. (2019). Estimation of conditional average treatment effects with high-dimensional data. *arXiv:1908.02399*.

[Firpo, 2007] Firpo, S. (2007). Efficient semiparametric estimation of quantile treatment effects. *Econometrica*, 75(1):259–276.

[Fischer and Steinwart, 2020] Fischer, S. and Steinwart, I. (2020). Sobolev norm learning rates for regularized least-squares algorithms. *Journal of Machine Learning Research*, 21:205–1.

[Flores et al., 2012] Flores, C. A., Flores-Lagunes, A., Gonzalez, A., and Neumann, T. C. (2012). Estimating the effects of length of exposure to instruction in a training program: The case of Job Corps. *Review of Economics and Statistics*, 94(1):153–171.
[Fukumizu et al., 2013] Fukumizu, K., Song, L., and Gretton, A. (2013). Kernel Bayes’ rule: Bayesian inference with positive definite kernels. *Journal of Machine Learning Research*, 14(1):3753–3783.

[Galvao and Wang, 2015] Galvao, A. F. and Wang, L. (2015). Uniformly semiparametric efficient estimation of treatment effects with a continuous treatment. *Journal of the American Statistical Association*, 110(512):1528–1542.

[Grünewälder et al., 2013] Grünewälder, S., Gretton, A., and Shawe-Taylor, J. (2013). Smooth operators. In *International Conference on Machine Learning*, pages 1184–1192.

[Hotz et al., 2005] Hotz, V. J., Imbens, G. W., and Mortimer, J. H. (2005). Predicting the efficacy of future training programs using past experiences at other locations. *Journal of Econometrics*, 125(1-2):241–270.

[Huber et al., 2020] Huber, M., Hsu, Y.-C., Lee, Y.-Y., and Lettry, L. (2020). Direct and indirect effects of continuous treatments based on generalized propensity score weighting. *Journal of Applied Econometrics*.

[Imai and Van Dyk, 2004] Imai, K. and Van Dyk, D. A. (2004). Causal inference with general treatment regimes: Generalizing the propensity score. *Journal of the American Statistical Association*, 99(467):854–866.

[Imbens, 2000] Imbens, G. W. (2000). The role of the propensity score in estimating dose-response functions. *Biometrika*, 87(3):706–710.

[Kallus and Zhou, 2018] Kallus, N. and Zhou, A. (2018). Policy evaluation and optimization with continuous treatments. In *International Conference on Artificial Intelligence and Statistics*, pages 1243–1251.
[Kanagawa and Fukumizu, 2014] Kanagawa, M. and Fukumizu, K. (2014). Recovering distributions from Gaussian RKHS embeddings. In *Artificial Intelligence and Statistics*, pages 457–465.

[Kennedy, 2020] Kennedy, E. H. (2020). Optimal doubly robust estimation of heterogeneous causal effects. *arXiv:2004.14497*.

[Kennedy et al., 2017] Kennedy, E. H., Ma, Z., McHugh, M. D., and Small, D. S. (2017). Nonparametric methods for doubly robust estimation of continuous treatment effects. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 79(4):1229.

[Kimeldorf and Wahba, 1971] Kimeldorf, G. and Wahba, G. (1971). Some results on Tchebycheffian spline functions. *Journal of Mathematical Analysis and Applications*, 33(1):82–95.

[Li, 1986] Li, K.-C. (1986). Asymptotic optimality of CL and generalized cross-validation in ridge regression with application to spline smoothing. *The Annals of Statistics*, pages 1101–1112.

[Luedtke and van der Laan, 2016a] Luedtke, A. R. and van der Laan, M. J. (2016a). Statistical inference for the mean outcome under a possibly non-unique optimal treatment strategy. *Annals of Statistics*, 44(2):713.

[Luedtke and van der Laan, 2016b] Luedtke, A. R. and van der Laan, M. J. (2016b). Super-learning of an optimal dynamic treatment rule. *The International Journal of Biostatistics*, 12(1):305–332.

[Micchelli and Pontil, 2005] Micchelli, C. A. and Pontil, M. (2005). On learning vector-valued functions. *Neural Computation*, 17(1):177–204.
[Muandet et al., 2021] Muandet, K., Kanagawa, M., Saengkyongam, S., and Marukatat, S. (2021). Counterfactual mean embeddings. *Journal of Machine Learning Research*, 22(162):1–71.

[Newey, 1994] Newey, W. K. (1994). Kernel estimation of partial means and a general variance estimator. *Econometric Theory*, pages 233–253.

[Nie and Wager, 2021] Nie, X. and Wager, S. (2021). Quasi-oracle estimation of heterogeneous treatment effects. *Biometrika*, 108(2):299–319.

[Park and Muandet, 2020] Park, J. and Muandet, K. (2020). A measure-theoretic approach to kernel conditional mean embeddings. *Advances in Neural Information Processing Systems*, 33:21247–21259.

[Pearl, 1993] Pearl, J. (1993). Comment: Graphical models, causality and intervention. *Statistical Science*, 8(3):266–269.

[Pearl, 1995] Pearl, J. (1995). Causal diagrams for empirical research. *Biometrika*, 82(4):669–688.

[Pearl, 2009] Pearl, J. (2009). *Causality*. Cambridge University Press.

[Pillaud-Vivien et al., 2018] Pillaud-Vivien, L., Rudi, A., and Bach, F. (2018). Statistical optimality of stochastic gradient descent on hard learning problems through multiple passes. In *Advances in Neural Information Processing Systems*, pages 8114–8124.

[Quiñoñero-Candela et al., 2009] Quiñoñero-Candela, J., Sugiyama, M., Lawrence, N. D., and Schwaighofer, A. (2009). *Dataset Shift in Machine Learning*. MIT Press.

[Rasmussen and Williams, 2006] Rasmussen, C. E. and Williams, C. K. (2006). *Gaussian Processes for Machine Learning*, volume 2. MIT Press.
[Robins, 1986] Robins, J. (1986). A new approach to causal inference in mortality studies with a sustained exposure period—application to control of the healthy worker survivor effect. *Mathematical Modelling*, 7(9-12):1393–1512.

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

[Rubin and van der Laan, 2005] Rubin, D. and van der Laan, M. J. (2005). A general imputation methodology for nonparametric regression with censored data. Technical report, UC Berkeley Division of Biostatistics.

[Rubin and van der Laan, 2006] Rubin, D. and van der Laan, M. J. (2006). Extending marginal structural models through local, penalized, and additive learning. Technical report, UC Berkeley Division of Biostatistics.

[Schochet et al., 2008] Schochet, P. Z., Burghardt, J., and McConnell, S. (2008). Does Job Corps work? Impact findings from the national Job Corps study. *American Economic Review*, 98(5):1864–86.

[Semenova and Chernozhukov, 2021] Semenova, V. and Chernozhukov, V. (2021). Debiased machine learning of conditional average treatment effects and other causal functions. *The Econometrics Journal*, 24(2):264–289.

[Simon-Gabriel et al., 2020] Simon-Gabriel, C.-J., Barp, A., and Mackey, L. (2020). Metrizing weak convergence with maximum mean discrepancies. *arXiv:2006.09268*.

[Singh, 2021] Singh, R. (2021). Debiased kernel methods. *arXiv:2102.11076*.
[Singh et al., 2019] Singh, R., Sahani, M., and Gretton, A. (2019). Kernel instrumental variable regression. In *Advances in Neural Information Processing Systems*, pages 4595–4607.

[Singh et al., 2020] Singh, R., Xu, L., and Gretton, A. (2020). Kernel methods for policy evaluation: Treatment effects, mediation analysis, and off-policy planning. *arXiv:2010.04855*.

[Smale and Zhou, 2007] Smale, S. and Zhou, D.-X. (2007). Learning theory estimates via integral operators and their approximations. *Constructive Approximation*, 26(2):153–172.

[Smola et al., 2007] Smola, A., Gretton, A., Song, L., and Schölkopf, B. (2007). A Hilbert space embedding for distributions. In *International Conference on Algorithmic Learning Theory*, pages 13–31.

[Sriperumbudur, 2016] Sriperumbudur, B. (2016). On the optimal estimation of probability measures in weak and strong topologies. *Bernoulli*, 22(3):1839–1893.

[Sriperumbudur et al., 2010] Sriperumbudur, B., Fukumizu, K., and Lanckriet, G. (2010). On the relation between universality, characteristic kernels and RKHS embedding of measures. In *International Conference on Artificial Intelligence and Statistics*, pages 773–780.

[Steinwart and Christmann, 2008] Steinwart, I. and Christmann, A. (2008). *Support Vector Machines*. Springer Science & Business Media.

[Steinwart and Scovel, 2012] Steinwart, I. and Scovel, C. (2012). Mercer’s theorem on general domains: On the interaction between measures, kernels, and RKHSs. *Constructive Approximation*, 35(3):363–417.
[Sutherland, 2017] Sutherland, D. J. (2017). Fixing an error in Caponnetto and de Vito (2007). arXiv:1702.02982.

[Talwai et al., 2022] Talwai, P., Shameli, A., and Simchi-Levi, D. (2022). Sobolev norm learning rates for conditional mean embeddings. In International Conference on Artificial Intelligence and Statistics, pages 10422–10447.

[Tolstikhin et al., 2017] Tolstikhin, I., Sriperumbudur, B. K., and Muandet, K. (2017). Minimax estimation of kernel mean embeddings. The Journal of Machine Learning Research, 18(1):3002–3048.

[van der Laan and Dudoit, 2003] van der Laan, M. J. and Dudoit, S. (2003). Unified cross-validation methodology for selection among estimators and a general cross-validated adaptive epsilon-net estimator: Finite sample oracle inequalities and examples. Technical report, UC Berkeley Division of Biostatistics.

[Wahba, 1990] Wahba, G. (1990). Spline Models for Observational Data. SIAM.

[Welling, 2009] Welling, M. (2009). Herding dynamical weights to learn. In International Conference on Machine Learning, pages 1121–1128.

[Zimmert and Lechner, 2019] Zimmert, M. and Lechner, M. (2019). Nonparametric estimation of causal heterogeneity under high-dimensional confounding. arXiv:1908.08779.
Supplementary material

Appendix: Proofs and further discussion. (.pdf file)

Python code: Code to implement the novel algorithm described in the article. The job training data are publicly available. (.zip file)

A Counterfactual distributions

A.1 Definition

In the main text, we study causal functions defined as means of potential outcomes. In this section, we extend the estimators and analyses presented in the main text to counterfactual distributions of potential outcomes. A counterfactual distribution can be encoded by a kernel mean embedding using a new feature map \( \phi(y) \) for a new scalar valued RKHS \( \mathcal{H}_Y \).

We now allow \( Y \) to be a Polish space (Assumption 4).

**Definition 2** (Counterfactual distributions and embeddings). We define

1. Counterfactual distribution: \( \theta_0^{D:ATE}(d) := \mathbb{P}(Y^{(d)}) \) is the counterfactual distribution of outcomes given intervention \( D = d \) for the entire population.

2. Counterfactual distribution with distribution shift: \( \theta_0^{D:DS}(d, \tilde{P}) := \tilde{P}(Y^{(d)}) \) is the counterfactual distribution of outcomes given intervention \( D = d \) for an alternative population with data distribution \( \tilde{P} \) (elaborated in Assumption 2).

3. Conditional counterfactual distribution: \( \theta_0^{D:ATT}(d, d') := \mathbb{P}(Y^{(d')} | D = d) \) is the counterfactual distribution of outcomes given intervention \( D = d' \) for the subpopulation who actually received treatment \( D = d \).
4. Heterogeneous counterfactual distribution: \( \theta_0^{D:CATE}(d, v) := \mathbb{P}(Y(d)|V = v) \) is the counterfactual distribution of outcomes given intervention \( D = d \) for the subpopulation with covariate value \( V = v \).

Likewise we define counterfactual distribution embeddings, e.g. \( \tilde{\theta}_0^{D:ATE}(d) := \mathbb{E}[\phi(Y(d))] \).

Our strategy is to estimate the embedding of a counterfactual distribution. At that point, the analyst may use the embedding to (i) estimate moments of the counterfactual distribution [Kanagawa and Fukumizu, 2014] or (ii) sample from the counterfactual distribution [Welling, 2009]. Since we already analyze means in the main text, we focus on (ii) in this appendix.

A.2 Identification

The same identification results apply to counterfactual distributions.

**Lemma 2** (Identification of counterfactual distributions). If Assumption 1 holds then

1. \( [\theta_0^{D:ATE}(d)](y) = \int \mathbb{P}(y|d, x) d\mathbb{P}(x) \).

2. If in addition Assumption 2 holds, then \( [\theta_0^{D:DS}(d, \tilde{\mathbb{P}})](y) = \int \mathbb{P}(y|d, x) d\tilde{\mathbb{P}}(x) \).

3. \( [\tilde{\theta}_0^{D:ATT}(d, d')] (y) = \int \mathbb{P}(y|d', x) d\tilde{\mathbb{P}}(x|d) \) [Chernozhukov et al., 2013].

4. \( [\tilde{\theta}_0^{D:CATE}(d, v)](y) = \int \mathbb{P}(y|d, v, x) d\tilde{\mathbb{P}}(x|v) \).

Likewise for embeddings of counterfactual distributions. For example, if in addition Assumption 3 holds, then \( \tilde{\theta}_0^{D:ATE}(d) = \int \mathbb{E}[\phi(Y)|D = d, X = x] d\mathbb{P}(x) \).

The identification results for embeddings of counterfactual distributions resemble those presented in the main text. Define the generalized regressions \( \gamma_0(d, x) := \mathbb{E}[\phi(Y)|D = d, X = x] \) and \( \gamma_0(d, v, x) := \mathbb{E}[\phi(Y)|D = d, V = v, X = x] \). Then we can express these results in the familiar form, e.g. \( \tilde{\theta}_0^{D:ATE}(d) = \int \gamma_0(d, x) d\mathbb{P}(x) \).
A.3 Closed form solution

To estimate counterfactual distributions, we extend the RKHS construction in Section 4. As before, define scalar valued RKHSs for treatment $D$ and covariates $X$. Define an additional scalar valued RKHS for outcome $Y$. Because the regression $\gamma_0$ is now a conditional mean embedding, we present a construction involving a conditional expectation operator. Define the conditional expectation operator $E_3: \mathcal{H}_Y \to \mathcal{H}_D \otimes \mathcal{H}_X$, $f(\cdot) \mapsto \mathbb{E}[f(Y)|D = \cdot, X = \cdot]$. By construction $\gamma_0(d, x) = E_3^*[\phi(d) \otimes \phi(x)]$. As before, we replace $X$ with $(V, X)$ for $\theta_0^{D,CATE}$.

We place regularity conditions on this RKHS construction, similar to those in Section 4, to represent counterfactual distributions as evaluations of $E_3^*$. This representation allows for continuous treatment, unlike the representation in [Muandet et al., 2021, eq. 16, 17, 20].

Theorem 3 (Representation via kernel mean embeddings). Suppose the conditions of Lemma 2 hold. Further suppose Assumption 3 holds and $E_3 \in \mathcal{L}_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_X)$. Then

1. $\tilde{\theta}_0^{D,ATE}(d) = E_3^*[\phi(d) \otimes \mu_x]$ where $\mu_x := \int \phi(x) d\mathbb{P}(x)$.

2. $\tilde{\theta}_0^{D,DS}(d, \tilde{\mathbb{P}}) = E_3^*[\phi(d) \otimes \nu_x]$ where $\nu_x := \int \phi(x) d\tilde{\mathbb{P}}(x)$.

3. $\tilde{\theta}_0^{D,ATT}(d, d') = E_3^*[\phi(d') \otimes \mu_x(d)]$ where $\mu_x(d) := \int \phi(x) d\mathbb{P}(x|d)$.

4. $\tilde{\theta}_0^{D,CATE}(d, v) = E_3^*[\phi(d) \otimes \phi(v) \otimes \mu_x(v)]$ where $\mu_x(v) := \int \phi(x) d\mathbb{P}(x|v)$.

For $\theta_0^{D,CATE}$, we instead assume $E_3 \in \mathcal{L}_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_V \otimes \mathcal{H}_X)$.

See Appendix C for the proof. The mean embeddings are the same as in Theorem 1. They encode the reweighting distributions as elements in the RKHS such that the counterfactual distribution embeddings can be expressed as evaluations of $E_3^*$.

As in Section 4, the abstract representation helps to define estimators with closed form solutions that can be easily computed. In particular, the representation separates the
three steps necessary to estimate a counterfactual distribution: estimating a conditional
distribution, which may involve many covariates; estimating the distribution for reweighting;
and using one distribution to reweight another. For example, for \( \hat{\theta}^{D:CATE}(d, v) \), our estimator
is \( \hat{D:CATE}(d, v) = \hat{E}_v \phi(d) \otimes \phi(v) \otimes \mu_x(v) \). \( \hat{E}_v \) and \( \mu_x(v) \) are generalized kernel ridge
regressions, and the latter can be used to reweight the former by simply multiplying the
two. This algorithmic insight is a key innovation of the present work, and the reason why
our estimators have simple closed form solutions despite complicated causal reweighting.

Algorithm 2 (Estimation of counterfactual distribution embeddings). Denote the empirical
kernel matrices \( K_{DD}, K_{XX}, K_{YY} \in \mathbb{R}^{n \times n} \). Let \( \{\tilde{X}_i\}_{i \in [\tilde{n}]} \) be observations drawn from popu-
lation \( \tilde{P} \). Denote by \( \odot \) the elementwise product. The distribution embedding estimators
have the closed form solutions

1. \( \hat{\theta}^{D:ATE}(d)(y) = n^{-1} \sum_{i=1}^{n} K_{yy}(K_{DD} \odot K_{XX} + n\lambda_3 I)^{-1}(K_{Dd} \odot K_{Xx}) \);

2. \( \hat{\theta}^{D:DS}(d)(y) = \tilde{n}^{-1} \sum_{i=1}^{\tilde{n}} K_{yy}(K_{DD} \odot K_{XX} + n\lambda_3 I)^{-1}(K_{Dd} \odot K_{X\tilde{x}}) \);

3. \( \hat{\theta}^{D:ATT}(d, d')(y) = K_{yy}(K_{DD} \odot K_{XX} + n\lambda_3 I)^{-1}(K_{Dd'} \odot [K_{XX}(K_{DD} + n\lambda_1 I)^{-1}K_{Dd}]) \);

4. \( \hat{\theta}^{D:CATE}(d, v)(y) = K_{yy}(K_{DD} \odot K_{VV} \odot K_{XX} + n\lambda_3 I)^{-1}(K_{Dd} \odot K_{Vv} \odot [K_{XX}(K_{VV} + 
\quad n\lambda_2 I)^{-1}K_{Vv}]) \);

where \( (\lambda_1, \lambda_2, \lambda_3) \) are ridge regression penalty hyperparameters.

We derive these estimators in Appendix C. We give theoretical values for \( (\lambda_1, \lambda_2, \lambda_3) \)
that balance bias and variance in Theorem 2 below. Appendix D gives practical tuning
procedures based on generalized cross validation and leave-one-out cross validation to
empirically balance bias and variance. Note that \( \hat{D:DS} \) requires observations of covariates
from the alternative population \( \tilde{P} \). We avoid the estimation and inversion of propensity
scores in [Muandet et al., 2021 eq. 21].
Algorithm 2 estimates counterfactual distribution embeddings. The ultimate parameters of interest are counterfactual distributions. We present a deterministic procedure that uses the distribution embedding to provide samples \( \{\tilde{Y}_j\} \) from the distribution. In Theorem 5 below, we prove that these samples converge in distribution to the counterfactual distribution. The procedure is a variant of kernel herding [Welling, 2009, Muandet et al., 2021].

**Algorithm 3** (Estimation of counterfactual distributions). Recall that \( \hat{\theta}_0^{D:ATE}(d) \) is a mapping from \( \mathcal{Y} \) to \( \mathbb{R} \). Given \( \hat{\theta}_0^{D:ATE}(d) \), calculate

1. \( \tilde{Y}_1 = \arg\max_{y \in \mathcal{Y}} \left\{ \hat{\theta}_0^{D:ATE}(d)(y) \right\} \);
2. \( \tilde{Y}_j = \arg\max_{y \in \mathcal{Y}} \left\{ \hat{\theta}_0^{D:ATE}(d)(y) - \frac{1}{j+1} \sum_{\ell=1}^{j-1} k_y(\tilde{Y}_\ell, y) \right\} \) for \( j > 1 \).

Likewise for the other counterfactual distributions, replacing \( \hat{\theta}_0^{D:ATE}(d) \) with the other quantities in Algorithm 2.

By this procedure, samples from counterfactual distributions are straightforward to compute. With such samples, one may visualize a histogram as an estimator of the counterfactual density of potential outcomes. Alternatively, one may test statistical hypotheses.

### A.4 Convergence in distribution

Towards a guarantee of uniform consistency, we place regularity conditions on the original spaces as in Assumption 4. Importantly, we relax the condition that \( \mathcal{Y} \subset \mathbb{R} \); instead, we assume \( \mathcal{Y} \) is a Polish space. Next, we assume the regression \( \gamma_0 \) is smooth and quantify the spectral decay of its RKHS, parameterized in terms of the conditional expectation operator \( E_3 \). Likewise we assume the conditional mean embeddings \( \mu_x(d) \) and \( \mu_x(v) \) are smooth and quantify their spectral decay. With these assumptions, we arrive at our next main result.
Theorem 4 (Uniform consistency of counterfactual distribution embeddings). Suppose Assumptions 1, 3, 4, and 6 hold with $A_3 = Y$ and $B_3 = D \times X$ (or $B_3 = D \times V \times X$ for $\theta_0^{D:CATE}$). Set $(\lambda_1, \lambda_2, \lambda_3) = \left( n^{-1/(c_1+1/b_1)}, n^{-1/(c_2+1/b_2)}, n^{-1/(c_3+1/b_3)} \right)$.

1. Then with high probability
   $$
   \sup_{d \in D} \| \hat{\theta}_D^{D:ATE}(d) - \hat{\theta}_0^{D:ATE}(d) \|_{H_Y} = O \left( n^{-\frac{1}{2}} \frac{c_3^{-1}}{c_3+1/b_3} \right).
   $$

2. If in addition Assumption 2 holds, then with high probability
   $$
   \sup_{d \in D} \| \hat{\theta}_D^{D:DS}(d, \bar{\mathbb{P}}) - \hat{\theta}_0^{D:DS}(d, \bar{\mathbb{P}}) \|_{H_Y} = O \left( n^{-\frac{1}{2}} \frac{c_3^{-1}}{c_3+1/b_3} + \bar{n}^{-\frac{1}{2}} \right).
   $$

3. If in addition Assumption 6 holds with $A_1 = X$ and $B_1 = D$, then with high probability
   $$
   \sup_{d, d' \in D} \| \hat{\theta}_D^{D:ATT}(d, d') - \hat{\theta}_0^{D:ATT}(d, d') \|_{H_Y} = O \left( n^{-\frac{1}{2}} \frac{c_3^{-1}}{c_3+1/b_3} + n^{-\frac{1}{2}} \frac{c_1^{-1}}{c_1+1/b_1} \right).
   $$

4. If in addition Assumption 6 holds with $A_2 = X$ and $B_2 = V$, then with high probability
   $$
   \sup_{d \in D, v \in V} \| \hat{\theta}_D^{D:CATE}(d, v) - \hat{\theta}_0^{D:CATE}(d, v) \|_{H_Y} = O \left( n^{-\frac{1}{2}} \frac{c_3^{-1}}{c_3+1/b_3} + n^{-\frac{1}{2}} \frac{c_2^{-1}}{c_2+1/b_2} \right).
   $$

Explicit constants hidden by the $O(\cdot)$ notation are indicated in Appendix E as well as explicit specializations of Assumption 6. Again, these rates approach $n^{-1/4}$ when $(c_1, c_2, c_3) = 2$ and $(b_1, b_2, b_3) \to \infty$, i.e. when the regressions are smooth and when the effective dimensions are finite. Our assumptions do not include an assumption on the smoothness of an explicit density ratio, which appears in [Fukumizu et al., 2013, Theorem 11] and [Muandet et al., 2021, Assumption 3]. Finally, we state an additional regularity condition under which we can prove that the samples $\{\tilde{Y}_j\}$ calculated from the distribution embeddings weakly converge to the desired distribution.

Assumption 7 (Additional regularity). Assume
1. \( \mathcal{Y} \) is locally compact.

2. \( \mathcal{H}_\mathcal{Y} \subset \mathcal{C}_0 \), where \( \mathcal{C}_0 \) is the space of bounded, continuous, real valued functions that vanish at infinity.

As discussed by Simon-Gabriel et al., 2020, the combined assumptions that \( \mathcal{Y} \) is Polish and locally compact impose weak restrictions. In particular, if \( \mathcal{Y} \) is a Banach space, then to satisfy both conditions it must be finite dimensional. Trivially, \( \mathcal{Y} = \mathbb{R}^{\text{dim}(\mathcal{Y})} \) satisfies both conditions. We arrive at our final result of this section.

**Theorem 5** (Convergence in distribution of counterfactual distributions). Suppose the conditions of Theorem 4 hold, as well as Assumption 7. Suppose samples \( \{\tilde{Y}_j\} \) are calculated for \( \theta_0^{D:\text{ATE}}(d) \) as described in Algorithm 3. Then \( \{\tilde{Y}_j\} \xrightarrow{d} \theta_0^{D:\text{ATE}}(d) \). Likewise for the other counterfactual distributions, replacing \( \tilde{\theta}_0^{D:\text{ATE}}(d) \) with the other quantities in Algorithm 2.

See Appendix E for the proof. Note that samples are drawn for given value \( d \). Though our nonparametric consistency result is uniform across treatment values, this convergence in distribution result is for a fixed treatment value.

**B  Graphical models**

In the main text, we study causal functions defined in the potential outcomes framework and identified by selection on observables. In this appendix, we study causal functions and counterfactual distributions defined in the directed acyclic graph (DAG) framework and identified by Pearl’s front and back door criteria. We derive estimators, then prove uniform consistency and convergence in distribution.
B.1 DAG background

In computer science and epidemiology, DAGs provide another popular language for causal inference [Pearl, 2009]. Rather than reasoning about $\mathbb{P}(Y^{(d)})$, one reasons about $\mathbb{P}(Y|do(D = d))$. Both expressions $\mathbb{P}(Y^{(d)})$ and $\mathbb{P}(Y|do(D = d))$ are concerned with the distribution of outcome $Y$ given intervention $D = d$. For a specific setting, graphical criteria in terms of the DAG can help verify conditional independence statements in terms of potential outcomes.

In this section, we provide identification results in terms of causal DAGs, analogous to the identification results in terms of potential outcomes given in the main text. In doing so, we emphasize that our estimators also apply to a variety of settings that appear in computer science research. In particular, we focus on the front and back door criteria, which are the fundamental building blocks of DAG-based causal inference.

Assume the analyst has access to a causal DAG $G$ with vertex set $W$, partitioned into four disjoint sets $W = \{Y, D, X, U\}$. $Y$ is the outcome, $D$ is the set of treatments, $X$ is the set of covariates, and $U$ is the set of unobserved variables. Since counterfactual inquiries involve intervention on the graph $G$, we require notation for graph modification. Denote by $G_D$ the graph obtained by deleting from $G$ all arrows pointing into nodes in $D$. Denote by $G_D$ the graph obtained by deleting from $G$ all arrows emerging from nodes in $D$. We denote $d$-separation by $\perp_{d}$. Note that $d$-separation implies statistical independence. Throughout this section, we make the standard faithfulness assumption: $d$-connection implies statistical dependence.

B.2 Identification

We define causal functions and counterfactual distributions in terms of the $do$ operator on the DAG. For clarity of exposition, we focus on the case where $(D, Y)$ are nodes rather
than sets of nodes.

**Definition 3** (Causal function and counterfactual distribution: DAG). $\theta_d^{do}(d) := \mathbb{E}[Y|do(D = d)]$ is the counterfactual mean outcome given intervention $D = d$ for the entire population. Likewise we define the counterfactual distribution $\theta^{D:do}_0(d) := \mathbb{P}(Y|do(D = d))$ and counterfactual distribution embedding $\hat{\theta}_0^{D:do}(d) := \mathbb{E}[\phi(Y)|do(D = d)]$ as in Appendix A.

In seminal works, [Pearl, 1993, Pearl, 1995] states sufficient conditions under which such effects—philosophical quantities defined in terms of interventions on the graph—can be measured from empirical quantities such as outcomes $Y$, treatments $D$, and covariates $X$. We present two sets of sufficient conditions, known as the back door and front door criteria.

**Assumption 8** (Back door criterion). Assume

1. No node in $X$ is a descendent of $D$.

2. $X$ blocks every path between $D$ and $Y$ that contains an arrow into $D$: $(Y \perp_{d} D | X)_{G_D}$.

Intuitively, the analyst requires sufficiently many and sufficiently well placed covariates $X$ in the context of the graph $G$. Assumption 8 is satisfied if there is no unobserved confounder $U$, or if any unobserved confounder $U$ with a back door path into treatment $D$ is blocked by $X$.

**Assumption 9** (Front door criterion). Assume

1. $X$ intercepts all directed paths from $D$ to $Y$.

2. There is no unblocked back door path from $D$ to $X$.

3. All back door paths from $X$ to $Y$ are blocked by $D$.

4. $\mathbb{P}(d, x) > 0$. 

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Intuitively, these conditions ensure that $X$ serves to block all spurious paths from $D$ to $Y$; to leave all directed paths unperturbed; and to create no new spurious paths. As before, define the regression $\gamma_0(d, x) := \mathbb{E}[Y|D = d, X = x]$.

**Lemma 3** (Identification of causal function: DAG [Pearl, 1993; Pearl, 1995]). Depending on which criterion holds, the causal parameter $\theta_0^{do}(d)$ has different expressions.

1. If Assumption 8 holds then $\theta_0^{do}(d) = \int \gamma_0(d, x) dP(x)$.

2. If Assumption 9 holds then $\theta_0^{do}(d) = \int \gamma_0(d', x) dP(d') dP(x|d)$.

If in addition Assumption 3 holds then the analogous result holds for counterfactual distribution embeddings using $\gamma_0(d, x) := \mathbb{E}[\phi(Y)|D = d, X = x]$ instead, as in Appendix A.

Comparing Lemma 3 with Lemma 1, we see that if Assumption 8 holds then our dose response estimator $\hat{\theta}^{ATE}(d)$ in Section 4 is also a uniformly consistent estimator of $\theta_0^{do}(d)$. Similarly our counterfactual distribution estimator $\hat{\theta}^{D:ATE}(d)$ converges in distribution to $\hat{\theta}^{D:do}(d)$. In the remainder of this section, we therefore focus on what happens if Assumption 9 holds instead. We study the causal function and counterfactual distribution.

### B.3 Closed form solutions

We maintain notation from Section 4.

**Theorem 6** (Representation via kernel mean embedding: DAG). Suppose Assumptions 3 and 9 hold.

1. If an addition $\gamma_0 \in \mathcal{H}$ then $\theta_0^{do}(d) = \langle \gamma_0, \mu_d \otimes \mu_x(d) \rangle_{\mathcal{H}}$;

2. If in addition $E_3 \in L_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_X)$ then $\hat{\theta}_0^{do}(d) = E_3^\ast [\mu_d \otimes \mu_x(d)]$;

where $\mu_d := \int \phi(d) dP(d)$ and $\mu_x(d) := \int \phi(x) dP(x|d)$. 

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See Appendix C for the proof. The quantity $\mu_d := \int \phi(d) d\mathbb{P}(d)$ is the mean embedding of $\mathbb{P}(d)$. The quantity $\mu_x(d) := \int \phi(x) d\mathbb{P}(x|d)$ is the conditional mean embedding of $\mathbb{P}(x|d)$.

While this representation appears abstract, it helps to derive an estimator with a closed form solution as before. For $\theta_0^{do}(d)$, our estimator will be $\hat{\theta}^{FD}(d) = \langle \hat{\gamma}, \hat{\mu}_d \otimes \hat{\mu}_x(d) \rangle_H$. The estimator $\hat{\gamma}$ is a standard kernel ridge regression. The estimator $\hat{\mu}_d$ is an empirical mean. The estimator $\hat{\mu}_x(d)$ is an appropriately defined kernel ridge regression.

Algorithm 4 (Estimation of causal functions: DAG). Denote the empirical kernel matrices $K_{DD}, K_{XX}, K_{YY} \in \mathbb{R}^{n \times n}$ calculated from observations drawn from population $\mathbb{P}$. Denote by $\otimes$ the elementwise product. The front door criterion estimators have the closed form solutions

1. $\hat{\theta}^{FD}(d) = n^{-1} \sum_{i=1}^{n} Y_i^T (K_{DD} \otimes K_{XX} + n\lambda I)^{-1} (K_{Dd_i} \otimes \{ K_{XX} (K_{DD} + n\lambda_1 I)^{-1} K_{Dd_i} \})$

2. $[\hat{\theta}^{D:FD}(d)](y) = n^{-1} \sum_{i=1}^{n} K_{yY} (K_{DD} \otimes K_{XX} + n\lambda_3 I)^{-1} (K_{Dd_i} \otimes \{ K_{XX} (K_{DD} + n\lambda_1 I)^{-1} K_{Dd_i} \})$

where $(\lambda, \lambda_1, \lambda_3)$ are ridge regression penalty hyperparameters.

We derive this estimator in Appendix C. We give theoretical values for $(\lambda, \lambda_1, \lambda_3)$ that balance bias and variance in Theorem 7 below. Appendix D gives practical tuning procedures based on generalized cross validation and leave-one-out cross validation to empirically balance bias and variance.

**B.4 Uniform consistency and convergence in distribution**

Towards a guarantee of uniform consistency, we place the same assumptions as in Section 4.

**Theorem 7** (Uniform consistency of causal functions: DAG). Suppose the conditions of Theorem 6 hold, as well as Assumptions 4 and 6 with $A_1 = \mathcal{X}$ and $B_1 = \mathcal{D}$. Set $(\lambda, \lambda_1, \lambda_3) = (n^{-1/(c+1/b)}, n^{-1/(c_1+1/c_1)}, n^{-1/(c_3+1/b_3)})$. 

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1. If in addition Assumption 5 holds then with high probability

$$\|\hat{\theta}_F^D - \theta^d_0\|_\infty = O\left(n^{-\frac{1}{2} \frac{c_1-1}{c_1+c_1}} + n^{\frac{1}{2} \frac{c_1-1}{c_1+c_1}}\right).$$

2. If in addition Assumption 6 holds with \(A_3 = \mathcal{Y}\) and \(B_3 = \mathcal{D} \times \mathcal{X}\) then with high probability

$$\sup_{d \in \mathcal{D}} \|\hat{\theta}_D^{D,FD}(d) - \hat{\theta}_0^{D,do}(d)\|_{\mathcal{H}_\mathcal{Y}} = O\left(n^{-\frac{1}{2} \frac{c_3-1}{c_3+c_3}} + n^{-\frac{1}{2} \frac{c_1-1}{c_1+c_1}}\right).$$

Explicit constants hidden by the \(O(\cdot)\) notation are indicated in Appendix E. The rate is at best \(n^{-1/4}\) when \((c, c_1, c_3) = 2\) and \((b, b_1, b_3) \to \infty\), i.e. when the regressions are smooth and when the effective dimensions are finite. The slow rates reflect the challenge of a sup norm guarantee, which is much stronger than a mean square error guarantee. The sup norm guarantee encodes caution about worst case scenarios when informing policy decisions. Finally, we present a convergence in distribution result.

**Theorem 8** (Convergence in distribution of counterfactual distributions: DAG). Suppose the conditions of Theorem 7 hold, as well as Assumption 7. Suppose samples \(\{\tilde{Y}_j\}\) are calculated for \(\theta_D^{D,FD}(d)\) as described in Algorithm 3. Then \(\tilde{Y}_j \overset{d}{\to} \theta_0^{D,do}(d)\).

See Appendix E for the proof. Note that samples are drawn for given value \(d\). Though our nonparametric consistency result is uniform across treatment values, this convergence in distribution result is for a fixed treatment value.

**C Algorithm derivation**

In this appendix, we derive estimators for (i) causal functions, (ii) counterfactual distributions, and (iii) graphical models.
C.1 Causal functions

Proof of Theorem 1. In Assumption 3, we impose that the scalar kernels are bounded. This assumption has several implications. First, the feature maps are Bochner integrable \cite[Definition A.5.20]{Steinwart:2008}. Bochner integrability permits us to interchange expectation and inner product. Second, the mean embeddings exist. Third, the product kernel is also bounded and hence the tensor product RKHS inherits these favorable properties. By Lemma 1 and linearity of expectation,

\[
\theta_0^{ATE}(d) = \int \gamma_0(d, x) d\mathbb{P}(x)
= \int \langle \gamma_0, \phi(d) \otimes \phi(x) \rangle_{\mathcal{H}} d\mathbb{P}(x)
= \langle \gamma_0, \phi(d) \otimes \int \phi(x) d\mathbb{P}(x) \rangle_{\mathcal{H}}
= \langle \gamma_0, \phi(d) \otimes \mu_x \rangle_{\mathcal{H}}.
\]

Likewise for \(\theta_0^{DS}(d, \tilde{\mathbb{P}})\). Next,

\[
\theta_0^{ATT}(d, d') = \int \gamma_0(d', x) d\mathbb{P}(x|d)
= \int \langle \gamma_0, \phi(d') \otimes \phi(x) \rangle_{\mathcal{H}} d\mathbb{P}(x|d)
= \langle \gamma_0, \phi(d') \otimes \int \phi(x) d\mathbb{P}(x|d) \rangle_{\mathcal{H}}
= \langle \gamma_0, \phi(d') \otimes \mu_x(d) \rangle_{\mathcal{H}}.
\]

Finally,

\[
\theta_0^{CATE}(d, v) = \int \gamma_0(d, v, x) d\mathbb{P}(x|v)
= \int \langle \gamma_0, \phi(d) \otimes \phi(v) \otimes \phi(x) \rangle_{\mathcal{H}} d\mathbb{P}(x|v)
= \langle \gamma_0, \phi(d) \otimes \phi(v) \otimes \int \phi(x) d\mathbb{P}(x|v) \rangle_{\mathcal{H}}
= \langle \gamma_0, \phi(d) \otimes \phi(v) \otimes \mu_x(v) \rangle_{\mathcal{H}}.
\]
Lemma 4.34] guarantees that the derivative feature map 
\( \nabla_d \phi(d) \) exists, is continuous, and is Bochner integrable since

\[
\kappa'_d = \sqrt{\sup_{d,d' \in D} \nabla_d \nabla_d' k(d, d')} < \infty.
\]

Therefore the derivations remain valid for incremental functions. \( \Box \)

Derivation of Algorithm 1. By standard arguments [Kimeldorf and Wahba, 1971]

\[
\hat{\gamma}(d, x) = \langle \hat{\gamma}, \phi(d) \otimes \phi(x) \rangle_H = Y^\top (K_{DD} \otimes K_{XX} + n\lambda I)^{-1}(K_{Dd} \otimes K_{Xx}).
\]

The results for \( \hat{\theta}_{ATE}(d) \) holds by substitution:

\[
\hat{\mu}_x = \frac{1}{n} \sum_{i=1}^{n} \phi(x_i), \quad \hat{\theta}_{ATE}(d) = \langle \hat{\gamma}, \phi(d) \otimes \hat{\mu}_x \rangle_H.
\]

Likewise for \( \hat{\theta}_{DS}(d, \bar{P}) \).

The results for \( \hat{\theta}_{ATT}(d, d') \) and \( \hat{\theta}_{CATE}(d, v) \) use the closed form of the conditional mean embedding from [Singh et al., 2019, Algorithm 1]. Specifically,

\[
\hat{\mu}_x(d) = K_{X} (K_{DD} + n\lambda_1 I)^{-1} K_{Dd}, \quad \hat{\theta}_{ATT}(d, d') = \langle \hat{\gamma}, \phi(d') \otimes \hat{\mu}_x(d) \rangle_H
\]

and

\[
\hat{\mu}_x(v) = K_{X} (K_{VV} + n\lambda_2 I)^{-1} K_{Vv}, \quad \hat{\theta}_{CATE}(d, v) = \langle \hat{\gamma}, \phi(d) \otimes \phi(v) \otimes \hat{\mu}_x(v) \rangle_H.
\]

For incremental functions, replace \( \hat{\gamma}(d, x) \) with

\[
\nabla_d \hat{\gamma}(d, x) = \langle \hat{\gamma}, \nabla_d \phi(d) \otimes \phi(x) \rangle_H = Y^\top (K_{DD} \otimes K_{XX} + n\lambda I)^{-1}(\nabla_d K_{Dd} \otimes K_{Xx}).
\]
C.2 Counterfactual distributions

Proof of Theorem 3. Assumption 3 implies Bochner integrability, which permits the us to interchange expectation and evaluation. Therefore by Lemma 1 and linearity of expectation,

\[
\hat{\theta}_{0}^{D.ATE}(d) = \int \gamma_0(d, x) d\mathbb{P}(x) \\
= \int E_3^*[\phi(d) \otimes \phi(x)] d\mathbb{P}(x) \\
= E_3^*[\phi(d) \otimes \int \phi(x) d\mathbb{P}(x)] \\
= E_3^*[\phi(d) \otimes \mu_x].
\]

Likewise for \( \hat{\theta}_{0}^{D.DS}(d, \bar{\mathbb{P}}). \) Next,

\[
\hat{\theta}_{0}^{D.ATT}(d) = \int \gamma_0(d', x) d\mathbb{P}(x|d) \\
= \int E_3^*[\phi(d') \otimes \phi(x)] d\mathbb{P}(x|d) \\
= E_3^*[\phi(d') \otimes \int \phi(x) d\mathbb{P}(x|d)] \\
= E_3^*[\phi(d') \otimes \mu_x(d)].
\]

Finally,

\[
\hat{\theta}_{0}^{D.CATE}(d) = \int \gamma_0(d, v, x) d\mathbb{P}(x|v) \\
= \int E_3^*[\phi(d) \otimes \phi(v) \otimes \phi(x)] d\mathbb{P}(x|v) \\
= E_3^*[\phi(d) \otimes \phi(v) \otimes \int \phi(x) d\mathbb{P}(x|v)] \\
= E_3^*[\phi(d) \otimes \phi(v) \otimes \mu_x(v)].
\]

Derivation of Algorithm 2. By [Singh et al., 2019, Algorithm 1],

\[
\hat{\gamma}(d, x) = \hat{E}_3^*[\phi(d) \otimes \phi(x)] = K_Y (K_{DD} \otimes K_{XX} + n\lambda_3 I)^{-1} (K_{Dd} \otimes K_{Xx}).
\]
The result for $\hat{\theta}^{ATE}$ follows by substitution:

$$\hat{\mu}_x = \frac{1}{n} \sum_{i=1}^{n} \phi(x_i), \quad \hat{\theta}^{ATE}(d) = \hat{E}_3^* [\phi(d) \otimes \hat{\mu}_x].$$

Likewise for $\hat{\theta}^{DS}$. Both $\hat{\theta}^{ATT}$ and $\hat{\theta}^{CATE}$ appeal to the closed form for conditional mean embeddings from [Singh et al., 2019, Algorithm 1]. Specifically,

$$\hat{\mu}_x(d) = \mathbf{K}_X (\mathbf{K}_{DD} + n\lambda_1 \mathbf{I})^{-1} \mathbf{K}_{Dd}, \quad \hat{\theta}^{ATT}(d,d') = \hat{E}_3^* [\phi(d') \otimes \hat{\mu}_x(d)];$$

$$\hat{\mu}_x(v) = \mathbf{K}_X (\mathbf{K}_{VV} + n\lambda_2 \mathbf{I})^{-1} \mathbf{K}_{Vv}, \quad \hat{\theta}^{CATE}(d,v) = \hat{E}_3^* [\phi(d) \otimes \phi(v) \otimes \hat{\mu}_x(v)].$$

\hfill \Box

C.3 Graphical models

Proof of Theorem 6. Assumption 3 implies Bochner integrability, which permits the us to interchange expectation and inner product. Therefore

$$\hat{\theta}_0^{do}(d) = \int \gamma_0(d', x)d\mathbb{P}(d')d\mathbb{P}(x|d)$$

$$= \int \langle \gamma_0, \phi(d') \otimes \phi(x) \rangle_{H} d\mathbb{P}(d')d\mathbb{P}(x|d)$$

$$= \langle \gamma_0, \int \phi(d')d\mathbb{P}(d') \otimes \int \phi(x)d\mathbb{P}(x|d) \rangle_{H}$$

$$= \langle \gamma_0, \mu_d \otimes \mu_x(d) \rangle_{H}.$$ 

Similarly,

$$\tilde{\theta}_0^{d_{do}}(d) = \int \gamma_0(d', x)d\mathbb{P}(d')d\mathbb{P}(x|d)$$

$$= \int E_3^* [\phi(d') \otimes \phi(x)]d\mathbb{P}(d')d\mathbb{P}(x|d)$$

$$= E_3^* \left[ \int \phi(d')d\mathbb{P}(d') \otimes \int \phi(x)d\mathbb{P}(x|d) \right]$$

$$= E_3^* [\mu_d \otimes \mu_x(d)].$$
**Derivation of Algorithm 4.** Consider $\hat{\theta}^{do}$. By standard arguments [Kimeldorf and Wahba, 1971]

$$ \hat{\gamma}(d, x) = \langle \hat{\gamma}, \phi(d) \otimes \phi(x) \rangle_{\mathcal{H}} = Y^T(K_{DD} \otimes K_{XX} + n\lambda I)^{-1}(K_{Dd} \otimes K_{Xx}). $$

By [Singh et al., 2019, Algorithm 1], write the mean embedding and conditional mean embedding as

$$ \hat{\mu}_x = \frac{1}{n} \sum_{i=1}^n \phi(x_i), \quad \hat{\mu}_x(d) = K_X(K_{DD} + n\lambda_1 I)^{-1}K_{Dd}. $$

Substitute these quantities to obtain $\hat{\theta}^{do}(d) = \langle \hat{\gamma}, \hat{\mu}_d \otimes \hat{\mu}_x(d) \rangle_{\mathcal{H}}$. Next consider $\hat{\theta}^{D:do}$. By [Singh et al., 2019, Algorithm 1]

$$ \hat{\gamma}(d, x) = \hat{E}_3^*[\phi(d) \otimes \phi(x)] = K_Y(K_{DD} \otimes K_{XX} + n\lambda_3 I)^{-1}(K_{Dd} \otimes K_{Xx}). $$

Substitution of the mean embeddings gives $\hat{\theta}^{D:do}(d) = \hat{E}_3^*[\hat{\mu}_d \otimes \hat{\mu}_x(d)]$. 

\[\square\]

### D Tuning

In the present work, we propose a family of novel estimators that are combinations of kernel ridge regressions. As such, the same two kinds of hyperparameters that arise in kernel ridge regressions arise in our estimators: ridge regression penalties and kernel hyperparameters. In this section, we describe practical tuning procedures for such hyperparameters. To simplify the discussion, we focus on the regression of $Y$ on $W$. Recall that the closed form solution of the regression estimator using all observations is

$$ \hat{f}(w) = K_{ww}(K_{ww} + n\lambda I)^{-1}Y. $$

#### D.1 Ridge penalty

It is convenient to tune $\lambda$ by leave-one-out cross validation (LOOCV) or generalized cross validation (GCV), since the validation losses have closed form solutions.
Algorithm 5 (Ridge penalty tuning by LOOCV). Construct the matrices

\[ H_\lambda := I - K_{WW}(K_{WW} + n\lambda I)^{-1} \in \mathbb{R}^{n \times n}, \quad \tilde{H}_\lambda := diag(H_\lambda) \in \mathbb{R}^{n \times n} \]

where \( \tilde{H}_\lambda \) has the same diagonal entries as \( H_\lambda \) and off diagonal entries of 0. Then set

\[ \lambda^* = \arg \min_{\lambda \in \Lambda} \frac{1}{n} \| \tilde{H}_\lambda^{-1} H_\lambda Y \|_2^2, \quad \Lambda \subset \mathbb{R}. \]

Derivation. We prove that \( n^{-1} \| \tilde{H}_\lambda^{-1} H_\lambda Y \|_2^2 \) is the LOOCV loss. By definition, the LOOCV loss is

\[ E(\lambda) := n^{-1} \sum_{i=1}^n [Y_i - \hat{f}_{-i}(W_i)]^2 \]

where \( \hat{f}_{-i} \) is the regression estimator using all observations except the \( i \)-th observation.

Let \( \Phi \) be the matrix of features, with \( i \)-th row \( \phi(W_i)^\top \), and let \( Q := \Phi^\top \Phi + n\lambda I \). To lighten notation, we do not express functions and operators in bold font. By the regression first order condition,

\[ \hat{f} = Q^{-1}\Phi^\top Y, \quad \hat{f}_{-i} = \{ Q - \phi(W_i)\phi(W_i)^\top \}^{-1}\{ \Phi^\top Y - \phi(W_i)Y_i \}. \]

Recall the Sherman-Morrison formula for rank one updates:

\[ (A + uv^\top)^{-1} = A^{-1} - \frac{A^{-1}uv^\top A^{-1}}{1 + v^\top A^{-1}u}. \]

Hence

\[ \{ Q - \phi(W_i)\phi(W_i)^\top \}^{-1} = Q^{-1} + \frac{Q^{-1}\phi(W_i)\phi(W_i)^\top Q^{-1}}{1 - \phi(W_i)^\top Q^{-1}\phi(W_i)}. \]

Let \( \beta_i := \phi(W_i)^\top Q^{-1}\phi(W_i) \). Then

\[ \hat{f}_{-i}(W_i) = \phi(W_i)^\top \left\{ Q^{-1} + \frac{Q^{-1}\phi(W_i)\phi(W_i)^\top Q^{-1}}{1 - \beta_i} \right\} \{ \Phi^\top Y - \phi(W_i)Y_i \} \]

\[ = \phi(W_i)^\top \left\{ I + \frac{Q^{-1}\phi(W_i)\phi(W_i)^\top}{1 - \beta_i} \right\} \{ \hat{f} - Q^{-1}\phi(W_i)Y_i \} \]

\[ = \left\{ 1 + \frac{\beta_i}{1 - \beta_i} \right\} \phi(W_i)^\top \{ \hat{f} - Q^{-1}\phi(W_i)Y_i \} \]

\[ = \left\{ 1 + \frac{\beta_i}{1 - \beta_i} \right\} \{ \hat{f}(W_i) - \beta_i Y_i \} \]

\[ = \frac{1}{1 - \beta_i} \{ \hat{f}(W_i) - \beta_i Y_i \}. \]
i.e. $\hat{f}_{-i}$ can be expressed in terms of $\hat{f}$. Note that

$$Y_i - \hat{f}_{-i}(x_i) = Y_i - \frac{1}{1 - \beta_i} \{\hat{f}(W_i) - \beta_i Y_i\}$$

$$= Y_i + \frac{1}{1 - \beta_i} \{\beta_i Y_i - \hat{f}(W_i)\}$$

$$= \frac{1}{1 - \beta_i} \{Y_i - \hat{f}(W_i)\}.$$  

Substituting back into the LOOCV loss

$$\frac{1}{n} \sum_{i=1}^{n} \left[ Y_i - \hat{f}_{-i}(W_i) \right]^2 = \frac{1}{n} \sum_{i=1}^{n} \left[ \{Y_i - \hat{f}(W_i)\} \left\{ \frac{1}{1 - \beta_i} \right\} \right]^2$$

$$= \frac{1}{n} \|\tilde{H}^{-1} \{Y - K_{WW}(K_{WW} + n\lambda I)^{-1} Y\}\|_2^2$$

$$= \frac{1}{n} \|\tilde{H}^{-1} H_{\lambda} Y\|_2^2,$$

since

$$[\tilde{H}^{-1}]_{ii} = \frac{1}{[H_{\lambda}]_{ii}} = \frac{1}{[H_{\lambda}]_{ii}} = \frac{1}{1 - [K_{WW}(K_{WW} + n\lambda I)^{-1}]_{ii}}$$

and

$$K_{WW}(K_{WW} + n\lambda I)^{-1} = \Phi \Phi^\top (\Phi \Phi^\top + n\lambda I)^{-1} = \Phi (\Phi^\top \Phi + n\lambda I)^{-1} \Phi^\top = \Phi Q^{-1} \Phi^\top.$$ 

\[\square\]

**Algorithm 6** (Ridge penalty tuning by GCV). Construct the matrix

$$H_{\lambda} := I - K_{WW}(K_{WW} + n\lambda I)^{-1} \in \mathbb{R}^{n \times n}.$$  

Then set

$$\lambda^* = \arg\min_{\lambda \in \Lambda} \frac{1}{n} \|\{Tr(H_{\lambda})\}^{-1} \cdot H_{\lambda} Y\|_2^2, \quad \Lambda \subset \mathbb{R}.$$  

**Derivation.** We match symbols with the classic derivation of [Craven and Wahba, 1978].

Observe that

$$\begin{bmatrix} \hat{f}(W_1) \\ \vdots \\ f(W_n) \end{bmatrix} = K_{WW}(K_{WW} + n\lambda I)^{-1} Y = A_{\lambda} Y, \quad A_{\lambda} = K_{WW}(K_{WW} + n\lambda I)^{-1}.$$
Therefore
\[
H_\lambda = I - K_{WW}(K_{WW} + n\lambda I)^{-1} = I - A_\lambda.
\]

GCV can be viewed as a rotation invariant modification of LOOCV. In practice, we find that LOOCV and GCV provide almost identical hyperparameter values.

\section*{D.2 Kernel}

The exponentiated quadratic kernel is the most popular kernel among machine learning researchers:
\[
k(w, w') = \exp \left\{ -\frac{1}{2} \frac{||w - w'||^2}{\iota^2} \right\}.
\]
Importantly, this kernel satisfies the required properties; it is continuous, bounded, and characteristic.

\cite{Rasmussen2006} characterize the exponentiated quadratic RKHS as an attenuated series of the form
\[
H = \left\{ f = \sum_{j=1}^{\infty} f_j \varphi_j : \sum_{j=1}^{\infty} \frac{f_j^2}{\eta_j} < \infty \right\}, \quad \langle f, f' \rangle_H = \sum_{j=1}^{\infty} \frac{f_j f'_j}{\eta_j}.
\]
For simplicity, take \( \mathcal{W} = \mathbb{R} \) and take the measure \( \nu \) to be the standard Gaussian distribution (more generally, it can be the population distribution \( \mathbb{P} \)). Recall that the generalization of Mercer’s Theorem permits \( \mathcal{W} \) to be separable. Then the induced RKHS is characterized by
\[
\eta_j = \sqrt{\frac{2\bar{a}}{A}} \bar{B}^j, \quad \varphi_j(w) = \exp(-(\bar{c} - \bar{a})w^2)H_j(w\sqrt{2\bar{c}}).
\]
\( H_j \) is the \( j \)-th Hermite polynomial, and the constants \( (\bar{a}, \bar{b}, \bar{c}, \bar{A}, \bar{B}) > 0 \) are
\[
\bar{a} = \frac{1}{4}, \quad \bar{b} = \frac{1}{2\iota^2}, \quad \bar{c} = \sqrt{\bar{a}^2 + 2\bar{a}\bar{b}}, \quad \bar{A} = \bar{a} + \bar{b} + \bar{c}, \quad \bar{B} = \frac{\bar{b}}{\bar{A}} < 1.
\]
The eigenvalues \( \{\eta_j\} \) geometrically decay, and the series \( \{\varphi_j\} \) consists of weighted Hermite polynomials. For a function to belong to this RKHS, its coefficients on higher order weighted Hermite polynomials must be small.

Observe that the exponentiated quadratic kernel has a hyperparameter: the lengthscale \( \iota \). A convenient heuristic is to set the lengthscale equal to the median interpoint distance of \( \{W_i\}^n_{i=1} \), where the interpoint distance between observations \( i \) and \( j \) is \( \|W_i - W_j\|_W \). When the input \( W \) is multidimensional, we use the kernel obtained as the product of scalar kernels for each input dimension. For example, if \( W \subset \mathbb{R}^d \) then

\[
k(w, w') = \prod_{j=1}^d \exp \left\{ -\frac{1}{2} \frac{[w_j - w'_j]^2}{\iota_j^2} \right\}.
\]

Each lengthscale \( \iota_j \) is set according to the median interpoint distance for that input dimension.

In principle, we could instead use LOOCV or GCV to tune kernel hyperparameters in the same way that we use LOOCV or GCV to tune ridge penalties. However, given our choice of product kernel, this approach becomes impractical in high dimensions. For example, in the dose response curve design, \( D \in \mathbb{R} \) and \( X \in \mathbb{R}^{100} \) leading to a total of 101 lengthscales \( \{\iota_j\} \). Even with a closed form solution for LOOCV and GCV, searching over this high dimensional grid becomes cumbersome.

### E Uniform consistency proof

In this appendix, we (i) present an equivalent definition of smoothness and relate our key assumptions with previous work; (ii) present technical lemmas for regression, unconditional mean embeddings, and conditional mean embeddings; (iii) appeal to these lemmas to prove uniform consistency of causal functions as well as convergence in distribution for counterfactual distributions.
E.1 Assumptions revisited

E.1.1 Alternative representations of smoothness

Lemma 4 (Alternative representation of smoothness; Remark 2 of [Caponnetto and De Vito, 2007]).

If the input measure and Mercer measure are the same then there are equivalent formalisms for the source conditions in Assumptions 5 and 6.

1. The source condition in Assumption 5 holds if and only if the regression \( \gamma_0 \) is a particularly smooth element of \( \mathcal{H} \). Formally, define the covariance operator \( T \) for \( \mathcal{H} \). We assume there exists \( g \in \mathcal{H} \) such that \( \gamma_0 = T^{c-1/2} g, \ c \in (1,2], \) and \( \|g\|_\mathcal{H}^2 \leq \zeta \).

2. The source condition in Assumption 6 holds if and only if the conditional expectation operator \( E_\ell \) is a particularly smooth element of \( L_2(\mathcal{H}_{A_\ell}, \mathcal{H}_{B_\ell}) \). Formally, define the covariance operator \( T_\ell := E[\phi(B_\ell) \otimes \phi(B_\ell)] \) for \( L_2(\mathcal{H}_{A_\ell}, \mathcal{H}_{B_\ell}) \). We assume there exists \( G_\ell \in L_2(\mathcal{H}_{A_\ell}, \mathcal{H}_{B_\ell}) \) such that \( E_\ell = (T_\ell)^{c-1/2} \circ G_\ell, \ c \in (1,2], \) and \( \|G_\ell\|_{L_2(\mathcal{H}_{A_\ell}, \mathcal{H}_{B_\ell})}^2 \leq \zeta_\ell \).

Remark 1 (Covariance operator). The covariance operator \( T \) for the RKHS \( \mathcal{H} \) depends on the setting.

1. \( \theta_0^{ATE}, \theta_0^{DS}, \theta_0^{ATT} : T = \mathbb{E}[\{\phi(D) \otimes \phi(X)\} \otimes \{\phi(D) \otimes \phi(X)\}] ; \)

2. \( \theta_0^{CATE} : T = \mathbb{E}[\{\phi(D) \otimes \phi(V) \otimes \phi(X)\} \otimes \{\phi(D) \otimes \phi(V) \otimes \phi(X)\}] . \)

See [Singh et al., 2019] for the proof that \( T_\ell \) and its powers are well defined under Assumption 3.

E.1.2 Specific representations of smoothness

Next, we instantiate the source condition in Assumption 6 for the different settings considered in the main text.
Assumption 10 (Smoothness of mean embedding $\mu_x(d)$). Assume

1. The conditional expectation operator $E_1$ is well specified as a Hilbert-Schmidt operator between RKHSs, i.e. $E_1 \in L_2(\mathcal{H}_X, \mathcal{H}_D)$, where $E_1 : \mathcal{H}_X \to \mathcal{H}_D$, $f(\cdot) \mapsto \mathbb{E}[f(X)|D = \cdot]$.

2. The conditional expectation operator is a particularly smooth element of $L_2(\mathcal{H}_X, \mathcal{H}_D)$. Formally, define the covariance operator $T_1 := \mathbb{E}[\phi(D) \otimes \phi(D)]$ for $L_2(\mathcal{H}_X, \mathcal{H}_D)$. We assume there exists $G_1 \in L_2(\mathcal{H}_X, \mathcal{H}_D)$ such that $E_1 = (T_1)^{c_1-1} \circ G_1$, $c_1 \in (1, 2]$, and $\|G_1\|^2_{L_2(\mathcal{H}_X, \mathcal{H}_D)} \leq \zeta_1$.

Assumption 11 (Smoothness of mean embedding $\mu_x(v)$). Assume

1. The conditional expectation operator $E_2$ is well specified as a Hilbert-Schmidt operator between RKHSs, i.e. $E_2 \in L_2(\mathcal{H}_X, \mathcal{H}_Y)$, where $E_2 : \mathcal{H}_X \to \mathcal{H}_Y$, $f(\cdot) \mapsto \mathbb{E}[f(X)|V = \cdot]$.

2. The conditional expectation operator is a particularly smooth element of $L_2(\mathcal{H}_X, \mathcal{H}_Y)$. Formally, define the covariance operator $T_2 := \mathbb{E}[\phi(V) \otimes \phi(V)]$ for $L_2(\mathcal{H}_X, \mathcal{H}_Y)$. We assume there exists $G_2 \in L_2(\mathcal{H}_X, \mathcal{H}_Y)$ such that $E_2 = (T_2)^{c_2-1} \circ G_2$, $c_2 \in (1, 2]$, and $\|G_2\|^2_{L_2(\mathcal{H}_X, \mathcal{H}_Y)} \leq \zeta_2$.

Assumption 12 (Smoothness of conditional expectation operator $E_3$). Assume

1. The conditional expectation operator $E_3$ is well specified as a Hilbert-Schmidt operator between RKHSs, i.e. $E_3 \in L_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_X)$, where $E_3 : \mathcal{H}_Y \to \mathcal{H}_D \otimes \mathcal{H}_X$, $f(\cdot) \mapsto \mathbb{E}[f(Y)|D = \cdot, X = \cdot]$.

2. The conditional expectation operator is a particularly smooth element of $L_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_X)$. Formally, define the covariance operator $T_3 := \mathbb{E}[(\phi(D)\otimes\phi(X)) \otimes (\phi(D)\otimes\phi(X))]$ for $L_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_X)$. We assume there exists $G_3 \in L_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_X)$ such that $E_3 = (T_3)^{c_3-1} \circ G_3$, $c_3 \in (1, 2]$, and $\|G_3\|^2_{L_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_X)} \leq \zeta_3$. 61
E.1.3 Matching assumptions with previous work

Finally, we relate our approximation assumptions with previous work. Specifically, we match symbols with [Fischer and Steinwart, 2020].

Remark 2 (Matching assumptions). Recall our main approximation assumptions.

1. Source condition $c \in (1, 2]$. [Fischer and Steinwart, 2020] refer to the source condition as SRC parametrized by $\beta$. Matching symbols, $c = \beta$. A larger value of $c$ is a stronger assumption.

2. Effective dimension $b \geq 1$. [Fischer and Steinwart, 2020] refer to the effective dimension condition as EVD parametrized by $p$. Matching symbols, $b = 1/p$. A larger value of $b$ is a stronger assumption.

3. Embedding property $a \in (0, 1]$. [Fischer and Steinwart, 2020] place an additional assumption EMB parametrized by $\alpha \in (0, 1]$. In our setting of interest, $c \geq 1$ and the kernel is bounded. Together, these conditions imply $\alpha \leq 1$. Matching symbols, $a = \alpha$. A larger value of $a$ is a weaker assumption.

In our algorithm derivation, we have already assumed correct specification and bounded kernels, i.e. we have already assumed that $c \geq 1$, $b \geq 1$, and $a \leq 1$. By placing explicit source and effective dimension conditions, we derive rates that adapt to stronger assumptions $c > 1$ and $b > 1$.

It turns out that a further assumption of $a < 1$ does not improve the rate, so we omit that additional complexity. Observe that $c \geq 1$ and $b \geq 1$ imply $c + 1/b > 1 \geq a$ for any value $a \in (0, 1]$. The regime in which the inequality $c + 1/b > a$ holds is the regime in which the rate does not depend on $a$. [Fischer and Steinwart, 2020, Theorem 1.ii], so the weakest version of the embedding property is sufficient for our purpose. We pose as a question for
future work how to analyze the misspecified case, in which the stronger assumption of $a < 1$
may play an important role.

E.2 Lemmas

E.2.1 Regression

For expositional purposes, we summarize classic results for the kernel ridge regression estimator $\hat{\gamma}$
for $\gamma_0(w) := \mathbb{E}[Y|W = w]$. Consider the definitions

$$\gamma_0 = \arg\min_{\gamma \in \mathcal{H}} \mathcal{E}(\gamma), \quad \mathcal{E}(\gamma) = \mathbb{E}[(Y - \gamma(W))^2];$$

$$\hat{\gamma} = \arg\min_{\gamma \in \mathcal{H}} \hat{\mathcal{E}}(\gamma), \quad \hat{\mathcal{E}}(\gamma) = \frac{1}{n} \sum_{i=1}^{n} [Y_i - \gamma(W_i)]^2 + \lambda \|\gamma\|_{\mathcal{H}}^2.$$  

**Proposition 1** (Regression rate). Suppose Assumptions 3, 4, and 5 hold. Set $\lambda = \frac{n-1}{c+1/b}$. Then with probability $1 - \delta$, for $n$ sufficiently large, we have that

$$\|\hat{\gamma} - \gamma_0\|_{\mathcal{H}} \leq r_{\gamma}(n, \delta, b, c) := C \ln(4/\delta) \cdot n^{-\frac{c+1}{2c+1}},$$

where $C$ is a constant independent of $n$ and $\delta$.

Remark 5 in the subsequent, technical appendix elaborates on the meaning of the phrase $n$ sufficiently large.

**Proof.** We verify the conditions of [Fischer and Steinwart, 2020, Theorem 1.ii]. By Assumption 3, the kernel is bounded and measurable. Separability of the original spaces together with boundedness of the kernel imply that $\mathcal{H}$ is separable [Steinwart and Christmann, 2008, Lemma 4.33]. By Assumption 4, $\int y^2d\mathbb{P}(y) < \infty$. Since Assumption 5 implies $\gamma_0 \in \mathcal{H}$, we have that $\|\gamma_0\|_{\infty} \leq \kappa_w \|\gamma_0\|_{\mathcal{H}}$ by Cauchy-Schwarz inequality.

Next, we verify the assumptions called EMB, EVD, SRC, and MOM. Boundedness of the kernel implies EMB with $a = 1$. EVD is the assumption we call effective dimension,
parametrized by $b \geq 1$. SRC is the assumption we call the source condition, parametrized by $c \in (1, 2]$ in our case. MOM is a Bernstein moment condition satisfied by hypothesis. We study the RKHS norm guarantee, which corresponds to Hilbert scale equal to one. We are in regime (ii) of the theorem, since $c + 1/b > 1$. For the exact finite sample constant, see [Fischer and Steinwart, 2020, Theorem 16].

**E.2.2 Unconditional mean embedding**

For expositional purposes, we summarize classic results for the unconditional mean embedding estimator $\hat{\mu}_w$ for $\mu_w := \mathbb{E}[\phi(W)]$.

**Lemma 5** (Bennett inequality; Lemma 2 of [Smale and Zhou, 2007]). Let $\{\xi_i\}$ be i.i.d. random variables drawn from distribution $\mathbb{P}$ taking values in a real separable Hilbert space $\mathcal{K}$. Suppose there exists $M$ such that $\|\xi_i\|_\mathcal{K} \leq M < \infty$ almost surely and $\sigma^2(\xi_i) := \mathbb{E}\|\xi_i\|_\mathcal{K}^2$. Then for all $n \in \mathbb{N}$ and for all $\delta \in (0, 1)$,

$$
P\left[\left\|\frac{1}{n} \sum_{i=1}^{n} \xi_i - \mathbb{E}\xi_i\right\|_{\mathcal{K}} \leq \frac{2M \ln(2/\delta)}{n} + \sqrt{\frac{2\sigma^2(\xi) \ln(2/\delta)}{n}}\right] \geq 1 - \delta.
$$

**Proposition 2** (Mean embedding rate). Suppose Assumptions 3 and 4 hold. Then with probability $1 - \delta$,

$$
\|\hat{\mu}_w - \mu_w\|_{\mathcal{H}_W} \leq r_{\mu}(n, \delta) := \frac{4\kappa_w \ln(2/\delta)}{\sqrt{n}}.
$$

**Proof.** The result follows from Lemma 5 with $\xi_i = \phi(W_i)$, since

$$
\left\|\frac{1}{n} \sum_{i=1}^{n} \phi(W_i) - \mathbb{E}[\phi(W)]\right\|_{\mathcal{H}_W} \leq \frac{2\kappa_w \ln(2/\delta)}{n} + \sqrt{\frac{2\kappa_w^2 \ln(2/\delta)}{n}} \leq \frac{4\kappa_w \ln(2/\delta)}{\sqrt{n}}.
$$

[Altun and Smola, 2006, Theorem 15] originally prove this rate by McDiarmid inequality. See [Smola et al., 2007, Theorem 2] for an argument via Rademacher complexity. See [Tolstikhin et al., 2017, Proposition A.1] for an improved constant and the proof that the rate is minimax optimal.
Remark 3 (Kernel bound). Note that in various applications, $\kappa_w$ varies.

1. $\theta_0^{ATE}$ and $\tilde{\theta}_0^{D:ATE}$: with probability $1 - \delta$, $\|\hat{\mu}_x - \mu_x\|_{\mathcal{H}_x} \leq r_\mu(n, \delta) := \frac{4\kappa_x \ln(2/\delta)}{\sqrt{n}}$.

2. $\theta_0^{DS}$ and $\tilde{\theta}_0^{D:DS}$: with probability $1 - \delta$, $\|\hat{\nu}_x - \nu_x\|_{\mathcal{H}_x} \leq r_\nu(\widetilde{n}, \delta) := \frac{4\kappa_x \ln(2/\delta)}{\sqrt{n}}$.

E.2.3 Conditional expectation operator and conditional mean embedding

Next, we present original results for the generalized kernel ridge regression estimator $\hat{E}_\ell$ of the conditional expectation operator $E_\ell : \mathcal{H}_{A_\ell} \to \mathcal{H}_{B_\ell}$, $f(\cdot) \mapsto \mathbb{E}[f(A_\ell)|B_\ell = \cdot]$. We prove these results and compare them with previous work in Appendix [F].

Consider the definitions

$$E_\ell = \arg\min_{E \in L_2(\mathcal{H}_{A_\ell}, \mathcal{H}_{B_\ell})} \mathcal{E}(E), \quad \mathcal{E}(E) = \mathbb{E}[\{\phi(A_\ell) - E^*\phi(B_\ell)\}^2];$$

$$\hat{E}_\ell = \arg\min_{E \in L_2(\mathcal{H}_{A_\ell}, \mathcal{H}_{B_\ell})} \hat{\mathcal{E}}(E), \quad \hat{\mathcal{E}}(E) = \frac{1}{n} \sum_{i=1}^{n} [\phi(A_{\ell i}) - E^*\phi(B_{\ell i})]^2 + \lambda_\ell \|E\|_{L_2(\mathcal{H}_{A_\ell}, \mathcal{H}_{B_\ell})}^2.$$  

Proposition 3 (Conditional mean embedding rate). Suppose Assumptions 3, 4, and 6 hold. Set $\lambda_\ell = n^{-1/(c_\ell + 1/b_\ell)}$. Then with probability $1 - \delta$, for $n$ sufficiently large,

$$\|\hat{E}_\ell - E_\ell\|_{L_2} \leq r_E(\delta, n, b_\ell, c_\ell) := C \ln(4/\delta) \cdot n^{-\frac{1}{2} \frac{1}{c_\ell + 1/b_\ell}},$$

where $C$ is a constant independent of $n$ and $\delta$. Moreover, for all $b \in B_\ell$

$$\|\hat{\mu}_a(b) - \mu_a(b)\|_{\mathcal{H}_{A_\ell}} \leq r_\mu(\delta, n, b_\ell, c_\ell) := \kappa_b \cdot r_E(\delta, n, b_\ell, c_\ell).$$

Remark 5 in the subsequent, technical appendix elaborates on the meaning of the phrase $n$ sufficiently large.

Proof. We delay the proof of this result to the next appendix due to its technicality.

Remark 4 (Kernel bounds). Note that in various applications, $\kappa_a$ and $\kappa_b$ vary.

1. $\theta_0^{ATT}$ and $\tilde{\theta}_0^{ATT}$: $\kappa_a = \kappa_x$, $\kappa_b = \kappa_d$;
2. $\theta_0^{\text{ATE}}$ and $\hat{\theta}_0^{\text{ATE}}$: $\kappa_a = \kappa_x$, $\kappa_b = \kappa_v$;

3. Counterfactual distributions: $\kappa_a = \kappa_y$, $\kappa_b = \kappa_d \kappa_x$.

**E.3 Main results**

Appealing to Propositions 1, 2, and 3, we now prove consistency for (i) causal functions, (ii) counterfactual distributions, and (iii) graphical models.

**E.3.1 Causal functions**

Proof of Theorem 2. We initially consider $\theta_0^{\text{ATE}}$.

$$
\hat{\theta}^{\text{ATE}}(d) - \theta_0^{\text{ATE}}(d) = \langle \hat{\gamma}, \phi(d) \otimes \hat{\mu}_x \rangle_{\mathcal{H}} - \langle \gamma_0, \phi(d) \otimes \mu_x \rangle_{\mathcal{H}} \\
= \langle \hat{\gamma}, \phi(d) \otimes [\hat{\mu}_x - \mu_x] \rangle_{\mathcal{H}} + \langle [\hat{\gamma} - \gamma_0], \phi(d) \otimes \mu_x \rangle_{\mathcal{H}} \\
= \langle [\hat{\gamma} - \gamma_0], \phi(d) \otimes [\hat{\mu}_x - \mu_x] \rangle_{\mathcal{H}} + \langle [\hat{\gamma} - \gamma_0], \phi(d) \otimes \mu_x \rangle_{\mathcal{H}}.
$$

Therefore by Propositions 1 and 2, with probability $1 - 2\delta$,

$$
|\hat{\theta}^{\text{ATE}}(d) - \theta_0^{\text{ATE}}(d)| \leq \|\hat{\gamma} - \gamma_0\|_{\mathcal{H}} \|\phi(d)\|_{\mathcal{H}} \|\hat{\mu}_x - \mu_x\|_{\mathcal{H}} \\
+ \|\gamma_0\|_{\mathcal{H}} \|\phi(d)\|_{\mathcal{H}} \|\hat{\mu}_x - \mu_x\|_{\mathcal{H}} \\
+ \|\hat{\gamma} - \gamma_0\|_{\mathcal{H}} \|\phi(d)\|_{\mathcal{H}} \|\mu_x\|_{\mathcal{H}} \\
\leq \kappa_d \cdot r_\gamma(n, \delta, b, c) \cdot r_\mu(n, \delta) + \kappa_d \cdot \|\gamma_0\|_{\mathcal{H}} \cdot r_\mu(n, \delta) + \kappa_d \kappa_x \cdot r_\gamma(n, \delta, b, c) \\
= O\left(n^{-\frac{1}{2} c+\frac{1}{2}} + \frac{\tilde{n}^{-\frac{1}{2}}}{\tilde{c}+\frac{1}{2}}\right).
$$

By the same argument, with probability $1 - 2\delta$,

$$
|\hat{\theta}^{\text{DS}}(d, \bar{P}) - \theta_0^{\text{DS}}(d, \bar{P})| \\
\leq \kappa_d \cdot r_\gamma(n, \delta, b, c) \cdot r_\nu(\tilde{n}, \delta) + \kappa_d \cdot \|\gamma_0\|_{\mathcal{H}} \cdot r_\nu(\tilde{n}, \delta) + \kappa_d \kappa_x \cdot r_\gamma(n, \delta, b, c) \\
= O\left(n^{-\frac{1}{2} c+\frac{1}{2}} + \frac{\tilde{n}^{-\frac{1}{2}}}{\tilde{c}+\frac{1}{2}}\right).
$$
Next, consider $\theta_0^{ATT}$.

\[
\hat{\theta}^{ATT}(d, d') - \theta_0^{ATT}(d, d') = \langle \hat{\gamma}, \phi(d') \otimes \hat{\mu}_x(d) \rangle_{\mathcal{H}} - \langle \gamma_0, \phi(d') \otimes \mu_x(d) \rangle_{\mathcal{H}} \\
= \langle \hat{\gamma}, \phi(d') \otimes [\hat{\mu}_x(d) - \mu_x(d)] \rangle_{\mathcal{H}} + \langle [\hat{\gamma} - \gamma_0], \phi(d') \otimes \mu_x(d) \rangle_{\mathcal{H}} \\
= \langle [\hat{\gamma} - \gamma_0], \phi(d') \otimes [\hat{\mu}_x(d) - \mu_x(d)] \rangle_{\mathcal{H}} \\
+ \langle \gamma_0, \phi(d') \otimes [\hat{\mu}_x(d) - \mu_x(d)] \rangle_{\mathcal{H}} \\
+ \langle [\hat{\gamma} - \gamma_0], \phi(d') \otimes \mu_x(d) \rangle_{\mathcal{H}}.
\]

Therefore by Propositions 1 and 3, with probability $1 - 2\delta$,

\[
|\hat{\theta}^{ATT}(d, d') - \theta_0^{ATT}(d, d')| \leq \|\hat{\gamma} - \gamma_0\|_{\mathcal{H}} \|\phi(d')\|_{\mathcal{H}_D} \|\hat{\mu}_x(d) - \mu_x(d)\|_{\mathcal{H}_X} \\
+ \|\gamma_0\|_{\mathcal{H}} \|\phi(d')\|_{\mathcal{H}_D} \|\hat{\mu}_x(d) - \mu_x(d)\|_{\mathcal{H}_X} \\
+ \|\hat{\gamma} - \gamma_0\|_{\mathcal{H}} \|\phi(d')\|_{\mathcal{H}_D} \|\mu_x(d)\|_{\mathcal{H}_X} \\
\leq \kappa_d \cdot r_\gamma(n, \delta, b, c) \cdot r_\mu^{ATT}(n, \delta, b_1, c_1) + \kappa_d \cdot \|\gamma_0\|_{\mathcal{H}} \cdot r_\mu^{ATT}(n, \delta, b_1, c_1) + \kappa_d \kappa_x \cdot r_\gamma(n, \delta, b, c) \\
= O \left( n^{-\frac{1}{2} \frac{s_1^{-1}}{s_1+1/\delta}} + n^{-\frac{1}{2} \frac{s_1^{-1}}{s_1+1/\delta}} \right).
\]

Finally, consider $\theta_0^{CATE}$.

\[
\hat{\theta}^{CATE}(d, v) - \theta_0^{CATE}(d, v) = \langle \hat{\gamma}, \phi(d) \otimes \phi(v) \otimes \hat{\mu}_x(v) \rangle_{\mathcal{H}} - \langle \gamma_0, \phi(d) \otimes \phi(v) \otimes \mu_x(v) \rangle_{\mathcal{H}} \\
= \langle \hat{\gamma}, \phi(d) \otimes \phi(v) \otimes [\hat{\mu}_x(v) - \mu_x(v)] \rangle_{\mathcal{H}} + \langle [\hat{\gamma} - \gamma_0], \phi(d) \otimes \phi(v) \otimes \mu_x(v) \rangle_{\mathcal{H}} \\
= \langle [\hat{\gamma} - \gamma_0], \phi(d) \otimes \phi(v) \otimes [\hat{\mu}_x(v) - \mu_x(v)] \rangle_{\mathcal{H}} \\
+ \langle \gamma_0, \phi(d) \otimes \phi(v) \otimes [\hat{\mu}_x(v) - \mu_x(v)] \rangle_{\mathcal{H}} \\
+ \langle [\hat{\gamma} - \gamma_0], \phi(d) \otimes \phi(v) \otimes \mu_x(v) \rangle_{\mathcal{H}}.
\]
Therefore by Propositions 1 and 3 with probability $1 - 2\delta$,

$$\left| \hat{\theta}^{CATE}(d, v) - \theta_0^{CATE}(d, v) \right| \leq \left\| \hat{\gamma} - \gamma_0 \right\|_{H} \left\| \phi(d) \right\|_{H_D} \left\| \phi(v) \right\|_{H_V} \left\| \hat{\mu}_x(v) - \mu_x(v) \right\|_{H_X}$$

$$+ \left\| \gamma_0 \right\|_{H} \left\| \phi(d) \right\|_{H_D} \left\| \phi(v) \right\|_{H_V} \left\| \hat{\mu}_x(v) - \mu_x(v) \right\|_{H_X}$$

$$+ \left\| \hat{\gamma} - \gamma_0 \right\|_{H} \left\| \phi(d) \right\|_{H_D} \left\| \phi(v) \right\|_{H_V} \left\| \mu_x(v) \right\|_{H_X}$$

$$\leq \kappa_d \delta \cdot r_{\gamma}(n, \delta, b, c) \cdot r_{\mu}^{CATE}(n, \delta, b_2, c_2)$$

$$+ \kappa_d \delta \cdot \left\| \gamma_0 \right\|_{H} \cdot r_{\mu}^{CATE}(n, \delta, b_2, c_2) + \kappa_d \delta \cdot \left\| \gamma_0 \right\|_{H} \cdot r_{\gamma}(n, \delta, b, c)$$

$$= O \left( n^{-\frac{1}{2} \frac{c_3 - 1}{c_3 + 17b_3}} + n^{-\frac{1}{2} \frac{c_3 - 1}{c_3 + 17b_3}} \right).$$

For incremental functions, replace $\phi(d)$ with $\nabla_d \phi(d)$ and hence replace $\left\| \phi(d) \right\|_{H_D} \leq \kappa_d$ with $\left\| \nabla_d \phi(d) \right\|_{H_D} \leq \kappa_d'$.

**E.3.2 Counterfactual distributions**

**Proof of Theorem 4** The argument is analogous to Theorem 2. By Propositions 2 and 3 for all $d \in \mathcal{D}$, with probability $1 - 2\delta$,

$$\left\| \hat{\theta}^{ATE}(d) - \theta_0^{ATE}(d) \right\|_{H_Y}$$

$$\leq \kappa_d \cdot r_{E}(n, \delta, b_3, c_3) \cdot r_{\mu}(n, \delta) + \kappa_d \cdot \left\| E_\delta \right\|_{L_2} \cdot r_{\mu}(n, \delta) + \kappa_d \cdot r_{E}(n, \delta, b_3, c_3)$$

$$= O \left( n^{-\frac{1}{2} \frac{c_3 - 1}{c_3 + 17b_3}} \right).$$

Likewise, with probability $1 - 2\delta$,

$$\left\| \hat{\theta}^{DS}(d, \bar{P}) - \theta_0^{DS}(d, \bar{P}) \right\|_{H_Y}$$

$$\leq \kappa_d \cdot r_{E}(n, \delta, b_3, c_3) \cdot r_{\nu}(\tilde{n}, \delta) + \kappa_d \cdot \left\| E_\delta \right\|_{L_2} \cdot r_{\nu}(\tilde{n}, \delta) + \kappa_d \cdot r_{E}(n, \delta, b_3, c_3)$$

$$= O \left( n^{-\frac{1}{2} \frac{c_3 - 1}{c_3 + 17b_3}} + \tilde{n}^{-\frac{1}{2}} \right).$$
By Proposition 3, for all \(d, d' \in D\), with probability \(1 - 2\delta\),

\[
\|\hat{\theta}^{D:ATT}(d, d') - \hat{\theta}_0^{D:ATT}(d, d')\|_{\mathcal{H}_Y} \\
\leq \kappa_d \cdot r_E(n, \delta, b_3, c_3) \cdot r^{ATT}_\mu(n, \delta, b_1, c_1) \\
+ \kappa_d \cdot \|E_3\|_2 \cdot r^{ATT}_\mu(n, \delta, b_1, c_1) + \kappa_d \kappa_x \cdot r_E(n, \delta, b_3, c_3) \\
= O \left( n^{-\frac{1}{2} \frac{c_3 - 1}{c_3 + 1/\delta_3} + n^{-\frac{1}{2} \frac{c_3 - 1}{c_3 + 1/\delta_3}}} \right). 
\]

By Proposition 3, for all \(d \in D\) and \(v \in V\) with probability \(1 - 2\delta\),

\[
\|\hat{\theta}^{D:CATE}(d, v) - \hat{\theta}_0^{D:CATE}(d, v)\|_{\mathcal{H}_Y} \leq \kappa_d \kappa_v \cdot r_E(n, \delta, b_3, c_3) \cdot r^{CATE}_\mu(n, \delta, b_2, c_2) \\
+ \kappa_d \kappa_v \cdot \|E_3\|_2 \cdot r^{CATE}_\mu(n, \delta, b_2, c_2) \\
+ \kappa_d \kappa_v \kappa_x \cdot r_E(n, \delta, b_3, c_3) \\
= O \left( n^{-\frac{1}{2} \frac{c_2 - 1}{c_2 + 1/\delta_2}} + n^{-\frac{1}{2} \frac{c_3 - 1}{c_3 + 1/\delta_3}} \right). 
\]

**Proof of Theorem 5** Fix \(d\). By Theorem 4

\[
\|\hat{\theta}^{D:ATE}(d) - \hat{\theta}_0^{D:ATE}(d)\|_{\mathcal{H}_Y} = O_p \left( n^{-\frac{1}{2} \frac{c_3 - 1}{c_3 + 1/\delta_3}} \right). 
\]

Denote the samples constructed by Algorithm 3 by \(\{\hat{Y}_j\}_{j \in [m]}\). Then by [Bach et al., 2012][section 4.2],

\[
\left\| \hat{\theta}^{D:ATE}(d) - \frac{1}{m} \sum_{j=1}^m \phi(\hat{Y}_j) \right\|_{\mathcal{H}_Y} = O(m^{-\frac{1}{2}}). 
\]

Therefore by triangle inequality,

\[
\left\| \frac{1}{m} \sum_{j=1}^m \phi(\hat{Y}_j) - \hat{\theta}_0^{D:ATE}(d) \right\|_{\mathcal{H}_Y} = O_p \left( n^{-\frac{1}{2} \frac{c_3 - 1}{c_3 + 1/\delta_3}} + m^{-\frac{1}{2}} \right). 
\]

The desired result follows from [Sriperumbudur, 2016][as quoted by Simon-Gabriel et al., 2020][Theorem 1.1]. The argument for other counterfactual distributions identical.
E.3.3 Graphical models

**Proposition 4.** If Assumptions 3, 4, and 6 hold with $A_1 = \mathcal{X}$ and $B_1 = \mathcal{D}$, then with probability $1 - 2\delta$,

$$||\hat{\mu}_d \otimes \hat{\mu}_x(d) - \mu_d \otimes \mu_x(d)||_{\mathcal{H}_D \otimes \mathcal{H}_X} \leq \kappa_x \cdot r_{\mu}(n, \delta) + \kappa_d \cdot r^{\text{ATT}}_{\mu}(n, \delta, b_1, c_1),$$

where $r_{\mu}$ is as defined in Proposition 2 (with $\kappa_w = \kappa_d$) and $r^{\text{ATT}}_{\mu}$ is as defined in Proposition 3.

**Proof.** By triangle inequality,

$$||\hat{\mu}_d \otimes \hat{\mu}_x(d) - \mu_d \otimes \mu_x(d)||_{\mathcal{H}_D \otimes \mathcal{H}_X} \leq ||\hat{\mu}_d \otimes \hat{\mu}_x(d) - \hat{\mu}_d \otimes \mu_x(d)||_{\mathcal{H}_D \otimes \mathcal{H}_X} + ||\hat{\mu}_d \otimes \mu_x(d) - \mu_d \otimes \mu_x(d)||_{\mathcal{H}_D \otimes \mathcal{H}_X}.$$

Focusing on the former term, by Proposition 3,

$$||\hat{\mu}_d \otimes \hat{\mu}_x(d) - \hat{\mu}_d \otimes \mu_x(d)||_{\mathcal{H}_D \otimes \mathcal{H}_X} \leq ||\hat{\mu}_d||_{\mathcal{H}_D} \cdot ||\hat{\mu}_x(d) - \mu_x(d)||_{\mathcal{H}_X} \leq \kappa_d \cdot r^{\text{ATT}}_{\mu}(n, \delta, b_1, c_1).$$

Focusing on the latter term, by Proposition 2,

$$||\hat{\mu}_d \otimes \mu_x(d) - \mu_d \otimes \mu_x(d)||_{\mathcal{H}_D \otimes \mathcal{H}_X} \leq ||\hat{\mu}_d - \mu_d||_{\mathcal{H}_D} \cdot ||\mu_x(d)||_{\mathcal{H}_X} \leq \kappa_x \cdot r_{\mu}(n, \delta).$$

**Proof of Theorem 7.** To begin, write

$$\hat{\theta}^{\text{FD}}(d) - \hat{\theta}_0^{\text{do}}(d) = \langle \hat{\gamma}, \hat{\mu}_d \otimes \hat{\mu}_x(d) \rangle_{\mathcal{H}} - \langle \gamma_0, \mu_d \otimes \mu_x(d) \rangle_{\mathcal{H}}$$

$$= \langle \hat{\gamma}, [\hat{\mu}_d \otimes \hat{\mu}_x(d) - \mu_d \otimes \mu_x(d)] \rangle_{\mathcal{H}} + \langle [\hat{\gamma} - \gamma_0], \mu_d \otimes \mu_x(d) \rangle_{\mathcal{H}}$$

$$= \langle [\hat{\gamma} - \gamma_0], [\hat{\mu}_d \otimes \hat{\mu}_x(d) - \mu_d \otimes \mu_x(d)] \rangle_{\mathcal{H}}$$

$$+ \langle \gamma_0, [\hat{\mu}_d \otimes \hat{\mu}_x(d) - \mu_d \otimes \mu_x(d)] \rangle_{\mathcal{H}}$$

$$+ \langle [\hat{\gamma} - \gamma_0], \mu_d \otimes \mu_x(d) \rangle_{\mathcal{H}}.$$
Therefore by Propositions 1, 2, 3, and 4 with probability $1 - 3\delta$,

\[
\left| \hat{\theta}_{\text{FD}}(d) - \theta_0^{\text{FD}}(d) \right| \leq \| \hat{\gamma} - \gamma_0 \|_H \| \hat{\mu}_d \otimes \hat{\mu}_x(d) - \mu_d \otimes \mu_x(d) \|_{H_D \otimes H_X}
\]

\[
+ \| \gamma_0 \|_H \| \hat{\mu}_d \otimes \hat{\mu}_x(d) - \mu_d \otimes \mu_x(d) \|_{H_D \otimes H_X}
\]

\[
+ \| \hat{\gamma} - \gamma_0 \|_H \| \mu_d \|_{H_D} \| \mu_x(d) \|_{H_X}
\]

\[
\leq r_E(n, \delta, b, c) \left\{ \kappa_x \cdot r_\mu(n, \delta) + \kappa_d \cdot r_\mu^{\text{ATT}}(n, \delta, b_1, c_1) \right\}
\]

\[
+ \| \gamma_0 \|_H \left\{ \kappa_x \cdot r_\mu(n, \delta) + \kappa_d \cdot r_\mu^{\text{ATT}}(n, \delta, b_1, c_1) \right\}
\]

\[
+ \kappa_d \kappa_x \cdot r_E(n, \delta, b, c)
\]

\[
= \mathcal{O}\left( n^{-\frac{1}{2}} \frac{c-1}{c+1} + n^{-\frac{1}{2}} \frac{c_1-1}{c_1+1} \right).
\]

The argument for $\hat{\theta}_{\text{D:FD}}$ is analogous. By Propositions 2, 3, and 4 for all $d \in D$, with probability $1 - 3\delta$,

\[
\| \hat{\theta}_{\text{D:FD}}(d) - \theta_0^{\text{D:FD}}(d) \|_{H_Y}
\]

\[
\leq r_E(n, \delta, b_3, c_3) \left\{ \kappa_x \cdot r_\mu(n, \delta) + \kappa_d \cdot r_\mu^{\text{ATT}}(n, \delta, b_1, c_1) \right\}
\]

\[
+ \| E_3 \|_{L_2} \left\{ \kappa_x \cdot r_\mu(n, \delta) + \kappa_d \cdot r_\mu^{\text{ATT}}(n, \delta, b_1, c_1) \right\}
\]

\[
+ \kappa_d \kappa_x \cdot r_E(n, \delta, b_3, c_3)
\]

\[
= \mathcal{O}\left( n^{-\frac{1}{2}} \frac{c_3-1}{c_3+1} + n^{-\frac{1}{2}} \frac{c_1-1}{c_1+1} \right).
\]

Proof of Theorem 3. The argument is identical to the proof of Theorem 5.

F Conditional mean embedding rate proof

In this appendix, we prove Proposition 3, improving the rate of [Singh et al., 2019] from

\[ n^{-\frac{1}{2}} \frac{c-1}{c+1} \]

to

\[ n^{-\frac{1}{2}} \frac{c_1-1}{c_1+1} \].

Our consideration of Hilbert-Schmidt norm departs from [Park and Muandet, 2020].
Talwai et al., 2022], who study surrogate risk and operator norm, respectively. Our assumptions also depart from [Singh et al., 2019, Park and Muandet, 2020, Talwai et al., 2022]. Instead, we directly generalize the assumptions of [Fischer and Steinwart, 2020] from the standard kernel ridge regression to the generalized kernel ridge regression that we use to estimate a conditional mean embedding.

To lighten notation, we suppress the indexing of conditional expectation operators and conditional mean embeddings by \( \ell \). Furthermore, to lighten notation, we abbreviate \( L_2 = L_2(\mathcal{H}_A, \mathcal{H}_B) \). In the simplified notation,

\[
E_0 = \arg\min_{E \in \mathcal{L}_2} \mathcal{E}(E), \quad \mathcal{E}(E) = \mathbb{E}[\{\phi(A) - E^* \phi(B)\}^2];
\]

\[
E_\lambda = \arg\min_{E \in \mathcal{L}_2} \mathcal{E}(E) + \lambda \|E\|_{L_2}^2;
\]

\[
\hat{E} = \arg\min_{E \in \mathcal{L}_2} \hat{\mathcal{E}}(E), \quad \hat{\mathcal{E}}(E) = \frac{1}{n} \sum_{i=1}^n [\phi(A_{\ell i}) - E^* \phi(B_{\ell i})]^2 + \lambda \|E\|_{L_2}^2.
\]

F.1 Bias

**Proposition 5** (Conditional expectation operator bias; Theorem 6 of [Singh et al., 2019]).

Suppose Assumptions 3, 4, and the source condition in 6 hold. Then with probability one,

\[
\|E_\lambda - E_0\|_{L_2} \leq \lambda^{\frac{\nu-1}{2}} \sqrt{\zeta},
\]

where \( \zeta \) is defined in Lemma 4.

F.2 Variance

**Lemma 6** (Helpful bounds). Suppose Assumptions 3, 4, and 6 hold. Let \( \mu^\lambda_a(b) = E_\lambda^* \phi(b) \).

We adopt the language of [Caponnetto and De Vito, 2007].

1. The generalized reconstruction error is \( B(\lambda) = \sup_{b \in \mathcal{B}} \|\mu^\lambda_a(b) - \mu_a(b)\|_{\mathcal{H}_A}^2 \leq \kappa_b^2 \zeta \cdot \lambda^{\nu-1} \).
2. The generalized effective dimension is \( N(\lambda) = Tr\{(T + \lambda I)^{-1}T\} \leq C_{\frac{n/b}{\sin(\pi/b)}}^{1/b}. \)

Proof. The first result is a corollary of Proposition 5. The second result follows from Sutherland, 2017, eq. f], appealing to the effective dimension condition in Assumption 6. \( \square \)

Lemma 7 (Decomposition of variance). Let \( T_{AB} = \mathbb{E}[\phi(A) \otimes \phi(B)] \) and let \( \mathbb{E}_n[\cdot] = n^{-1} \sum_{i=1}^{n}[\cdot] \). The following bound holds:

\[
\|\hat{E} - E\|_{L^2} \leq \|\{\hat{T}_{AB} - T_{AB}(T_{BB} + \lambda I)^{-1}(\hat{T}_{BB} + \lambda I)\}(T_{BB} + \lambda I)^{-1/2}\|_{L^2} \\
\cdot \|(T_{BB} + \lambda I)^{1/2}(\hat{T}_{BB} + \lambda I)^{-1}(T_{BB} + \lambda I)^{1/2}\|_{op} \\
\cdot \|(T_{BB} + \lambda I)^{-1/2}\|_{op}.
\]

Moreover, in the first factor,

\[
\hat{T}_{AB} - T_{AB}(T_{BB} + \lambda I)^{-1}(\hat{T}_{BB} + \lambda I) \\
= \mathbb{E}_n[\{\phi(A) - \mu_a^\lambda(B)\} \otimes \phi(B)] - \mathbb{E}[\{\phi(A) - \mu_a^\lambda(B)\} \otimes \phi(B)].
\]

Proof. The result mirrors Fischer and Steinwart, 2020, eq. 44 and Talwai et al., 2022, eq. 34, strengthening the RKHS norm to Hilbert-Schmidt norm via Singh et al., 2019, Proposition 22. \( \square \)

Lemma 8 (Bounding the first factor). Suppose Assumptions 3 and 4 hold. Then with probability \( 1 - \delta/2 \), the first factor in Lemma 7 is bounded as

\[
\|\{\hat{T}_{AB} - T_{AB}(T_{BB} + \lambda I)^{-1}(\hat{T}_{BB} + \lambda I)\}(T_{BB} + \lambda I)^{-1/2}\|_{L^2} \leq 4 \ln(4/\delta) \left[ \frac{\kappa_a \kappa_b}{n \lambda^{1/2}} + \frac{\kappa_b \mathcal{B}(\lambda)^{1/2}}{n \lambda^{1/2}} + \frac{\kappa_a \mathcal{N}(\lambda)^{1/2}}{n^{1/2}} + \frac{\mathcal{B}(\lambda)^{1/2} \mathcal{N}(\lambda)^{1/2}}{n^{1/2}} \right].
\]

Proof. We verify the conditions of Lemma 5. Let

\[
\xi_i = \{\phi(A_i) - \mu_a^\lambda(B_i)\} \otimes \phi(B_i)(T_{BB} + \lambda I)^{-1/2}.
\]

We proceed in steps.
1. First moment.

Observe that

\[\|\xi_i\|_{L^2} = \|\{\phi(A_i) - \mu_{a}(B_i)\} \otimes \phi(B_i)(T_{BB} + \lambda I)^{-1/2}\|_{L^2}\]

\[= \|T_{BB} + \lambda I\|^{-1/2}[\phi(B_i) \otimes \{\phi(A_i) - \mu_{a}(B_i)\}]\|_{L^2}\]

\[= \|T_{BB} + \lambda I\|^{-1/2}\phi(B_i)\|_{H^S} \cdot \|\phi(A_i) - \mu_{a}(B_i)\|_{H_A} \cdot\]

Moreover

\[\|T_{BB} + \lambda I\|^{-1/2}\phi(B_i)\|_{H^S} \leq \|T_{BB} + \lambda I\|^{-1/2}\|_{op}\|\phi(B_i)\|_{H^S} \leq \frac{k_b}{\lambda^{1/2}}\]

and

\[\|\phi(A_i) - \mu_{a}(B_i)\|_{H_A} \leq \|\phi(A_i) - \mu_{a}(B_i)\|_{H_A} + \|\mu_{a}(B_i) - \mu_{a}(B_i)\|_{H_A} \leq 2\kappa_a + \sqrt{B(\lambda)}\]

In summary,

\[\|\xi_i\|_{L^2} \leq \frac{k_b}{\lambda^{1/2}} \left\{ 2\kappa_a + \sqrt{B(\lambda)} \right\} .\]

2. Second moment.

Next, write

\[\mathbb{E}[\|\xi_i\|_{L^2}^2]\]

\[= \int Tr(\{\phi(a) - \mu_{a}(b)\} \otimes \phi(b)(T_{BB} + \lambda I)^{-1}[\phi(b) \otimes \{\phi(a) - \mu_{a}(b)\}]d\mathbb{P}(a, b)\]

\[= \int Tr(\{\phi(a) - \mu_{a}(b)\} \langle \phi(b), (T_{BB} + \lambda I)^{-1}\phi(b) \rangle_{H^S} \{\phi(a) - \mu_{a}(b)\}, \cdot\rangle_{H_A})d\mathbb{P}(a, b)\]

\[= \int Tr(\langle \phi(b), (T_{BB} + \lambda I)^{-1}\phi(b) \rangle_{H^S} \{\phi(a) - \mu_{a}(b)\}, \{\phi(a) - \mu_{a}(b)\}\rangle_{H_A})d\mathbb{P}(a, b)\]

\[\leq \sup_{a, b} \|\phi(a) - \mu_{a}(b)\|_{H_A}^2 \cdot \int Tr(\langle \phi(b), (T_{BB} + \lambda I)^{-1}\phi(b) \rangle_{H^S} d\mathbb{P}(b)\).

Focusing on the former factor,

\[\|\phi(a) - \mu_{a}(b)\|_{H_A} \leq \|\phi(a) - \mu_{a}(b)\|_{H_A} + \|\mu_{a}(b) - \mu_{a}(b)\|_{H_A} \leq 2\kappa_a + \sqrt{B(\lambda)}\].
Therefore

\[ \sup_{a,b} \| \phi(a) - \mu^\lambda_a(b) \|^2_{\mathcal{H}_a} \leq \left\{ 2\kappa_a + \sqrt{\mathcal{B}(\lambda)} \right\}^2. \]

Focusing on the latter factor,

\[
\int \operatorname{Tr}((\phi(b), (T_{BB} + \lambda I)^{-1} \phi(b))_{\mathcal{H}_b} d\mathbb{P}(b) = \int \operatorname{Tr}((T_{BB} + \lambda I)^{-1} [\phi(b) \otimes \phi(b)] d\mathbb{P}(b)
= \operatorname{Tr}((T_{BB} + \lambda I)^{-1} T_{BB})
= \mathcal{N}(\lambda).
\]

In summary,

\[ \mathbb{E}[\| \xi \|^2_{L^2}] \leq \mathcal{N}(\lambda) \left\{ 2\kappa_a + \sqrt{\mathcal{B}(\lambda)} \right\}^2. \]

3. Concentration.

Therefore with probability \( 1 - \delta/2 \),

\[
\| \mathbb{E}_n[\xi] - \mathbb{E}[\xi] \|_{L^2} \leq \frac{2 \ln(4/\delta)}{n} \frac{\kappa_b}{\lambda^{1/2}} \left\{ 2\kappa_a + \sqrt{\mathcal{B}(\lambda)} \right\} + \sqrt{\frac{2 \ln(4/\delta)}{n} \frac{2 \ln(4/\delta)}{n} \frac{\kappa_a \mathcal{N}(\lambda)^{1/2}}{n^{1/2}} + \frac{\mathcal{B}(\lambda)^{1/2} \mathcal{N}(\lambda)^{1/2}}{n^{1/2}}}.\]

\[
\leq 4 \ln(4/\delta) \left[ \frac{\kappa_a \kappa_b}{n \lambda^{1/2}} + \frac{\kappa_b \mathcal{B}(\lambda)^{1/2}}{n \lambda^{1/2}} + \frac{\kappa_a \mathcal{N}(\lambda)^{1/2}}{n^{1/2}} + \frac{\mathcal{B}(\lambda)^{1/2} \mathcal{N}(\lambda)^{1/2}}{n^{1/2}} \right].
\]

\[ \square \]

Remark 5 (Sufficiently large \( n \)). In the finite sample, we assume a certain inequality holds when bounding the second factor:

\[ n \geq 8\kappa_b^2 \ln(4/\delta) \cdot \lambda \cdot \ln \left[ 2e \cdot \mathcal{N}(\lambda) \frac{\| T \|_{op} + \lambda}{\| T \|_{op}} \right]. \tag{5} \]

Ultimately, we will choose \( \lambda = n^{-1/(c+1/b)} \) in Proposition 3. This choice of \( \lambda \) together with the bound on generalized effective dimension \( \mathcal{N}(\lambda) \) in Lemma 6 imply that there exists an \( n_0 \) such that for all \( n \geq n_0 \), (5) holds, as argued by Fischer and Steinwart, 2020. Proof of
Theorem 1. We use the phrase \textit{n sufficiently large} when we appeal to this logic, and we summarize the final bound using $O(\cdot)$ notation.

\textbf{Lemma 9} (Bounding the second factor). Suppose Assumptions \textit{3} and \textit{4} hold. Further assume \textit{(5)} holds. Then probability $1 - \delta/2$, the second factor in Lemma \textit{7} is bounded as

$$
\| (T_{BB} + \lambda I)^{1/2}(\hat{T}_{BB} + \lambda I)^{-1}(T_{BB} + \lambda I)^{1/2}\|_{op} \leq 3.
$$

\textit{Proof}. The result follows from \cite[eq. 44b, 47]{Fischer and Steinwart, 2020}. In particular, our assumptions suffice for the properties used in \cite[Lemma 17]{Fischer and Steinwart, 2020} to hold. Separability of $B$ together with boundedness of the kernel $k_B$ imply that $\mathcal{H}_B$ is separable \cite[Lemma 4.33]{Steinwart and Christmann, 2008}. Next, we verify the assumptions called EMB, EVD, and SRC. Boundedness of the kernel implies EMB with $a = 1$. EVD is the assumption we call effective dimension, parametrized by $b \geq 1$. SRC is the assumption we call the source condition, parametrized by $c \in (1, 2]$ in our case. \hfill \Box

\textbf{Lemma 10} (Bounding the third factor). With probability one, the third factor in Lemma \textit{7} is bounded as

$$
\| (T_{BB} + \lambda I)^{-1/2}\|_{op} \leq \lambda^{-1/2}.
$$

\textit{Proof}. The result follows from the definition of operator norm. \hfill \Box

\textbf{Proposition 6} (Conditional expectation operator variance). Suppose Assumptions \textit{3}, \textit{4} and \textit{6} hold. Further assume \textit{(5)} holds and $\lambda \leq 1$. Then with probability $1 - \delta$,

$$
\| \hat{E} - E_\lambda \|_{L_2} \leq C \ln(4/\delta) \left[ \frac{1}{n\lambda} + \frac{1}{n^{1/2}\lambda^{1/b+1/2}} \right].
$$

\textit{Proof}. We combine the previous lemmas. By Lemmas \textit{7}, \textit{8}, \textit{9} and \textit{10} if \textit{(5)} holds, then
with probability $1 - \delta$

$$\|\hat{E} - E\|_{L_2} \leq \frac{12 \ln(4/\delta)}{\lambda^{1/2}} \left[ \kappa_a \kappa_b \beta(\lambda)^{1/2} \frac{n \lambda^{1/2} + \kappa_a \nu \nu(\lambda)^{1/2}}{n^{1/2}} + \frac{\kappa_a \nu \nu(\lambda)^{1/2}}{n^{1/2}} + \frac{B(\lambda)^{1/2} \nu \nu(\lambda)^{1/2}}{n^{1/2}} \right].$$

Next, recall the bounds in Lemma 6. Note that when $\lambda \leq 1$,

$$\sqrt{\beta(\lambda)} \leq \kappa_b \sqrt{\zeta} \lambda \frac{c+1}{2} \leq \kappa_b \sqrt{\zeta}.$$ 

For brevity, write

$$\nu \nu(\lambda)^{1/2} \leq C^\prime \lambda^{-1/2}.$$ 

Therefore when $\lambda \leq 1$ the bound simplifies as

$$\|\hat{E} - E\|_{L_2} \leq C \ln(4/\delta) \left[ \frac{1}{n \lambda} + \frac{1}{n^{1/2} \lambda^{1/(2b)+1/2}} \right].$$ 

\[ \square \]

### F.3 Collecting results

**Proof of Proposition 3.** We combine and simplify Propositions 5 and 6. Take $\lambda = n^{-1/(c+1/b)}$. For sufficiently large $n$, (5) holds and $\lambda \leq 1$ as explained in Remark 5. By triangle inequality, with probability $1 - \delta$,

$$\|\hat{E} - E\|_{L_2} \leq \|\hat{E} - E\|_{L_2} + \|E - E_0\|_{L_2} \leq C \ln(4/\delta) \left[ \frac{1}{n \lambda} + \frac{1}{n^{1/2} \lambda^{1/(2b)+1/2}} \right] + C \lambda \frac{c+1}{2}.$$ 

Each term on the RHS simplifies as follows:

$$n^{-1} \lambda^{-1} = n^{-1} n^{1/(c+1/b)} = n^{1/(c+1/b)-1} = n^{1-1/c+1/b} = n^{-\frac{1}{2} \frac{2(c+1/b)}{c+1/b}} \leq n^{-\frac{1}{2} \frac{c+1/b}{c+1/b}};$$

$$n^{-1/2} \lambda^{-1/(1/(2b)+1/2)} = n^{-1/2} n^{\frac{1/(2b)+1/2}{c+1/b}} = n^{-\frac{1}{2} \frac{1 (c+1/b+1)}{c+1/b}} = n^{-\frac{1}{2} \frac{1 (c+1/b+1)}{c+1/b}} = n^{-\frac{1}{2} \frac{c+1/b}{c+1/b}};$$

$$\lambda^{c+1} = n^{-\frac{1}{c+1/b} \frac{c+1}{2}} = n^{-\frac{1}{2} \frac{c+1/b}{c+1/b}}.$$ 

\[ \square \]
G Simulation details

In this appendix, we provide simulation details for (i) the dose response design, and (ii) the heterogeneous treatment effect design.

G.1 Dose response curve

A single observation consists of the triple \((Y, D, X)\) for outcome, treatment, and covariates where \(Y, D \in \mathbb{R}\) and \(X \in \mathbb{R}^{100}\). A single observation is generated is as follows. Draw unobserved noise as \(\nu, \epsilon \overset{i.i.d.}{\sim} \mathcal{N}(0, 1)\). Define the vector \(\beta \in \mathbb{R}^{100}\) by \(\beta_j = j^{-2}\). Define the matrix \(\Sigma \in \mathbb{R}^{100 \times 100}\) such that \(\Sigma_{ii} = 1\) and \(\Sigma_{ij} = \frac{1}{2} \cdot 1\{|i - j| = 1\}\) for \(i \neq j\). Then draw \(X \sim \mathcal{N}(0, \Sigma)\) and set

\[
D = \Phi(3X^\top \beta) + 0.75\nu, \quad Y = 1.2D + 1.2X^\top \beta + D^2 + DX_1 + \epsilon.
\]

We implement our estimator \(\hat{\theta}_{ATE}(d)\) (RKHS) described in Section 4, with the tuning procedure described in Appendix D. Specifically, we use ridge penalties determined by leave-one-out cross validation, and product exponentiated quadratic kernel with lengthscales set by the median heuristic. We implement [Kennedy et al., 2017] (DR1) using the default settings of the command \texttt{ctseff} in the \texttt{R} package \texttt{npcausal}. We implement [Colangelo and Lee, 2020] (DR2) using default settings in \texttt{Python} code shared by the authors. Specifically, we use random forest for prediction, with the suggested hyperparameter values. For the Nadaraya-Watson smoothing, we select bandwidth that minimizes out-of-sample MSE. We implement [Semenova and Chernozhukov, 2021] (DR-series) by modifying \texttt{ctseff}, as instructed by the authors. Importantly, we give DR-series the advantage of correct specification of the true dose response curve as a quadratic function.
G.2 Heterogeneous treatment effect

A single observations consists of the tuple \((Y, D, V, X)\), where outcome, treatment, and covariate of interest \(Y, D, V \in \mathbb{R}\) and other covariates \(X \in \mathbb{R}^3\). A single observation is generated as follows. Draw unobserved noise as \(\{\epsilon_j\}_{j=1:4} \sim \text{i.i.d. } U(-1/2, 1/2)\) and \(\nu \sim \mathcal{N}(0, 1/16)\). Then set

\[
V = \epsilon_1, \quad X = \begin{bmatrix}
1 + 2V + \epsilon_2 \\
1 + 2V + \epsilon_3 \\
(V - 1)^2 + \epsilon_4
\end{bmatrix}.
\]

Draw \(D \sim \text{Bernoulli}(\Lambda(1/2 \cdot [V + X_1 + X_2 + X_3]))\) where \(\Lambda\) is the logistic link function. Finally set

\[
Y = \begin{cases}
0 & \text{if } D = 0; \\
V \cdot X_1 \cdot X_2 \cdot X_3 + \nu & \text{if } D = 1.
\end{cases}
\]

Note that [Abrevaya et al., 2015] also present a simpler version of this design.

We implement our estimator \(\hat{\theta}_{\text{CATE}}(d, v) (\text{RKHS})\) described in Section 4, with the tuning procedure described in Appendix D. Specifically, we use ridge penalties determined by leave-one-out cross validation. For multivariate functions, we use products of scalar kernels. For the binary treatment \(D\), we use the binary kernel. For continuous variables, we use (product) exponentiated quadratic kernel with lengthscales set by the median heuristic. We implement [Abrevaya et al., 2015] (IPW) using default settings in the MATLAB code shared by the authors. We implement [Semenova and Chernozhukov, 2021] (DR-series) using the default settings of the command \texttt{best_linear_projection} in the R package \texttt{grf}. Importantly, we give DR-series the advantage of correct specification of the true heterogeneous treatment effect as the appropriate polynomial.
H Application details

We implement our nonparametric estimators $\hat{\theta}_{ATE}(d)$, $\hat{\theta}_{CATE}(d,v)$ described in Section 4. We also implement the semiparametric estimator of [Singh, 2021] (DML3) with 95% confidence intervals. Specifically, we reduce the continuous treatment into a discrete treatment that takes nine values corresponding to the roughly equiprobable bins $[40, 250]$, $(250, 500]$, $(500, 750]$, $(750, 1000]$, $(1000, 1250]$, $(1250, 1500]$, $(1500, 1750]$, and $(1750, 2000]$ class hours. Across estimators, we use the tuning procedure described in Appendix D. Specifically, we use ridge penalties determined by leave-one-out cross validation, and product exponentiated quadratic kernel with lengthscales set by the median heuristic.

![Class-hours distribution](image)

(a) $D \geq 40$ and $Y > 0$  
(b) $D \geq 40$

Figure 3: Class hours for different samples

We use the dataset published by [Huber et al., 2020]. In the main text, we focus on the $n = 3,906$ observations for which $D \geq 40$, i.e. individuals who completed at least one week of training. In this section, we verify that our results are robust to the choice of sample. Specifically, we consider the sample with $D \geq 40$ and $Y > 0$, i.e. the $n = 2,989$ individuals who completed at least one week of training and who found employment.
Figure 4: Effect of job training on employment: \( D \geq 40 \) and \( Y > 0 \)

For each sample, we visualize class hours \( D \) with a histogram in Figure 3. The class hour distribution in the sample with \( D \geq 40 \) and \( Y > 0 \) is similar to the class hour distribution in the sample with \( D \geq 40 \) that we use in the main text. Next, we estimate the dose response curve, heterogeneous treatment effect, and incremental response curve for the new sample choice. Figure 4 visualizes results. For the sample with \( D \geq 40 \) and \( Y > 0 \), the results mirror the results of the sample with \( D \geq 40 \) presented in the main text. Excluding observations for which \( Y = 0 \) leads to estimates that have the same shape but higher magnitudes, confirming the robustness of the results we present in the main text.