Kernel Methods for Multistage Causal Inference: Mediation Analysis and Dynamic Treatment Effects

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Abstract

We propose simple estimators for mediation analysis and dynamic treatment effects over short horizons based on kernel ridge regression. We study both nonparametric response curves and semiparametric treatment effects, allowing treatments, mediators, and covariates to be continuous or discrete in general spaces. Our key innovation is a new RKHS technique called sequential mean embedding, which facilitates the construction of simple estimators for complex causal estimands, including new estimands without existing alternatives. In particular, we propose machine learning estimators of dynamic dose response curves and dynamic counterfactual distributions without restrictive linearity, Markov, or no-effect-modification assumptions. Our simple estimators preserve the generality of classic identification while also achieving nonasymptotic uniform rates for causal functions and semiparametric efficiency for causal scalars. In nonlinear simulations with many covariates, we demonstrate state-of-the-art performance. We estimate mediated and dynamic response curves of the US Job Corps program for disadvantaged youth, and share a data set that may serve as a benchmark in future work.

Keywords: reproducing kernel Hilbert space, dose response curve, uniform consistency, semiparametric efficiency, counterfactual distribution

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1 Introduction and related work

We study mediation analysis and dynamic treatment effects. Mediation analysis asks, how much of the total effect of the treatment $D$ on the outcome $Y$ is mediated by a particular mechanism $M$ that takes place between treatment and outcome? Dynamic analysis asks, what would be the effect of a sequence of treatments $D_{1:T}$ on the outcome $Y$, even when that sequence was not actually implemented? When treatments are continuous, we consider nonparametric causal functions. For example, the dynamic dose response curve of two continuous treatments is the function $\theta_{0}^{GF}(d_1, d_2) := \mathbb{E}\{Y^{(d_1, d_2)}\}$. When treatments are discrete, we consider semiparametric causal scalars.

In seminal works, [Imai et al., 2010] and [Robins, 1986] rigorously develop identification theory for mediation analysis and dynamic treatment effects. A rich class of mediated and dynamic treatment effects are estimable in principle if the analyst has access to a sufficiently rich set of covariates over time $X_{1:T}$. Treatment may be discrete or continuous; relationships among outcome, treatment, and covariates may be nonlinear; and dependence may be interwoven in a way that modifies effects [Gill and Robins, 2001]. For example, under standard assumptions, the dynamic dose response is identified as the nested integral $\theta_{0}^{GF}(d_1, d_2) = \int \gamma_0(d_1, d_2, x_1, x_2) \text{d}\mathbb{P}(x_2|d_1, x_1) \text{d}\mathbb{P}(x_1)$, where $\gamma_0(d_1, d_2, x_1, x_2) = \mathbb{E}(Y|D_1 = d_1, D_2 = d_2, X_1 = x_1, X_2 = x_2)$ [Robins, 1986].

While mediated and dynamic treatment effects are identified in theory, they are challenging to estimate in practice. Popular estimators restrict attention to binary treatment, parametric models, Markov simplifications, or restricted effect modification for tractability, and may even redefine the estimand. See [Vansteelandt and Joffe, 2014] for a review. Each of these restrictions simplifies the nested integral in order to simplify estimation. Our research question is: can we devise simple machine learning estimators that preserve the richness of the integral, and therefore the generality of classic identification, while also achieving nonasymptotic uniform rates for causal functions and semiparametric efficiency for causal scalars?

For the continuous treatment case, existing nonparametric estimators for mediated response curves [Huber et al., 2020] [Ghassami et al., 2021] use density estimation, which can be challenging as dimension increases. Existing machine learning estimators for dy-
namic dose response curves [Lewis and Syrgkanis, 2020] rely on restrictive linearity, Markov, and no-effect-modification assumptions, which imply additive effects of treatments. For the binary treatment case, a rich literature characterizes abstract conditions for $n^{-1/2}$ consistent semiparametric estimation, on which we build; see e.g. [Scharfstein et al., 1999, van der Laan and Rubin, 2006, Zheng and van der Laan, 2011, van der Laan and Gruber, 2012, Tchetgen Tchetgen and Shpitser, 2012, Molina et al., 2017, Luedtke et al., 2017, Rotnitzky et al., 2017, Chernozhukov et al., 2018, Farbmacher et al., 2020, Bodory et al., 2020, Singh, 2021b] and references therein. Still, estimators that preserve the full generality of the mediated and dynamic treatment effect identification are not widely used in empirical research [Vansteelandt and Joffe, 2014], perhaps due to the complexity of their subroutines.

In this paper, we match the generality of mediation analysis and dynamic treatment effect identification with the flexibility and simplicity of kernel ridge regression estimation. We propose a new family of nonparametric and semiparametric estimators for multistage causal inference over short horizons. Our algorithms are combinations of kernel ridge regressions, and so they inherit the practical and theoretical virtues that make kernel ridge regression popular in machine learning. The algorithms are simple; even the dynamic dose response curve trained on text and images in a medical record has a one line, closed form solution. In nonlinear simulations over short horizons, the algorithms reliably outperform some state-of-the-art alternatives, justifying their use in a real world program evaluation of the US Job Corps. The key approximation assumption that underpins their performance is smoothness, which departs from the sparsity assumption popular in high dimensional causal inference. Crucially, we preserve the nonlinearity, dependence, and effect modification of identification theory. There are three aspects of our contribution.

First, we introduce an algorithmic technique that appears to be an innovation in the RKHS literature: sequential embeddings, i.e. RKHS representations of mediator and covariate conditional distributions given a hypothetical treatment sequence. For example, we introduce the sequential embedding $\mu_{x_1, x_2}(d_1)$ such that the inner product $\langle f, \mu_{x_1, x_2}(d_1) \rangle$ in an appropriately defined Hilbert space equals the nested integral $\int f(x_1, x_2) d\mathbb{P}(x_2 | d_1, x_1) d\mathbb{P}(x_1)$. Our new technique leads to estimators with closed form solutions that are combinations of simple kernel ridge regressions, and in this sense we extend the recursive regression insight of [Bang and Robins, 2005] to machine learning. For continuous treatment, we use
sequential embeddings to propose a machine learning estimator of dynamic dose response curves without restrictive linearity, Markov, or no-effect-modification assumptions, which to our knowledge is new. We extend these results to propose what appear to be the first unrestricted incremental response curves and counterfactual distributions for multistage settings, relaxing the restrictions of the structural nested distribution model [Robins, 1992]. For discrete treatment, we use sequential embeddings to propose new and simpler subroutines for known procedures that deliver confidence intervals. In particular, we avoid multiple levels of sample splitting and iterative fitting.

Second, we prove that our simple estimators based on sequential mean embedding achieve nonasymptotic uniform rates for causal functions and semiparametric efficiency for causal scalars. Specifically, for the continuous treatment case, we prove uniform consistency with finite sample rates that combine well-known fast rates for kernel ridge regression [Caponnetto and De Vito, 2007] [Fischer and Steinwart, 2020] [Li et al., 2022]. The rates do not directly depend on the data dimension, but rather smoothness and effective dimension. We extend these results to multistage incremental response curves and multistage counterfactual outcome distributions. For the discrete treatment case, we prove $n^{-1/2}$ consistency, finite sample Gaussian approximation, and semiparametric efficiency, which imply validity of the confidence intervals. We articulate a double spectral robustness for the multistage setting whereby some kernels may have higher effective dimensions as long as others have sufficiently low effective dimensions. The same assumptions and techniques drive both nonparametric and semiparametric analysis.

Third, for a broad statistics audience, we illustrate the practicality of our approach by conducting comparative simulations and estimating the mediated and dynamic response curves of the Jobs Corps, the largest job training program for disadvantaged youth in the US. Access to the program was randomized from November 1994 to February 1996 and several rounds of surveys were collected over a short horizon [Schochet et al., 2008]. Individuals could decide whether to participate and for how many hours, possibly over multiple years. We model class-hours in different years as a sequence of continuous treatments and conduct a program evaluation. Using direct and indirect dose response curves, we find that job training reduces arrests via social mechanisms besides employment. By allowing for continuous treatment and dynamic confounding, we uncover that relatively few class-hours in the first
year and no class-hours in the second year confer most of the benefit to counterfactual employment. Of independent interest, we clean and share a data set that may serve as a benchmark for new, flexible approaches to dynamic dose response curve estimation.

Unlike previous work that incorporates the RKHS into causal inference, we provide a framework for *multistage* estimands. Existing work incorporates the RKHS into one-stage causal inference. [Nie and Wager, 2021] [Kennedy et al., 2017] [Foster and Syrgkanis, 2019] propose methods based on orthogonal loss minimization for heterogeneous treatment effect, and [Wong and Chan, 2018] [Zhao, 2019] [Kallus, 2020] [Hirshberg et al., 2019] [Singh, 2021a] propose methods based on balancing weights for average treatment effect. [Muandet et al., 2017] propose counterfactual distributions for binary treatment, while [Singh et al., 2020] propose dose responses and counterfactual distributions for continuous treatment. Whereas previous work studies the one-stage setting, we study the multistage setting and prove equally strong results despite additional complexity in the chain of causal influence and scope for nonlinearity.\(^1\)

The structure of this paper is as follows. Section 2 presents our assumptions, which are standard in RKHS learning theory. Section 3 presents nonparametric and semiparametric theory for mediation analysis. Section 4 presents nonparametric and semiparametric theory for dynamic response curves and treatment effects. Section 5 conducts comparative simulation experiments and a program evaluation. Section 6 concludes. In Appendix A, we provide a glossary of the new estimators and guarantees. We extend the nonparametric results to counterfactual distributions in Appendix B and longer horizons in Appendix C.

## 2 RKHS assumptions

We summarize RKHS notation, interpretation, and assumptions that we use in this paper. A reproducing kernel Hilbert space (RKHS) \( \mathcal{H} \) has elements that are functions \( f : \mathcal{W} \to \mathbb{R} \) where \( \mathcal{W} \) is a Polish space, which we formally define below. Let \( k : \mathcal{W} \times \mathcal{W} \to \mathbb{R} \) be a

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function that is continuous, symmetric, and positive definite. We call \( k \) the kernel, and we call \( \phi : w \mapsto k(w, \cdot) \) the feature map. The kernel is the inner product of features: \( k(w, w') = \langle \phi(w), \phi(w') \rangle_{\mathcal{H}} \). The RKHS is the closure of the span of the features \( \{ \phi(w) \}_{w \in \mathcal{W}} \).

As such, the features are interpretable as the dictionary of basis functions for the RKHS: for \( f \in \mathcal{H} \), we have that \( f(w) = \langle f, \phi(w) \rangle_{\mathcal{H}} \).

Kernel ridge regression uses the RKHS \( \mathcal{H} \) as the hypothesis space in an infinite dimensional optimization problem with a ridge penalty. This infinite dimensional optimization problem has a well-known closed form solution:

\[
\hat{f} := \arg\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \{ Y_i - f(W_i) \}^2 + \lambda \| f \|_{\mathcal{H}}^2; \quad \hat{f}(w) = Y^T(WW + n\lambda I)^{-1}K_{Ww}, \tag{1}
\]

where \( K_{Ww} \in \mathbb{R}^{n \times n} \) is the kernel matrix with \((i, j)\)-th entry \( k(W_i, W_j) \) and \( K_{Ww} \in \mathbb{R}^n \) is the kernel vector 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 \cite{Li, 1986}. To analyze the bias and variance of kernel ridge regression, the statistical learning literature places assumptions on the smoothness of \( f_0 \) and effective dimension of \( \mathcal{H} \). Both assumptions are spectral in nature, so we present the spectral view of the RKHS before introducing them.

The kernel gets its name from its role within an integral operator. Denote by \( \mathbb{L}^2_\nu(W) \) the space of square integrable functions with respect to measure \( \nu \). Consider the convolution operator in which \( k \) serves as the kernel, i.e. \( L : \mathbb{L}^2_\nu(W) \to \mathbb{L}^2_\nu(W), f \mapsto \int k(\cdot, w)f(w)\,d\nu(w) \).

By the spectral theorem, we write \( Lf = \sum_{j=1}^{\infty} \eta_j \langle \varphi_j, f \rangle_{\mathbb{L}^2_\nu(W)} \cdot \varphi_j \) where \( \eta_j \) are weakly decreasing eigenvalues and \( \varphi_j \) are orthonormal eigenfunctions that form a basis of \( \mathbb{L}^2_\nu(W) \).

To interpret how the RKHS \( \mathcal{H} \) compares to \( \mathbb{L}^2_\nu(W) \), we express both function spaces in terms of the orthonormal basis \( \{ \varphi_j \} \). In other words, we present the spectral view of the RKHS. For any \( f, g \in \mathbb{L}^2_\nu(W) \), write \( f = \sum_{j=1}^{\infty} f_j \varphi_j \) and \( g = \sum_{j=1}^{\infty} g_j \varphi_j \). Then

\[
\mathbb{L}^2_\nu(W) = \left( f = \sum_{j=1}^{\infty} f_j \varphi_j : \sum_{j=1}^{\infty} f_j^2 < \infty \right), \quad \langle f, g \rangle_{\mathbb{L}^2_\nu(W)} = \sum_{j=1}^{\infty} f_j g_j;
\]

\[
\mathcal{H} = \left( f = \sum_{j=1}^{\infty} f_j \varphi_j : \sum_{j=1}^{\infty} f_j^2 \eta_j < \infty \right), \quad \langle f, g \rangle_{\mathcal{H}} = \sum_{j=1}^{\infty} \frac{f_j g_j}{\eta_j}.
\]

\( \mathcal{H} \) is the subset of \( \mathbb{L}^2_\nu(W) \) for which higher order terms in \( \langle \varphi_j \rangle \) have a smaller contribution, subject to \( \nu \) satisfying the conditions of Mercer’s theorem \cite{Steinwart and Scovel, 2012}. 

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An analyst can place assumptions on the spectral properties of a statistical target \( f_0 \) estimated in the RKHS \( \mathcal{H} \): smoothness and effective dimension \cite{CaponnettoDeVito2007, FischerSteinwart2020}. These assumptions are formalized by parameters \((b,c)\):

\[
f_0 \in \mathcal{H}^c := \left\{ f = \sum_{j=1}^{\infty} f_j \varphi_j : \sum_{j=1}^{\infty} \frac{f_j^2}{\eta_j} < \infty \right\} \subset \mathcal{H}, \quad c \in (1,2]; \quad \eta_j \leq C j^{-b}, \quad b \geq 1. \tag{2}
\]

The value \( c \) quantifies how well the leading terms in \((\varphi_j)\) approximate \( f_0 \); a larger value of \( c \) corresponds to a smoother target \( f_0 \). A larger value of \( b \) corresponds to a faster rate of spectral decay and therefore a lower effective dimension. Both \((b,c)\) are joint assumptions on the kernel and data distribution. Correct specification implies \( c \geq 1 \) and a bounded kernel implies \( b \geq 1 \) \cite[Lemma 10]{FischerSteinwart2020}. Minimax optimal rates for regression are governed by \((b,c)\) \cite{FischerSteinwart2020, Li2022}, with faster rates corresponding to higher values. In our analysis of causal estimands, we obtain nonparametric rates and semiparametric rate conditions that combine minimax optimal regression rates, which are therefore in terms of \((b,c)\).

Spectral assumptions are easy to interpret in the context of Sobolev spaces \cite{FischerSteinwart2020}. Let \( \mathcal{W} \subset \mathbb{R}^p \). Denote by \( \mathbb{H}_2^s \) the Sobolev space with \( s > p/2 \) square integrable derivatives. \( \mathbb{H}_2^s \) can be generated by the Matèrn kernel. Suppose \( \mathcal{H} = \mathbb{H}_2^s \) is chosen as the RKHS for estimation. If \( f_0 \in \mathbb{H}_2^{s_0} \), then \( c = s_0/s \); \( c \) quantifies the additional smoothness of \( f_0 \) relative to \( \mathcal{H} \). In this Sobolev space, \( b = 2s/p > 1 \). The effective dimension is increasing in the original dimension \( p \) and decreasing in the degree of smoothness \( s \). The minimax optimal regression rates are

\[
n^{-\frac{1}{2} c+1/2} = n^{-\frac{s_0}{2q_0+p}} \text{ in } L^2 \text{ norm,} \quad n^{-\frac{1}{2} c-1} = n^{-\frac{2q_0-s}{2q_0+p}} \text{ in Sobolev norm,} \tag{3}
\]

and both are achieved by kernel ridge regression with \( \lambda = n^{-\frac{1}{c+1/2}} = n^{-\frac{2s}{2q_0+p}} \).

With notation and interpretation of the RKHS in hand, we are ready to state the five types of assumptions we place in this paper, generalizing the standard RKHS learning theory assumptions from kernel ridge regression to multistage causal inference.

**Identification.** We assume variants of selection on observables in order to express direct, indirect, and dynamic effects as reweightings of a regression function. We allow the marginal distribution of treatments and covariates to shift.
**RKHS regularity.** We construct an RKHS for the regression function that facilitates the analysis of partial means. Our RKHS construction requires kernels that are bounded and characteristic. For incremental responses, we require kernels that are differentiable.

**Original space regularity.** We allow treatment, mediator, and covariates to be discrete or continuous in general Polish spaces. For simplicity, we assume the outcome is bounded.

**Smoothness.** We estimate regression functions, propensity scores, and conditional expectation operators by kernel ridge regression. To analyze the bias from ridge regularization, we assume smoothness conditions for each object estimated by a kernel ridge regression.

**Effective dimension.** To analyze the variance from ridge regularization, we assume effective dimension conditions for each object estimated by a kernel ridge regression.

We formally instantiate these assumptions for mediation analysis (Section 3), dynamic analysis (Section 4), and counterfactual distributions (Appendix B). We uncover a double spectral robustness in the semiparametric inferential theory: some kernels may have higher effective dimensions, as long as other kernels have lower effective dimensions.

### 3 Mediation analysis

#### 3.1 Definition and identification

Mediation analysis seeks to decompose the total effect of treatment $D$ on outcome $Y$ into the direct effect versus the indirect effect mediated via mechanism $M$. The problem is multistage in the sense that $D$ causes $M$ and $Y$, then $M$ also causes $Y$. We denote the counterfactual mediator $M^{(d)}$ given a hypothetical intervention on treatment $D = d$. We denote the counterfactual outcome $Y^{(d,m)}$ given a hypothetical intervention on not only treatment $D = d$ but also mediator $M = m$.

**Definition 1** (Mediation analysis [Robins and Greenland, 1992]). We define

1. $\theta_{0TE}^{TE}(d, d') := \mathbb{E}[Y^{\{d', M^{(d')}\}}] - Y^{\{d, M^{(d)}\}}]$ is the total effect of new treatment value $d'$ compared to old value $d$.

2. $\theta_{0IE}^{IE}(d, d') := \mathbb{E}[Y^{\{d', M^{(d')}\}}] - Y^{\{d, M^{(d)}\}}]$ is the indirect effect of new treatment value $d'$ compared to old value $d$, i.e. the component of total effect mediated by $M$. 


3. \(\theta^D_0(d, d') := \mathbb{E}[Y_{d', M(d)}] - Y_{d, M(d)}\) is the direct effect of new treatment value \(d'\) compared to old value \(d\).

4. \(\theta^M_0(d, d') := \mathbb{E}[Y_{d', M(d)}]\) is the counterfactual mean outcome in the thought experiment that treatment is set at a new value \(D = d'\) but the mediator \(M\) follows the distribution it would have followed if treatment were set at its old value \(D = d\).

Likewise we define incremental response curves and effects, e.g. \(\theta^{ME}_0(d, d') := \mathbb{E}[\nabla d Y_{d', M(d)}]\).

\(\theta^{TE}_0(d, d')\) generalizes average total effects. Average total effect of a binary treatment \(D \in \{0, 1\}\) is \(\mathbb{E}[Y_{1, M(1)}] - Y_{0, M(0)}\). For treatment that is continuous, the vector \(\mathbb{E}[Y_{d, M(d)}]\) may be infinite dimensional, which makes this problem fully nonparametric.

\(\theta^{TE}_0(d, d')\) captures the concept of total effect, but the total effect may be mostly mediated by some mechanism \(M\). An analyst may therefore wish to measure how much of the total effect is indirect: how much of the total effect would be achieved by simply intervening on the mediator distribution? For example, in Section 5, we investigate the extent to which employment mediates the effect of job training on arrests. With binary treatment, the indirect effect is \(\mathbb{E}[Y_{1, M(1)}] - \mathbb{E}[Y_{1, M(0)}]\). In the former term, the mediator follows the counterfactual distribution under intervention \(D = 1\), and in the latter, it follows the counterfactual distribution under intervention \(D = 0\).

The remaining component of total effect is the direct effect, which answers: if the mediator were held at the original distribution corresponding to \(D = d\), what would be the impact of treatment \(D = d'\)? For example, in Section 5, we investigate the effect of job training on arrests holding employment at the original distribution. With binary treatment, the direct effect is \(\mathbb{E}[Y_{1, M(0)}] - \mathbb{E}[Y_{0, M(0)}]\).

The final target parameter is \(\theta^{ME}_0(d, d')\). It is useful because \(\theta^{TE}_0(d, d'), \theta^{IE}_0(d, d')\), and \(\theta^{DE}_0(d, d')\) can be expressed in terms of \(\theta^{ME}_0(d, d')\). With binary treatment, this quantity would be a matrix in \(\mathbb{R}^{2 \times 2}\). In our nonparametric approach, it is a surface over \(D \times D\).

**Proposition 1.** Mediated response curves and effects can be expressed in terms of \(\theta^{ME}_0(d, d')\).

1. \(\theta^{TE}_0(d, d') = \theta^{DE}_0(d, d') + \theta^{IE}_0(d, d') = \theta^{ME}_0(d', d') - \theta^{ME}_0(d, d)\);

2. \(\theta^{IE}_0(d, d') = \theta^{ME}_0(d', d') - \theta^{ME}_0(d, d')\);
3. $\theta_0^{DE}(d,d') = \theta_0^{ME}(d,d') - \theta_0^{ME}(d,d)$. 

Under the assumption of no interference, defined below, $\theta_0^{TE}(d,d') = \mathbb{E}\{Y(d',M) - Y(d,M)\}$.

In seminal work, [Imai et al., 2010] state sufficient conditions under which mediated effects can be measured from outcomes $Y$, treatments $D$, mediators $M$, and covariates $X$. We refer to this collection of sufficient conditions as selection on observables for mediation.

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

1. No interference: if $D = d$ then $M = M(d)$; if $D = d$ and $M = m$ then $Y = Y(d,m)$.

2. Conditional exchangeability: $\{M(d), Y(d',m)\} \perp D | X$ and $\{Y(d',m)\} \perp M | D, X$.

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

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, treatment assignment is as good as random. Moreover, conditional on treatment and covariates, mediator assignment is as good as random. Overlap ensures that there is no covariate stratum $X = x$ such that treatment has a restricted support, and there is no treatment-covariate stratum $(D, X) = (d, x)$ such that mediator has a restricted support.

We generalize a classic identification result. Whereas [Imai et al., 2010] identify $\theta_0^{ME}(d,d')$, we also identify the incremental version $\theta_0^{ME,N}(d,d')$, which appears to be a new result. Define the regression $\gamma_0(d,m,x) := \mathbb{E}(Y|D = d, M = m, X = x)$.

**Theorem 1** (Identification of mediated response curves and effects). If Assumption 1 holds, then

1. $\theta_0^{ME}(d,d') = \int \gamma_0(d',m,x) d\mathbb{P}(m|d,x)d\mathbb{P}(x)$ [Imai et al., 2010].

2. $\theta_0^{ME,N}(d,d') = \int \nabla d' \gamma_0(d',m,x) d\mathbb{P}(m|d,x)d\mathbb{P}(x)$.

See Appendix D for the proof. Proposition 1 identifies the other quantities in Definition 1. For subsequent analysis, it helps to define $\omega_0(d,d';x) := \int \gamma_0(d',m,x) d\mathbb{P}(m|d,x)$, so that $\theta_0^{ME}(d,d') = \mathbb{E}\{\omega_0(d,d';X)\}$.
3.2 Algorithm

Theorem 1 makes precise how each mediated response curve and effect is identified as a nested integral of the form
\[ \int \gamma_0(d', m, x) dQ \]
for the distribution \( Q = P(m|d, x)P(x) \).

Since \( x \) appears in \( \gamma_0(d', m, x) \), \( P(m|d, x) \), and \( P(x) \), the nested integral is coupled and therefore challenging to estimate. Our key insight is that, with the appropriate RKHS construction, the components \( \gamma_0(d', m, x) \), \( P(m|d, x) \), and \( P(x) \) can be decoupled. Moreover, the multistage distribution \( Q \) can be encoded by a *sequential mean embedding*, which appears to be an innovation. We use these techniques to reduce multistage causal inference into the combination of kernel ridge regressions, which then allows us to propose estimators with closed form solutions.

To begin, we construct the appropriate RKHS for \( \gamma_0 \). In our construction, we define RKHSs for treatment \( D \), mediator \( M \), and covariates \( X \), then assume that the regression is an element of a certain composite space. To lighten notation, we will suppress subscripts when arguments are provided. We assume the regression \( \gamma_0 \) is an element of the RKHS \( H \) with the kernel
\[ k_D(d, d') \cdot k_M(m, m') \cdot k_X(x, x') \]
Formally, this choice of kernel corresponds to the tensor product: \( \gamma_0 \in H := H_D \otimes H_M \otimes H_X \), with the tensor product dictionary of basis functions \( \phi(d) \otimes \phi(m) \otimes \phi(x) \). As such, \( \gamma_0(d, m, x) = \langle \gamma_0, \phi(d) \otimes \phi(m) \otimes \phi(x) \rangle_H \) and \( \|\phi(d) \otimes \phi(m) \otimes \phi(x)\|_H = \|\phi(d)\|_{H_D} \cdot \|\phi(m)\|_{H_M} \cdot \|\phi(x)\|_{H_X} \).

We place regularity conditions on this RKHS construction in order to prove our decoupling result. Anticipating Appendix B, we include conditions for an outcome RKHS in parentheses.

**Assumption 2 (RKHS regularity conditions).** Assume

1. \( k_D, k_M, k_X \) (and \( k_Y \)) are continuous and bounded. Formally, \( \sup_{d \in D} \|\phi(d)\|_{H_D} \leq \kappa_d \), \( \sup_{m \in M} \|\phi(m)\|_{H_M} \leq \kappa_m \), \( \sup_{x \in X} \|\phi(x)\|_{H_X} \leq \kappa_x \) (and \( \sup_{y \in Y} \|\phi(y)\|_{H_Y} \leq \kappa_y \)).

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

3. \( k_M, k_X \) (and \( k_Y \)) are characteristic [Sriperumbudur et al., 2010].

For incremental responses, further assume \( D \subset \mathbb{R} \) is an open set and \( \nabla_d \nabla_d' k_D(d, d') \) exists and is continuous, hence \( \sup_{d \in D} \|\nabla_d \phi(d)\|_H \leq \kappa'_d \). When treatment is discrete, take \( k_D(d, d') = 1_{d=d'} \) instead.
Commonly used kernels are continuous and bounded. Measurability is a similarly weak condition. The characteristic property means that different distributions will have different embeddings in the RKHS. For example, the indicator kernel is characteristic over a discrete domain, while the exponentiated quadratic kernel is characteristic over a continuous domain.

**Theorem 2** (Decoupling of mediated response curves). Suppose the conditions of Theorem 1 hold. Further suppose Assumption 2 holds and \( \gamma_0 \in \mathcal{H} \). Then

1. \( \omega_0(d, d'; X) = \langle \gamma_0, \phi(d') \otimes \mu_m(d, X) \otimes \phi(X) \rangle_{\mathcal{H}} \);
2. \( \theta_0^{ME}(d, d') = \mathbb{E}\{\omega_0(d, d'; X)\} = \langle \gamma_0, \phi(d') \otimes \mu_{m,x}(d) \rangle_{\mathcal{H}}, \)
3. \( \theta_0^{ME, \nabla}(d, d') = \mathbb{E}\{\nabla_d \omega_0(d, d'; X)\} = \langle \gamma_0, \nabla_d \phi(d') \otimes \mu_{m,x}(d) \rangle_{\mathcal{H}}, \)

where \( \mu_m(d, x) := \int \phi(m)d\mathbb{P}(m|d, x) \) and \( \mu_{m,x}(d) := \int \{\mu_m(d, x) \otimes \phi(x)\}d\mathbb{P}(x) \).

**Proof sketch.** Consider \( \omega_0(d, d', x) \). Exchanging integration and inner product,

\[
\omega_0(d, d'; x) = \int \langle \gamma_0, \phi(d') \otimes \phi(m) \otimes \phi(x) \rangle_{\mathcal{H}}d\mathbb{P}(m|d, x) = \langle \gamma_0, \phi(d') \otimes \mu_m(d, x) \otimes \phi(x) \rangle_{\mathcal{H}}.
\]

See Appendix E for the proof. The quantity \( \mu_m(d, x) := \int \phi(m)d\mathbb{P}(m|d, x) \) embeds the conditional distribution \( \mathbb{P}(m|d, x) \) as an element of the RKHS \( \mathcal{H}_M \), which is a popular technique in the RKHS literature. It has the property that, for \( f \in \mathcal{H}_M \), \( \langle f, \mu_m(d, x) \rangle_{\mathcal{H}_M} = \int f(m)d\mathbb{P}(m|d, x) \). The quantity \( \mu_{m,x}(d) \) is a sequential mean embedding that encodes the counterfactual distribution of mediator \( M \) and covariates \( X \) when treatment is \( D = d \), and it appears to be an innovation. It has the property that, for \( f \in \mathcal{H}_M \otimes \mathcal{H}_X \), \( \langle f, \mu_{m,x}(d) \rangle_{\mathcal{H}_M \otimes \mathcal{H}_X} = \int f(m, x)d\mathbb{P}(m|d, x)d\mathbb{P}(x) \).

Theorem 2 decouples \( \gamma_0(d', m, x), \mathbb{P}(m|d, x), \) and \( \mathbb{P}(x) \). As such, it provides a blueprint for estimation that avoids density estimation and nested integration. Our estimator will be \( \hat{\theta}^{ME}(d, d') = \langle \hat{\gamma}, \phi(d') \otimes \mu_{m,x}(d) \rangle_{\mathcal{H}} = \langle \hat{\gamma}, \phi(d') \otimes n^{-1}\sum_{i=1}^n \{\mu_m(d, X_i) \otimes \phi(X_i)\} \rangle_{\mathcal{H}} \). The estimator \( \hat{\gamma} \) is a standard kernel ridge regression. The estimator \( \hat{\mu}_m(d, x) \) is an appropriately generalized kernel ridge regression. We combine them by averaging and taking the product.

**Algorithm 1** (Nonparametric estimation of mediated response curves). Denote the kernel matrices by \( K_{DD}, K_{MM}, K_{XX} \in \mathbb{R}^{n \times n} \). Let \( \otimes \) mean elementwise product. Mediated response curves have closed form solutions:
1. \(\hat{\omega}(d, d'; x) = Y^\top(K_{DD} \odot K_{MM} \odot K_{XX} + n\lambda I)^{-1}[K_{Da'} \odot \{K_{MM}(K_{DD} \odot K_{XX} + n\lambda I)^{-1}(K_{Dd} \odot K_{Xx})\} \odot K_{Xx}]\);

2. \(\hat{\theta}^{ME}(d, d') = n^{-1}\sum_{i=1}^{n}\hat{\omega}(d, d'; X_i)\)

where \((\lambda, \lambda_1)\) are ridge regression penalty parameters. For mediated incremental response curve estimators, we replace \(K_{Da'}\) with \(\nabla_d k(D_i, d')\) where \((\nabla_d k(D_i, d'))_i = \nabla_d k(D_i, d')\).

**Derivation sketch.** Consider \(\omega_0(d, d'; x)\). Analogously to [1], the kernel ridge regression estimators of the regression \(\gamma_0\) and the conditional mean embedding \(\mu_m(d, x)\) are

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

\[
\hat{E} = \arg\min_{E \in \mathcal{L}(\mathcal{H}_M, \mathcal{H}_D \otimes \mathcal{H}_X)} \frac{1}{n}\sum_{i=1}^{n}[\phi(M_i) - E^*\{\phi(D_i) \otimes \phi(X_i)\}]^2 + \lambda_1\|E\|_{\mathcal{L}_2(\mathcal{H}_M, \mathcal{H}_D \otimes \mathcal{H}_X)}^2,
\]

where \(\hat{\mu}_m(d, x) = \hat{E}^*\{\phi(d) \otimes \phi(x)\}\) and \(E^*\) is the adjoint of \(E\). The closed forms are

\[
\hat{\gamma}(d', \cdot, x) = Y^\top(K_{DD} \odot K_{MM} \odot K_{XX} + n\lambda I)^{-1}(K_{Da'} \odot K_{M} \odot K_{Xx}),
\]

\[
[\hat{\mu}_m(d, x)](\cdot) = K_{M}(K_{DD} \odot K_{XX} + n\lambda I)^{-1}(K_{Dd} \odot K_{Xx}).
\]

To arrive at the main result, match the empty arguments (\(\cdot\)) of the kernel ridge regressions.

We derive this algorithm in Appendix [E]. We give theoretical values for \((\lambda, \lambda_1)\) that optimally balance bias and variance in Theorem [3] below. Appendix [H] gives practical tuning procedures with closed form solutions to empirically balance bias and variance, one of which is asymptotically optimal. We formally define the operator space \(\mathcal{L}_2(\mathcal{H}_M, \mathcal{H}_D \otimes \mathcal{H}_X)\) below.

Next we turn to semiparametric estimation and inference. We quote the doubly robust moment function for mediation analysis parametrized to avoid density estimation.

**Lemma 1** (Doubly robust moment of mediated effects [Tchetgen, Tchetgen and Shpitser, 2012]).

Suppose treatment \(D\) is binary, so that \(d, d' \in \{0, 1\}\). If Assumption [1] holds then

\[
\hat{\theta}^{ME}(d, d') = \mathbb{E}\{\psi^{ME}(d, d'; \gamma_0, \omega_0, \pi_0, \rho_0; W)\} \text{ where } W = (Y, D, M, X)\]

\[
\psi^{ME}(d, d'; \gamma, \omega, \pi, \rho; W) = \omega(d, d'; X) + \frac{1_{D=d'}}{\pi(d'; M, X)} \frac{\rho(d; M, X)}{\pi(d; M, X)}\{Y - \gamma(d', M, X)\}
\]

\[
+ \frac{1_{D=d}}{\pi(d; X)} \{\gamma(d', M, X) - \omega(d, d'; X)\}.
\]
The function $\gamma_0$ is a regression and $\omega_0(d, d'; X) = \int \gamma_0(d', m, X)d\mathcal{P}(m|d, X)$ is its partial mean, while $\pi_0(d; X) = \mathbb{P}(d|X)$ and $\rho_0(d; M, X) = \mathbb{P}(d|M, X)$ are propensity scores.

This equation is doubly robust with respect to the nonparametric quantities $(\gamma_0, \omega_0, \pi_0, \rho_0)$ in the sense that it continues to hold if $(\gamma_0, \omega_0)$ or $(\pi_0, \rho_0)$ are misspecified. As a consequence, our semiparametric results continue to hold if one of $(\gamma_0, \omega_0, \pi_0, \rho_0)$ is not actually an element of an RKHS. This parametrization, widely used in the targeted machine learning literature, suits our approach since the technique of sequential mean embeddings allows us to estimate $\omega_0$ without explicitly estimating the conditional density $f(m|d, x)$.

The semiparametric procedure uses our new nonparametric estimator from Algorithm 1 as a subroutine within a meta procedure that combines the doubly robust moment function from Lemma 1 and sample splitting. The meta algorithm of using the doubly robust moment function [Robins and Rotnitzky, 1995] and sample splitting [Klaassen, 1987], without specifying the nonparametric subroutines, is a variant of targeted [Zheng and van der Laan, 2011] and debiased [Chernozhukov et al., 2018] machine learning for mediation analysis.

Algorithm 2 (Semiparametric inference of mediated effects [Zheng and van der Laan, 2011, Chernozhukov et al., 2018]). Partition the sample into folds $(I_\ell)_{\ell=1:L}$. Denote by $I_\ell$ observations not in fold $I_\ell$.

1. For each fold $\ell$, estimate $(\hat{\gamma}_\ell, \hat{\omega}_\ell, \hat{\pi}_\ell, \hat{\rho}_\ell)$ from observations in $I_\ell$.

2. Estimate $\hat{\theta}^{ME}(d, d') = n^{-1} \sum_{\ell=1}^L \sum_{i \in I_\ell} \psi^{ME}(d, d'; \hat{\gamma}_\ell, \hat{\omega}_\ell, \hat{\pi}_\ell, \hat{\rho}_\ell; W_i)$.

3. Estimate its $(1 - a) \cdot 100\%$ confidence interval as $\hat{\theta}^{ME}(d, d') \pm \zeta_a \hat{\sigma}(d, d') n^{-1/2}$ where $\hat{\sigma}^2(d, d') = n^{-1} \sum_{\ell=1}^L \sum_{i \in I_\ell} \{\psi^{ME}(d, d'; \hat{\gamma}_\ell, \hat{\omega}_\ell, \hat{\pi}_\ell, \hat{\rho}_\ell; W_i) - \hat{\theta}^{ME}(d, d')\}^2$ and $\zeta_a$ is the $1 - a/2$ quantile of the standard Gaussian.

Unlike [Farbmacher et al., 2020, Algorithm 2], our procedure does not require multiple levels of sample splitting. Our algorithmic innovation is to propose and analyze a new subroutine $\hat{\omega}$ in Algorithm 1 based on the idea of sequential mean embedding, that does not require sample splitting of its own. Note that $\hat{\omega}$ is computed according to Algorithm 1 with regularization parameters $(\lambda, \lambda_1)$. $(\hat{\gamma}, \hat{\pi}, \hat{\rho})$ are standard kernel ridge regressions with regularization parameters $(\lambda, \lambda_2, \lambda_3)$. See Appendix E for explicit computations. We give theoretical values for regularization parameters that optimally balance bias and variance.
in Theorem 4 below. Appendix H gives practical tuning procedures with closed form
solutions to empirically balance bias and variance, one of which is asymptotically optimal.
Proposition 1 and the delta method imply confidence intervals for other quantities in
Definition 1.

3.3 Uniform consistency and semiparametric inference

Towards a guarantee of uniform consistency, we place regularity conditions on the original
spaces. Anticipating Appendix B, we include conditions for the outcome in parentheses.

Assumption 3 (Original space regularity conditions). Assume

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

2. \( \mathcal{Y} \subset \mathbb{R} \) and \( |Y| \leq C \) almost surely.

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 even texts,
graphs, or images. Boundedness of \( Y \) can be relaxed. Next, we place assumptions on the
smoothness of the regression \( \gamma_0 \) and the effective dimension of \( \mathcal{H} \) the sense of (2).

Assumption 4 (Smoothness and effective dimension of regression). Assume \( \gamma_0 \in \mathcal{H}^c \) where \( c \in (1, 2] \), and \( \eta_j(\mathcal{H}) \leq C j^{-b} \) where \( b \geq 1 \).

See Appendix F for alternative ways of writing and interpreting Assumption 4 in the
tensor product space \( \mathcal{H} \). We place similar conditions on the conditional mean embedding
\( \mu_m(d, x) \), which is a generalized regression. 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 \( b \in \mathcal{B}_{\ell} \). As such, all
one has to do is specify \( \mathcal{A}_{\ell} \) and \( \mathcal{B}_{\ell} \) to specialize the assumption. For \( \mu_m(d, x), \mathcal{A}_1 = \mathcal{M} \) and
\( \mathcal{B}_1 = \mathcal{D} \times \mathcal{X} \). We parametrize the effective dimension and smoothness of \( \mu_a(b) \) by \( (b_{\ell}, c_{\ell}) \).

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

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

where \( E_{\ell}^* \) is the adjoint of \( E_{\ell} \). We denote the space of Hilbert-Schmidt operators be-
tween \( \mathcal{H}_{\mathcal{A}_{\ell}} \) and \( \mathcal{H}_{\mathcal{B}_{\ell}} \) by \( L_2(\mathcal{H}_{\mathcal{A}_{\ell}}, \mathcal{H}_{\mathcal{B}_{\ell}}) \). \( L_2(\mathcal{H}_{\mathcal{A}_{\ell}}, \mathcal{H}_{\mathcal{B}_{\ell}}) \) is an RKHS in its own right, for
which we place smoothness and effective dimension assumptions in the sense of [2]. See [Grünewälder et al., 2013, Appendix B] and [Singh et al., 2019, Appendix A.3] for details.

**Assumption 5** (Smoothness and effective dimension of conditional mean embedding). Assume $E_\ell \in L^2(\mathcal{H}_A, \mathcal{H}_B^\ell)$ where $c_\ell \in (1, 2]$ and $\eta_j(\mathcal{H}_B^\ell) \leq C_j - b_\ell$ where $b_\ell \geq 1$.

Just as we place approximation assumptions for $\gamma_0$ in terms of $\mathcal{H}$, which provides the features onto which we project $Y$, we place approximation assumptions for $E_\ell$ in terms of $\mathcal{H}_B^\ell$, which provides the features $\phi(B_\ell)$ onto which we project $\phi(A_\ell)$. Under these conditions, we arrive at our first main theoretical guarantee.

**Theorem 3** (Nonparametric consistency of mediated response curves). Suppose Assumptions 1, 2, 3, 4, and 5 hold with $A_1 = M$ and $B_1 = D \times X$. Set $(\lambda, \lambda_1) = \left( n^{-\frac{1}{2}} \frac{c_1}{c + 1/8} + n^{-\frac{1}{2}} \frac{c_1 - 1}{c_1 + 1/8}, n^{-\frac{1}{2}} \frac{c_1}{c + 1/8} + n^{-\frac{1}{2}} \frac{c_1 - 1}{c_1 + 1/8} \right)$, which is rate optimal regularization. Then

1. $\|\hat{\theta}_{ME} - \theta_{ME}^0\|_\infty = O_p \left( n^{-\frac{1}{2}} \frac{c_1}{c + 1/8} + n^{-\frac{1}{2}} \frac{c_1 - 1}{c_1 + 1/8} \right)$;
2. $\|\hat{\theta}_{ME,\nabla} - \theta_{ME,\nabla}^0\|_\infty = O_p \left( n^{-\frac{1}{2}} \frac{c_1}{c + 1/8} + n^{-\frac{1}{2}} \frac{c_1 - 1}{c_1 + 1/8} \right)$.

See Appendix [F] for the proof. By Proposition 1 the various quantities in Definition 1 are uniformly consistent with the same rate, which combines optimal rates for standard [Fischer and Steinwart, 2020, Theorem 2] and generalized [Li et al., 2022, Theorem 3] kernel ridge regression in RKHS norm. The exact finite sample rate is given in Appendix [F] as well as the explicit specialization of Assumption 5. The rate is at best $n^{-\frac{1}{4}}$ when $(c, c_1) = 2$ and $(b, b_1) \to \infty$, i.e. when $(\gamma_0, \mu_m)$ are very smooth with finite effective dimensions. The rates reflect the challenge of a sup norm guarantee, which is much stronger than an $L^2$ norm guarantee and which encodes caution about worst case scenarios when informing policy decisions. See (3) to specialize these rates for Sobolev spaces.

In the semiparametric case where $D$ is binary, $\theta_{0,ME}^0(d, d')$ is a matrix in $\mathbb{R}^{2 \times 2}$. Theorem 3 simplifies to a guarantee on the maximum element of the matrix of differences $|\hat{\theta}_{ME}^0(d, d') - \theta_{ME}^0(d, d')|$. For the semiparametric case, we improve the rate from $n^{-\frac{1}{4}}$ to $n^{-\frac{1}{2}}$ by using Algorithm 2 and imposing additional assumptions. In particular, we place additional assumptions on the propensity scores.

**Assumption 6** (Bounded propensities). Propensity scores $\pi_0(d; X)$ and $\rho_0(d; M, X)$, and estimators $\hat{\pi}(d; X)$ and $\hat{\rho}(d; M, X)$, are bounded away from zero and one almost surely.
The first part of Assumption 6 is a mild strengthening of the overlap condition in Assumption 1. The second part can be imposed by trimming the estimators $(\hat{\pi}, \hat{\rho})$, which only improves prediction quality since $(\pi_0, \rho_0)$ are bounded. Assumption 6 is not specific to the RKHS setting. We now place smoothness and spectral decay assumptions that are specific to the RKHS setting. Specifically, we assume propensity scores are smooth and belong to RKHSs with quantifiable effective dimension in the sense of (2).

**Assumption 7 (Smoothness and effective dimension of propensities). Assume**

1. $\pi_0 \in \mathcal{H}_X^{c_2}$ where $c_2 \in (1, 2]$, and $\eta_j(\mathcal{H}_X) \leq C_j j^{-b_2}$ where $b_2 \geq 1$;

2. $\rho_0 \in (\mathcal{H}_M \otimes \mathcal{H}_X)^{c_3}$ where $c_3 \in (1, 2]$ and $\eta_j(\mathcal{H}_M \otimes \mathcal{H}_X) \leq C_j j^{-b_3}$ where $b_3 \geq 1$.

Finally, we prove our main result for semiparametric mediated effects.

**Theorem 4 (Semiparametric consistency, Gaussian approximation, and efficiency of mediated effects). Suppose the conditions of Theorem 3 hold, as well as Assumptions 6 and 7. Set**

$$(\lambda, \lambda_1, \lambda_2, \lambda_3) = (n^{-\epsilon_1 + 1/3}, n^{-\epsilon_1 + 1/3}, n^{-\epsilon_2 + 1/3}, n^{-\epsilon_3 + 1/3}),$$

which is rate optimal regularization. Then for any $c, c_1, c_2 \in (1, 2]$ and $b, b_1, b_2 \geq 1$ satisfying

$$\min \left( \frac{c - 1}{c + 1/b}, \frac{c_1 - 1}{c_1 + 1/b_1} \right) + \frac{c_2}{c_2 + 1/b_2} > 1,$$

we have that $\hat{\theta}^{ME}(d, d') \overset{p}{\to} \theta_0^{ME}(d, d'), \sqrt{n} \sigma(\hat{\sigma})^{-1}(\hat{\theta}^{ME}(d, d') - \theta_0^{ME}(d, d')) \overset{d}{\to} \mathcal{N}(0, 1)

$$\mathbb{P}\left[ \theta_0^{ME}(d, d') \in \left\{ \hat{\sigma}^{ME}(d, d') \pm \varsigma_{a} \hat{\sigma}(d, d') n^{-1/2} \right\} \right] \to 1 - a.$$
quantified by \((b, b_1, b_2)\) must be sufficiently fast relative to the smoothness of the various nonparametric objects \((c, c_1, c_2)\). See (3) to specialize these conditions for Sobolev spaces. See [Singh, 2021b, Corollary 6.2] to translate the semiparametric Gaussian approximation into pointwise nonparametric inference.

4 Dynamic dose responses and treatment effects

4.1 Definition and identification

So far we have considered the effect of a one-off treatment \(D\). Next, we consider the effect of a sequence of treatments \(D_{1:T} = d_{1:T}\) on counterfactual outcome \(Y^{(d_{1:T})}\). If the sequence of treatment values \(d_{1:T}\) is observed in the data, this problem may be called on policy planning; if not, it may be called off policy planning.

**Definition 2** (Dynamic response curves and effects). We define

1. \(\theta_{GF}^0(d_{1:T}) := E\{Y^{(d_{1:T})}\}\) is the counterfactual mean outcome given interventions \(D_{1:T} = d_{1:T}\) for the entire population.

2. \(\theta_{DS}^0(d_{1:T}, \tilde{P}) := E_{\tilde{P}}\{Y^{(d_{1:T})}\}\) is the counterfactual mean outcome given interventions \(D_{1:T} = d_{1:T}\) for an alternative population with data distribution \(\tilde{P}\) (elaborated in Assumption 9 below).

Likewise we define incremental response curves and effects, e.g. \(\theta_{GF}^{dT}(d_{1:T}) := E\{\nabla_{dT} Y^{(d_{1:T})}\}\).

Whereas much of the semiparametric literature restricts \(d_t \in \{0, 1\}\), we allow \(d_t\) to be discrete or continuous and consider a nonparametric approach to dynamic response curves [Gill and Robins, 2001]. For example, in Section 5 we estimate the effect of \(d_1\) job training hours in year one, and \(d_2\) job training hours in year two, on counterfactual employment. In the spirit of off policy planning, we consider a distribution shift from \(P\) to \(\tilde{P}\).

For clarity, we focus on the deterministic, static counterfactual policy \(d_{1:T}\). It is deterministic in that it is nonrandom. It is static in that it does not depend on the observed sequence of covariates \(X_{1:T}\). Impressively, the causal inference literature on dynamic treatment effects extends to policies that may be randomized and that may be
dynamic [Robins, 1986]. Our approach may extend to randomized and dynamic policies
with additional notation.\footnote{To accommodate randomized dynamic policies, the product in Theorem 5 will include factors for the conditional distributions of treatments. Specifically, the integral will replace \( d_t \) with \( g_t : \{d_{1:(t-1)}, x_{1:t}\} \mapsto G\{d_t|d_{1:(t-1)}, x_{1:t}\} \) where \( G \) is the distribution induced by the randomized dynamic policy \( g_t \).}

In seminal work, \cite{Robins1986} states sufficient conditions under which dynamic responses and effects can be measured from outcomes \( Y \), treatments \( D_{1:T} \), and covariates \( X_{1:T} \). This collection of conditions is known as sequential selection on observables.

**Assumption 8** (Sequential selection on observables). Assume

1. No interference: if \( D_{1:T} = d_{1:T} \) then \( Y = Y^{(d_{1:T})} \).
2. Conditional exchangeability: \( \{Y^{(d_{1:T})}\} \perp D_t | D_{1:(t-1)}, X_{1:t}, \forall 1 \leq t \leq T. \)
3. Overlap: if \( \{d_{1:(t-1)}, x_{1:t}\} > 0 \) then \( f\{d_t|d_{1:(t-1)}, x_{1:t}\} > 0 \), where \( f\{d_{1:(t-1)}, x_{1:t}\} \) and \( f\{d_t|d_{1:(t-1)}, x_{1:t}\} \) are densities.

Assumption 8 is a sequential generalization of the familiar, one-stage selection on observables. To handle \( \theta^0_{DS} \), we generalize a standard assumption in transfer learning.

**Assumption 9** (Distribution shift). Assume

1. \( \tilde{P}(Y, D_{1:T}, X_{1:T}) = P(Y|D_{1:T}, X_{1:T})\tilde{P}(D_{1:T}, X_{1:T}); \)
2. \( \tilde{P}(D_{1:T}, X_{1:T}) \) is absolutely continuous with respect to \( P(D_{1:T}, X_{1:T}) \).

The difference between \( P \) and \( \tilde{P} \) is only in the distribution of treatments and covariates. Moreover, the support of \( P \) contains the support of \( \tilde{P} \). An immediate consequence is that the regression function \( \gamma_0(d_{1:T}, x_{1:T}) := E(Y|D_{1:T} = d_{1:T}, X_{1:T} = x_{1:T}) \) remains the same across the different populations \( P \) and \( \tilde{P} \). We generalize a classic identification result due to \cite{Robins1986, GillRobins2001} in two ways: we consider distribution shift, and we consider incremental responses and effects. These extensions appear to be new.

**Theorem 5** (Identification of dynamic response curves and effects). If Assumption 8 holds, then

\[ \theta^0_{G}(d_{1:T}) = \int \gamma_0(d_{1:T}, x_{1:T}) d\tilde{P}(x_1) \prod_{t=2}^{T} d\tilde{P}\{x_t|d_{1:(t-1)}, x_{1:(t-1)}\} \] \cite{Robins1986}.\footnote{To accommodate randomized dynamic policies, the product in Theorem 5 will include factors for the conditional distributions of treatments. Specifically, the integral will replace \( d_t \) with \( g_t : \{d_{1:(t-1)}, x_{1:t}\} \mapsto G\{d_t|d_{1:(t-1)}, x_{1:t}\} \) where \( G \) is the distribution induced by the randomized dynamic policy \( g_t \).}
Theorem 6

Theorem 5 makes precise how each dynamic response and effect is identified as a nested integral. Further suppose Assumption 2 holds and

\[ \prod_{t=2}^{T} \mathbb{P}\{x_t|d_{1:(t-1)}, x_{1:(t-1)}\}. \]

For incremental response curves and effects, we replace \( \gamma_0(d_{1:T}, x_{1:T}) \) with \( \nabla_{d_t} \gamma_0(d_{1:T}, x_{1:T}) \).

See Appendix D for the proof. The nested integral is the famous g-formula from biostatistics stated for sequences of treatments that may be discrete or continuous. We consider a fully nonparametric g-formula that allows for distribution shift. Theorem 5 handles auxiliary Markov restrictions as special cases. For example, if covariates follow a Markov process, then \( \theta_0^{\text{GP}} \) simplifies by setting \( \mathbb{P}\{x_t|d_{1:(t-1)}, x_{1:(t-1)}\} = \mathbb{P}(x_t|d_{t-1}, x_{t-1}) \).

4.2 Algorithm

Theorem 4 makes precise how each dynamic response and effect is identified as a nested integral of the form \( \int \gamma_0(d_{1:T}, x_{1:T})dQ \) for the distribution \( Q = \mathbb{P}(x_1) \prod_{t=2}^{T} \mathbb{P}\{x_t|d_{1:(t-1)}, x_{1:(t-1)}\} \) or \( Q = \tilde{\mathbb{P}}(x_1) \prod_{t=2}^{T} \tilde{\mathbb{P}}\{x_t|d_{1:(t-1)}, x_{1:(t-1)}\}. \) Since \( x_1 \) appears in \( \gamma_0(d_{1:T}, x_{1:T}) \), \( \mathbb{P}\{x_t|d_{1:(t-1)}, x_{1:(t-1)}\} \), and \( \mathbb{P}(x_1) \), the components of the nested integral are coupled and therefore challenging to estimate. As in Section 3, our key insight is to construct an appropriate RKHS to decouple these components, then to encode \( Q \) by a sequential mean embedding. With these techniques, we again reduce multistage causal inference into the combination of kernel ridge regressions. For clarity, we present the algorithm with \( T = 2 \), and we define \( \omega_0(d_1, d_2; x_1) = \int \gamma_0(d_1, d_2, x_1, x_2)d\mathbb{P}(x_2|d_1, x_1) \) so that \( \theta_0^{\text{GP}}(d_1, d_2) = \mathbb{E}\{\omega_0(d_1, d_2; X_1)\} \). We consider \( T > 2 \) in Appendix C which also showcases the role of Markov assumptions and demonstrates the connection to Bang and Robins, 2005.

As before, we begin by constructing the appropriate RKHS for \( \gamma_0 \). We define RKHSs for each treatment \( D_t \) and each covariate \( X_t \). Using identical notation as Section 3 we assume the regression \( \gamma_0 \) is an element of the RKHS \( \mathcal{H} \) with the kernel \( k(d_1, d_2, x_1, x_2; d_1', d_2', x_1', x_2') = k_D(d_1, d_1') \cdot k_D(d_2, d_2') \cdot k_X(x_1, x_1') \cdot k_X(x_2, x_2'), \) i.e. \( \gamma_0 \in \mathcal{H} := \mathcal{H}_D \otimes \mathcal{H}_D \otimes \mathcal{H}_X \otimes \mathcal{H}_X \). As such, \( \gamma_0(d_1, d_2, x_1, x_2) = \langle \gamma_0, \phi(d_1) \otimes \phi(d_2) \otimes \phi(x_1) \otimes \phi(x_2) \rangle_{\mathcal{H}} \) and \( \|\phi(d_1) \otimes \phi(d_2) \otimes \phi(x_1) \otimes \phi(x_2)\|_{\mathcal{H}} = \|\phi(d_1)\|_{\mathcal{H}_D} \cdot \|\phi(d_2)\|_{\mathcal{H}_D} \cdot \|\phi(x_1)\|_{\mathcal{H}_X} \cdot \|\phi(x_2)\|_{\mathcal{H}_X} \). Under regularity conditions on this RKHS construction, we prove an analogous decoupling result.

**Theorem 6** (Decoupling of dynamic response curves). Suppose the conditions of Theorem 5 hold. Further suppose Assumption 2 holds and \( \gamma_0 \in \mathcal{H} \). Then
Algorithm 3 (Nonparametric estimation of dynamic response curves). Denote the kernel matrices $K_{D_1 D_1}, K_{D_2 D_2}, K_{X_1 X_1}, K_{X_2 X_2} \in \mathbb{R}^{n \times n}$ calculated from observations of population $\mathbb{P}$. Denote the kernel matrices $K_{\tilde{D}_1 \tilde{D}_1}, K_{\tilde{D}_2 \tilde{D}_2}, K_{\tilde{X}_1 \tilde{X}_1}, K_{\tilde{X}_2 \tilde{X}_2} \in \mathbb{R}^{\tilde{n} \times \tilde{n}}$ calculated from observations of population $\mathbb{\tilde{P}}$. Let $\odot$ mean elementwise product. Dynamic dose response curve estimators are

1. $\hat{\omega}(d_1, d_2; X_1) = Y^\top (K_{D_1 D_1} \odot K_{D_2 D_2} \odot K_{X_1 X_1} \odot K_{X_2 X_2} + n\lambda I)^{-1}$
   
   $[K_{D_1 d_1} \odot K_{D_2 d_2} \odot K_{X_1 x_1} \odot \{K_{X_2 X_2}(K_{D_1 D_1} \odot K_{X_1 X_1} + n\lambda I)^{-1}(K_{D_1 d_1} \odot K_{X_1 x_1})\}]$;

2. $\hat{\theta}^{GF}(d_1, d_2) = n^{-1} \sum_{i=1}^{n} \hat{\omega}(d_1, d_2; X_{1i})$;

3. $\hat{\theta}^{DS}(d_1, d_2; \mathbb{\tilde{P}}) = \tilde{n}^{-1} \sum_{i=1}^{\tilde{n}} Y^\top (K_{D_1 D_1} \odot K_{D_2 D_2} \odot K_{X_1 X_1} \odot K_{X_2 X_2} + n\lambda I)^{-1}$
   
   $[K_{D_1 d_1} \odot K_{D_2 d_2} \odot K_{X_1 \tilde{x}_1} \odot \{K_{X_2 \tilde{x}_2}(K_{D_1 D_1} \odot K_{\tilde{X}_1 \tilde{x}_1} + \tilde{n}\lambda_5 I)^{-1}(K_{D_1 d_1} \odot K_{X_1 \tilde{x}_1})\}]$.

where $(\lambda, \lambda_4, \lambda_5)$ are ridge regression penalty parameters. For incremental responses, we replace $K_{D_2 d_2}$ with $\nabla_d K_{D_2 d_2}$ where $(\nabla_d K_{D_2 d_2})_i = \nabla_d k(D_{2i}, d_2)$.
We derive these algorithms in Appendix E. We give theoretical values for $(\lambda, \lambda_4, \lambda_5)$ that optimally balance bias and variance in Theorem 7 below. Appendix H gives practical tuning procedures with closed form solutions to empirically balance bias and variance, one of which is asymptotically optimal. Note that $\hat{\theta}^{DS}$ requires observations of treatments and covariates from the alternative population $\tilde{P}$.

Next we turn to semiparametric estimation and inference. We quote the doubly robust moment function for dynamic treatment effects parametrized to avoid density estimation.

Lemma 2 (Doubly robust moment of dynamic treatment effects [Scharfstein et al., 1999]). Suppose treatment $D_t$ is binary, so that $d_1, d_2 \in \{0, 1\}$. If Assumption 8 holds then

$$
\theta^{GF}(d_1, d_2) = E\{\psi^{GF}(d_1, d_2; \gamma_0, \omega_0, \pi_0, \rho_0; W)\}
$$

where $W = (Y, D_1, D_2, X_1, X_2)$ and

$$
\psi^{GF}(d_1, d_2; \gamma, \omega, \pi, \rho; W) = \omega(d_1, d_2; X_1) + \frac{1_{D_1=d_1} 1_{D_2=d_2}}{\pi(d_1; X_1)} \{Y - \gamma(d_1, d_2, X_1, X_2)\}
$$

$$
+ \frac{1_{D_1=d_1}}{\pi(d_1; X_1)} \{\gamma(d_1, d_2, X_1, X_2) - \omega(d_1, d_2; X_1)\}.
$$

The function $\gamma_0$ is a regression and $\omega_0(d_1, d_2; X_1) := \int \gamma_0(d_1, d_2, X_1, x_2)d\tilde{P}(x_2|d_1, X_1)$ is its partial mean, while $\pi_0(d_1; X_1) := \tilde{P}(d_1|X_1)$ and $\rho_0(d_2; d_1, X_1, X_2) := \tilde{P}(d_2|d_1, X_1, X_2)$ are propensity scores.

This equation is doubly robust with respect to the nonparametric quantities $(\gamma_0, \omega_0, \pi_0, \rho_0)$ in the sense that it continues to hold if $(\gamma_0, \omega_0)$ or $(\pi_0, \rho_0)$ are misspecified. As a consequence, our semiparametric results continue to hold if one of $(\gamma_0, \omega_0, \pi_0, \rho_0)$ is not actually an element of an RKHS. This parametrization, widely used in the targeted machine learning literature, suits our approach since the technique of sequential mean embeddings allows us to estimate $\omega_0$ without explicitly estimating the conditional density $f(x_2|d_1, x_1)$.

The semiparametric procedure combines our new nonparametric estimator from Algorithm 3 as a subroutine within a meta procedure that combines the doubly robust moment function from Lemma 2 and sample splitting. The meta algorithm, with abstract nonparametric subroutines, is a variant of targeted [Zheng and van der Laan, 2011] and debiased [Chernozhukov et al., 2018] machine learning for dynamic treatment effects.

Algorithm 4 (Semiparametric inference of dynamic treatment effects [Zheng and van der Laan, 2011, Chernozhukov et al., 2018]). Partition the sample into folds $(I_\ell)_{\ell=1:L}$. Denote by $I_\ell$ observations not in fold $I_\ell$. 

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1. For each fold \(\ell\), estimate \((\hat{\gamma}_\ell, \hat{\omega}_\ell, \hat{\pi}_\ell, \hat{\rho}_\ell)\) from observations in \(I^c_\ell\).

2. Estimate \(\hat{\theta}_{GF}(d_1, d_2) = n^{-1} \sum_{\ell=1}^{L} \sum_{i \in I_\ell} \psi_{GF}(d_1, d_2; \hat{\gamma}_\ell, \hat{\omega}_\ell, \hat{\pi}_\ell, \hat{\rho}_\ell; W_i)\).

3. Estimate its \((1 - a) \cdot 100\%\) confidence interval as \(\hat{\theta}_{GF}(d_1, d_2) \pm \varsigma_a \hat{\sigma}(d_1, d_2)n^{-1/2}\) where 
\[\hat{\sigma}^2(d_1, d_2) = n^{-1} \sum_{\ell=1}^{L} \sum_{i \in I_\ell} \left\{\psi_{GF}(d_1, d_2; \hat{\gamma}_\ell, \hat{\omega}_\ell, \hat{\pi}_\ell, \hat{\rho}_\ell; W_i) - \hat{\theta}_{GF}(d_1, d_2)\right\}^2\]
and \(\varsigma_a\) is the \(1 - a/2\) quantile of the standard Gaussian.

Unlike [Bodory et al., 2020, Algorithm 1], our procedure does not require multiple levels of sample splitting. Our algorithmic innovation is to propose and analyze a new estimator \(\hat{\omega}\) in Algorithm 3, based on the idea of sequential mean embedding, that does not require sample splitting of its own. Note that \(\hat{\omega}\) is computed according to Algorithm 3 with regularization parameters \((\lambda, \lambda_4)\). \((\hat{\gamma}, \hat{\pi}, \hat{\rho})\) are standard kernel ridge regressions with regularization parameters \((\lambda, \lambda_6, \lambda_7)\). See Appendix E for explicit computations. We give theoretical values for regularization parameters that optimally balance bias and variance in Theorem 8 below. Appendix H gives practical tuning procedures with closed form solutions to empirically balance bias and variance, one of which is asymptotically optimal.

4.3 Uniform consistency and semiparametric inference

Towards a guarantee of uniform consistency, we place regularity conditions on the RKHSs and original spaces via Assumptions 2 and 3. We also assume the regression \(\gamma_0\) is smooth and quantify the effective dimension of \(\mathcal{H}\) via Assumption 4. For the conditional mean embeddings \(\mu_{x_2}(d_1, x_1)\) and \(\nu_{x_2}(d_1, x_1)\), we place further smoothness and effective dimension conditions via Assumption 5. With these assumptions, we arrive at our next main result.

**Theorem 7** (Nonparametric consistency of dynamic response curves). Suppose Assumptions 8, 2, 3, and 4 hold. Set \((\lambda, \lambda_4, \lambda_5) = (n^{-\frac{1}{2+1/\beta}}, n^{-\frac{1}{2+1/\beta_4}}, \tilde{n}^{-\frac{1}{2+1/\beta_5}})\), which is rate optimal regularization.

1. If in addition Assumption 5 holds with \(A_4 = \mathcal{X}\) and \(B_4 = \mathcal{D} \times \mathcal{X}\), then \(\|\hat{\theta}_{GF} - \theta_0^{GF}\|_{\infty} = O_p\left(n^{-\frac{1}{2+1/\beta}} + n^{-\frac{1}{2+1/\beta_4}}\right)\).

2. If in addition Assumptions 9 and 5 hold with \(A_5 = \mathcal{X}\) and \(B_5 = \mathcal{D} \times \mathcal{X}\), then \(\|\hat{\theta}_{DS} - \theta_0^{DS}\|_{\infty} = O_p\left(n^{-\frac{1}{2+1/\beta}} + \tilde{n}^{-\frac{1}{2+1/\beta_5}}\right)\).
Likewise for incremental responses, e.g. 
\[\|\hat{\theta}^{GF,\nabla} - \theta_0^{GF,\nabla}\|_\infty = O_p\left(n^{-\frac{1}{2}} \epsilon^{-1} + n^{-\frac{1}{2} \epsilon^{-c_4^{-1}}/b}\right).\]

See Appendix [4] for the proof, exact finite sample rates, and explicit specializations of Assumption [5]. As before, these rates are at best \(n^{-\frac{1}{4}}\) when \((c, c_4, c_5) = 2\) and \((b, b_4, b_5) \to \infty\). See (3) for the Sobolev special case.

In the semiparametric case where \((D_1, D_2)\) are binary, \(\theta_0^{GF}(d_1, d_2)\) is a matrix in \(\mathbb{R}^{2 \times 2}\).

Theorem [7] simplifies to a guarantee on the maximum element of the matrix of differences \(|\hat{\theta}^{GF}(d_1, d_2) - \theta_0^{GF}(d_1, d_2)|\). For the semiparametric case, we are able to improve the rate from \(n^{-\frac{1}{4}}\) to \(n^{-\frac{1}{2}}\) by using Algorithm [4] and imposing additional assumptions. In particular, we place additional assumptions on the propensity scores.

**Assumption 10** (Bounded propensities and density ratio). Assume that, almost surely

1. Propensity scores \(\pi_0(d_1; X_1)\) and \(\rho_0(d_2; D_1, X_1, X_2)\), and their estimators \(\hat{\pi}(d_1; X_1)\) and \(\hat{\rho}(d_2; D_1, X_1, X_2)\), are bounded away from zero and one;

2. The density ratio \(f(x_2|d_1, X_1)/f(x_2|d'_1, X_1)\) is bounded for any values \(d_1, d'_1 \in \mathcal{D}\).

The first part of Assumption [10] is a mild strengthening of the overlap condition in Assumption [8]. The second part can be imposed by trimming the estimators \((\hat{\pi}, \hat{\rho})\), which only improves prediction quality since \((\pi_0, \rho_0)\) are bounded. The third part is a weak regularity condition that simplifies the proof technique. Assumption [10] is not specific to the RKHS setting. We now place smoothness and spectral decay assumptions that are specific to the RKHS setting. Specifically, we assume propensity scores are smooth and belong to RKHSs with quantifiable effective dimension in the sense of (2).

**Assumption 11** (Smoothness and effective dimension of propensities). Assume

1. \(\pi_0 \in \mathcal{H}_{\mathcal{X}}^{c_6}\) where \(c_6 \in (1, 2]\), and \(\eta_j(\mathcal{H}_{\mathcal{X}}) \leq C_j^{-b_6}\) where \(b_6 \geq 1\).

2. \(\rho_0 \in (\mathcal{H}_{\mathcal{D}} \otimes \mathcal{H}_{\mathcal{X}} \otimes \mathcal{H}_{\mathcal{X}})^{c_7}\) where \(c_7 \in (1, 2]\), and \(\eta_j(\mathcal{H}_{\mathcal{D}} \otimes \mathcal{H}_{\mathcal{X}} \otimes \mathcal{H}_{\mathcal{X}}) \leq C_j^{-b_7}\) where \(b_7 \geq 1\).

Finally, we prove our main result for semiparametric dynamic treatment effects.
Theorem 8 (Semiparametric consistency, Gaussian approximation, and efficiency of dynamic treatment effects). Suppose the conditions of Theorem 7 hold, as well as Assumptions 10 and 11. Set \((\lambda, \lambda_4, \lambda_6, \lambda_7) = (n^{-\frac{1}{2+c}} \cdot n^{-\frac{1}{4+c_4}}, n^{-\frac{1}{6+c_6}}, n^{-\frac{1}{7+c_7}})\), which is rate optimal regularization. Then for any \(c, c_4, c_6 \in (1, 2]\) and \(b, b_4, b_6 \geq 1\) satisfying

\[
\min \left( \frac{c-1}{c+1/b}, \frac{c_4-1}{c_4+1/b_4} \right) + \frac{c_6}{c_6+1/b_6} > 1,
\]

we have that \(\hat{\theta}^{GF}(d_1, d_2) \overset{p}{\to} \theta_0^{GF}(d_1, d_2)\), \(n^{1/2} \sigma(d_1, d_2)^{-1} \{\hat{\theta}^{GF}(d_1, d_2) - \theta_0^{GF}(d_1, d_2)\} \overset{d}{\to} \mathcal{N}(0, 1)\), and

\[
P \left[ \theta_0^{GF}(d_1, d_2) \in \{\hat{\theta}^{GF}(d_1, d_2) \pm \varsigma_a \hat{\sigma}(d_1, d_2)n^{-1/2}\} \right] \to 1 - a.
\]

Moreover, the estimator is semiparametrically efficient.

See Appendix G for the proof and a stronger finite sample guarantee. In the favorable case that \((c, c_4, c_6) = 2\) i.e. \((\gamma_0, \mu_{x_2}, \pi_0)\) are very smooth, the conditions simplify: either \((b, b_4) > 1\) or \(b_6 > 1\). We require *either* the kernels of \((\gamma_0, \mu_{x_2})\) or the kernel of \(\pi_0\) to have low effective dimension. We uncover double spectral robustness that is again similar in spirit to double sparsity robustness of lasso estimators for one-stage treatment effects. More generally, there is a trade-off among the smoothness and effective dimension assumptions across nonparametric objects. The spectral decay quantified by \((b, b_4, b_6)\) must be sufficiently fast relative to the smoothness of the various nonparametric objects \((c, c_4, c_6)\). See [3] for the Sobolev special case. See [Singh, 2021b, Corollary 6.2] to translate the semiparametric Gaussian approximation into pointwise nonparametric inference.

5 Simulations and application

5.1 Simulations

We evaluate the empirical performance of our estimators on various nonparametric and semiparametric designs with varying sample sizes over short horizons. For each nonparametric design and sample size, we implement 100 simulations and calculate mean square error (MSE) with respect to the true counterfactual function. Figure I visualizes results. Note that a lower MSE is desirable. For each semiparametric design and sample size, we
implement 100 simulations and calculate coverage with respect to the true counterfactual values. Note that 95% coverage is desirable. See Appendix I for the data generating processes, implementation details, and coverage tables.

Figure 1: Nonparametric mean square error simulations

The mediated dose response design [Huber et al., 2020] involves learning the nonlinear counterfactual function $\theta_{ME}^0(d, d') = 0.3d' + 0.09d + 0.15dd' + 0.25 \cdot (d')^3$. A single observation consists of the tuple $(Y, D, M, X)$ for outcome, treatment, mediator, and covariates where $Y, D, M, X \in \mathbb{R}$. In addition to our estimator (RKHS), we implement the estimator of [Huber et al., 2020] (IPW), which involves Nadaraya-Watson density estimation en route to a generalized inverse propensity estimate. By the Wilcoxon rank sum test, RKHS significantly outperforms IPW at all sample sizes with p-values < 0.001.

Next, we propose a dynamic dose response design, extending the design of [Colangelo and Lee, 2020] to the multistage setting. The nonlinear counterfactual function is $\theta_{GF}^0(d_1, d_2) = 0.6d_1 + 0.5d_2^2 + 1.2d_2 + d_2^2$. A single observation consists of the tuple $(Y, D_{1:2}, X_{1:2})$ for outcome, treatments, and covariates where $Y, D_t \in \mathbb{R}$ and $X_t \in \mathbb{R}^{100}$. In addition to this high dimensional setting, we consider low and moderate dimensional settings in Appendix I. Our machine learning approach for dynamic dose response curves allows for nonlinearity, dependence over time, and effect modification, which appears to be new.

To illustrate why dynamic confounding and effect modification matter, we implement not only $\hat{\theta}_{GF}^0(d_1, d_2)$ \{RKHS(GF)\} but also estimators that ignore dynamic confounding
and effect modification to various degrees. Using the one-stage dose response estimator of \cite{Singh2020} \{RKHS(ATE)\}, we take treatment to be $D_2$ and misclassify $D_1$ as a covariate. Using the heterogeneous dose response estimator of \cite{Singh2020} \{RKHS(CATE)\}, we take treatment to be $D_2$ and misclassify $D_1$ as the low dimensional subcovariate with meaningful heterogeneity. We also implement the estimator of \cite{Lewis2020} (SNMM), which is a machine learning approach with linearity, Markov, and no-effect-modification assumptions that do not hold. By the Wilcoxon rank sum test, RKHS(GF) significantly outperforms alternatives at sample size 5000 with p-value $< 0.001$. The ability of RKHS(GF) to capture dynamic confounding and effect modification in the multistage setting confers benefits when the sample size is sufficiently large.

Finally, we implement semiparametric simplifications of both designs. The goal of the semiparametric mediated effect design is to learn $\theta_0^{ME}(d,d') = 0.09d + 0.55d' + 0.15dd'$. A single observation consists of the tuple $(Y,D,M,X)$ where now $D \in \{0,1\}$. The goal of the semiparametric dynamic treatment effect design is to learn $\theta_0^{GF}(d_1,d_2) = 1.1d_1 + 2.2d_2 + 0.5d_1d_2$. A single observation consists of the tuple $(Y,D_{1:2},X_{1:2})$ where now $D_t \in \{0,1\}$. We implement our semiparametric estimators with 95% confidence intervals. Over 100 simulations, we calculate 100 estimates with confidence intervals. We report (i) the average estimate (ii), the standard error of estimates, and (iii) the percentage of confidence intervals containing the true value, i.e. the coverage. Across designs and sample sizes, our confidence intervals achieve nominal coverage. As desired, the confidence intervals shrink as sample size increases. To conserve space, we report the coverage tables in Appendix I.

### 5.2 Application: US Job Corps

We estimate the mediated and dynamic dose responses of the Job Corps, the largest job training program for disadvantaged youth in the US. Financed by the US Department of Labor, the Job Corps 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 \cite{Schochet2008} for details. Though access to the program was randomized, individuals could decide whether to participate and for how many hours over multiple years. We assume that, conditional on observed covariates, those
decisions were as good as random in the sense of Assumptions 1 and 8.

We initially consider arrests to be the outcome of interest. We consider employment to be a possible mechanism through which class hours affect arrests \cite{Flores2012, Huber2020}. The covariates $X \in \mathbb{R}^{40}$ are measured at baseline; the treatment $D \in \mathbb{R}$ is total hours spent in academic or vocational classes in the first year after randomization; the mediator $M \in \mathbb{R}$ is the proportion of weeks employed in the second year after randomization; and the outcome $Y \in \mathbb{R}$ is the number of times an individual is arrested by police in the fourth year after randomization. We use the same covariates $X \in \mathbb{R}^{40}$ and sample as \cite{Colangelo2020}, with $n = 2,913$. Covariates 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. $\theta^{TE}_0(d,d')$ is the total effect of class-hours $d'$ relative to class-hours $d$ on arrests; $\theta^{DE}_0(d,d')$ is the direct effect of class-hours $d'$ relative to class-hours $d$ on arrests; and $\theta^{IE}_0(d,d')$ is the indirect effect of class-hours $d'$ relative to class-hours $d$ on arrests, as mediated by the mechanism of employment. Figure 2 visualizes the direct and indirect dose response curves.

![Figure 2: Total, direct, and indirect dose responses of job training on arrests](image)

(a) Total response  
(b) Direct response  
(c) Indirect response

The total effect of training on arrests is negative. At best, the total effect of receiving 1,600 class-hours (40 weeks) versus 480 class-hours (12 weeks) is a reduction of 0.1 arrests. The direct effect of class-hours on arrests is negative, with the same magnitude as the total effect. The indirect effect of class-hours on arrests, as mediated through employment, is essentially zero. Our results extend the findings of \cite{Huber2020}, allowing both $(d, d')$ to vary. We conclude that the effect of class-hours on arrests is purely direct; class-hours decrease arrests, but not via the mechanism of increasing employment. From a
policy perspective, there are benefits of the training program that are not explained by employment alone. These benefits, however, require many class-hours. In Appendix J we provide implementation details and verify that our results are robust to the sample choice.

Next, we evaluate the dynamic dose response of job training on employment. $X_1 \in \mathbb{R}^{65}$ are covariates at baseline; $D_1 \in \mathbb{R}$ is total class-hours in the first year; $X_2 \in \mathbb{R}^{30}$ are covariates observed at the end of the first year; $D_2 \in \mathbb{R}$ is total class-hours in the second year; and $Y \in \mathbb{R}$ is proportion of weeks employed in the fourth year. We use similar covariates and sample as [Colangelo and Lee, 2020], with $n = 3, 141$. $\theta_0^{GF}(d_1, d_2)$ is the counterfactual mean employment given $d_1$ class-hours in year one and $d_2$ class-hours in year two. $\theta_0^{GF,\nabla}(d_1, d_2)$ is the increment of counterfactual mean employment given $d_1$ class-hours in year one and incrementally more than $d_2$ class-hours in year two. Figure 3 visualizes the multistage dose response curve and its derivative with respect to the second dose.

![Dynamic and Incremental Responses](image)

Figure 3: Dynamic and incremental responses of job training on employment

The effect of training on employment is positive when the duration of training is relatively brief. At best, the effect of receiving job training is 64% employment, compared to receiving no class-hours at all which gives 56% employment. The maximum effect is achieved by 480-1280 class-hours (12-32 weeks) in year one and 0-480 (0-12 weeks) in year two. There $X_1 \in \mathbb{R}^{65}$ yet $X_2 \in \mathbb{R}^{30}$ for two reasons. First, the follow up interview was less extensive than the baseline interview. Second, when a variable never varies over time, e.g. race, we include it in $X_1$ but not $X_2$ so as not to clash with the characteristic property in our RKHS approach.
Table 1: Semiparametric dynamic effect of job training on employment

| year 2 / year 1 | ≤ 1000 class-hours | > 1000 class-hours |
|-----------------|---------------------|---------------------|
| > 1000 class-hours | 41.5 (0.75) | 44.5 (0.70) |
| ≤ 1000 class-hours | 53.9 (1.00) | 56.6 (0.95) |

is another local maximum of counterfactual employment achieved by 1200 class-hours (30 weeks) in both years. Class-hours in year one and year two are complementary at low levels, as visualized by the incremental response. The large plateau in counterfactual employment suggests that a successful yet cost-effective policy would be 480 class-hours (12 weeks) in the first year and an optional, brief follow-up in the second year, confirming the policy recommendation from one-stage analysis [Singh et al., 2020]. In Appendix J we provide implementation details and verify that our results are robust to the sample choice.

Finally, we implement the semiparametric dynamic treatment effect estimator with confidence intervals. Though class-hours \((D_1, D_2)\) are observed as continuous variables, we discretize them into the bins of \(≤ 1000\) class-hours and \(> 1000\) class-hours to transform the nonparametric problem into a semiparametric one. We choose a coarse grid because the simulations show that our procedure requires a sufficiently large sample size for good performance. Table 1 summarizes results, arrayed to mirror the quadrants of Figure 3. The semiparametric results corroborate our nonparametric results: most of the gain in counterfactual employment is achieved with few class-hours in both years. We also confirm our finding that many class-hours in the second year are unproductive and possibly even counterproductive for employment. These differences are statistically significant.

In summary, we find that many class-hours in the first year have the direct effect of modestly decreasing arrests in the fourth year; 1,600 class-hours (40 weeks) cause a reduction of 0.1 arrests. Meanwhile, few class-hours in the first and second years significantly increase employment in the fourth year; 480 class-hours (12 weeks) in both years causes an 8% increase in employment. We conclude that the US Job Corps provides two distinct benefits—reducing arrests and increasing employment—under different durations of class-hours. We provide clean data for further research. Whereas data for mediation analysis were available from [Huber et al., 2020], we clean the data ourselves for the dynamic response application.
from raw files provided by Schochet et al., 2008. Section III.A. This data set may serve as a benchmark for dynamic response curve estimation.

6 Conclusion

We propose a family of estimators for nonparametric estimation of mediated and dynamic response curves as well as semiparametric estimation of mediated and dynamic treatment effects over short horizons. Our estimators are easily implemented and yet respect the nonlinearity, dependence, and effect modification allowed by identification theory. As a contribution to the multistage treatment effect literature, we propose simple estimators with closed form solutions for complex causal estimands. As a contribution to the kernel methods literature, we propose a sequential mean embedding that facilitates multistage causal inference over short horizons. A question for future research is how to apply the sequential mean embedding in dynamic programming for optimal dynamic policy estimation.

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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 Glossary of estimators and results

#### Table 2: New estimators and guarantees for mediation analysis

| Causal parameter              | Symbol | Guarantee             | Best rate | Section |
|-------------------------------|--------|-----------------------|-----------|---------|
| Total dose response           | TE     | uniform consistency   | $n^{-\frac{1}{4}}$ | 3       |
| Direct dose response          | DE     | uniform consistency   | $n^{-\frac{1}{4}}$ | 3       |
| Indirect dose response        | IE     | uniform consistency   | $n^{-\frac{1}{4}}$ | 3       |
| Total incremental response    | TE,$\nabla$ | uniform consistency  | $n^{-\frac{1}{4}}$ | 3       |
| Direct incremental response   | DE,$\nabla$ | uniform consistency  | $n^{-\frac{1}{4}}$ | 3       |
| Indirect incremental response | IE,$\nabla$ | uniform consistency  | $n^{-\frac{1}{4}}$ | 3       |
| Total effect                  | TE     | Gaussian approx.      | $n^{-\frac{1}{2}}$ | 3       |
| Direct effect                 | DE     | Gaussian approx.      | $n^{-\frac{1}{2}}$ | 3       |
| Indirect effect               | IE     | Gaussian approx.      | $n^{-\frac{1}{2}}$ | 3       |
| Total counterfactual dist.    | DTE    | convergence in dist.  | $n^{-\frac{1}{2}}$ | B       |
| Direct counterfactual dist.   | DDE    | convergence in dist.  | $n^{-\frac{1}{2}}$ | B       |
| Indirect counterfactual dist. | DIE    | convergence in dist.  | $n^{-\frac{1}{2}}$ | B       |
### Table 3: New estimators and guarantees for dynamic treatment effects over short horizons

| Causal parameter                      | Symbol | Guarantee         | Best rate | Section |
|---------------------------------------|--------|-------------------|-----------|---------|
| Dynamic dose response                 | GF     | uniform consistency | $n^{-\frac{1}{4}}$ | 4       |
| Dynamic dose response with dist. shift| DS     | uniform consistency | $n^{-\frac{1}{4}}$ | 4       |
| Dynamic incremental response          | GF,∇  | uniform consistency | $n^{-\frac{1}{4}}$ | 4       |
| Dynamic incremental response with dist. shift | DS,∇ | uniform consistency | $n^{-\frac{1}{4}}$ | 4       |
| Dynamic effect                        | GF     | Gaussian approx.  | $n^{-\frac{1}{2}}$ | 4       |
| Dynamic effect with dist. shift       | DS     | Gaussian approx.  | $n^{-\frac{1}{2}}$ | 4       |
| Dynamic counterfactual dist.          | DGF    | convergence in dist. | $n^{-\frac{1}{4}}$ | B       |
| Dynamic counterfactual dist. with dist. shift | DDS | convergence in dist. | $n^{-\frac{1}{4}}$ | B       |

### B Counterfactual distributions

#### B.1 Definition and identification

In the main text, we study target parameters defined as means or increments of potential outcomes. In fact, our framework for nonparametric estimation extends to target parameters defined as distributions of potential outcomes. In this section, we extend the algorithms and analyses presented in the main text to counterfactual distributions. 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 $\mathcal{Y}$ to be a Polish space (Assumption 3).

**Definition 3** (Counterfactual distributions and embeddings). For mediation analysis, we define

1. $\theta_0^{DME}(d, d') := \mathbb{P}[Y^{d',M(d)}]$ is the counterfactual distribution of outcomes in the thought experiment that treatment is set at a new value $D = d'$ but the mediator $M$ follows the distribution it would have followed if treatment were set at its old value $D = d$.

For dynamic treatment effects, we define
1. $\theta_0^{DGF}(d_{1:T}) := \mathbb{P}\{Y^{(d_{1:T})}\}$ is the counterfactual distribution of outcomes given interventions $D_{1:T} = d_{1:T}$ for the entire population;

2. $\theta_0^{DDS}(d_{1:T}; \bar{P}) := \tilde{\mathbb{P}}\{Y^{(d_{1:T})}\}$ is the counterfactual distribution of outcomes given interventions $D_{1:T} = d_{1:T}$ for an alternative population with data distribution $\bar{P}$ (elaborated in Assumption 9).

Likewise we define embeddings of the counterfactual distributions, e.g. $\tilde{\theta}_0^{DME}(d, d') := \mathbb{E}(\phi[Y^{(d', M(d')]}])$.

The general strategy will be 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. The same identification results apply to counterfactual distributions.

**Theorem 9** (Identification of counterfactual distributions and embeddings). If Assumption 1 holds then

1. $\{\theta_0^{DME}(d, d')\}(y) = \int \mathbb{P}(y|d', m, x)d\mathbb{P}(m|d, x)d\mathbb{P}(x)$.

If Assumption 8 holds then

1. $\{\theta_0^{DGF}(d_{1:T})\}(y) = \int \mathbb{P}(y|d_{1:T}, x_{1:T})d\mathbb{P}(x_{1:T})\prod_{t=2}^{T} d\mathbb{P}\{x_t|d_{1:t-1}, x_{1:t-1}\}$.

2. If in addition Assumption 9 holds then $\{\theta_0^{DDS}(d_{1:T}; \bar{P})\}(y) = \int \mathbb{P}(y|d_{1:T}, x_{1:T})d\bar{P}(x_{1:T})\prod_{t=2}^{T} d\bar{P}\{x_t|d_{1:t-1}, x_{1:t-1}\}$.

Likewise for embedding of counterfactual distributions. For example, if in addition Assumption 2 holds then $\tilde{\theta}_0^{DME}(d, d') = \int \mathbb{E}(\phi(Y)|D = d', M = m, X = x)d\mathbb{P}(m|d, x)d\mathbb{P}(x)$.

The identification results for embedding of counterfactual distributions resemble those presented in the main text. Define the generalized regressions $\gamma_0(d, m, x) := \mathbb{E}\{\phi(Y)|D = d, M = m, X = x\}$ and $\gamma_0(d_{1:T}, x_{1:T}) := \mathbb{E}\{\phi(Y)|D_{1:T} = d_{1:T}, X_{1:T} = x_{1:T}\}$. Then we can express these results in the familiar form, e.g. $\tilde{\theta}_0^{DME}(d, d') = \int \gamma_0(d', m, x)d\mathbb{P}(m|d, x)d\mathbb{P}(x)$. 

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B.2 Algorithm

To estimate counterfactual distributions, we extend the RKHS constructions in Section 3 and 4. 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. For mediation analysis, define the conditional expectation operator $E_8 : \mathcal{H}_Y \to \mathcal{H}_D \otimes \mathcal{H}_M \otimes \mathcal{H}_X$, $f(\cdot) \mapsto \mathbb{E}\{f(Y)|D = \cdot, M = \cdot, X = \cdot\}$. Importantly, by construction, $\gamma_0(d,m,x) = E_8^* \left[ \phi(d) \otimes \phi(m) \otimes \phi(x) \right]$. Likewise, for dynamic treatment effects, define the conditional expectation operator $E_9 : \mathcal{H}_Y \to \mathcal{H}_D \otimes \mathcal{H}_D \otimes \mathcal{H}_X \otimes \mathcal{H}_X$, $f(\cdot) \mapsto \mathbb{E}\{f(Y)|D_1 = \cdot, D_2 = \cdot, X_1 = \cdot, X_2 = \cdot\}$. We place regularity conditions on this RKHS construction in order to prove a generalized decoupling result.

**Theorem 10** (Decoupling of counterfactual distribution embeddings). Suppose the conditions of Theorem 1 hold. Further suppose Assumption 2 holds and $E_8 \in L^2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_M \otimes \mathcal{H}_X)$. Then

1. $\tilde{\theta}_0^{DME}(d,d') = E_8^* [\phi(d') \otimes \mu_{m,x}(d)]$.

Suppose the conditions of Theorem 5 hold. Further suppose Assumption 2 holds and $E_9 \in L^2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_D \otimes \mathcal{H}_X \otimes \mathcal{H}_X)$. Then

1. $\tilde{\theta}_0^{DGF}(d_1,d_2) = E_9^* [\phi(d_1) \otimes \phi(d_2) \otimes \mu_{x_1,x_2}(d_1)]$;

2. $\tilde{\theta}_0^{DDS}(d_1,d_2; \tilde{P}) = E_9^* [\phi(d_1) \otimes \phi(d_2) \otimes \nu_{x_1,x_2}(d_1)]$.

See Appendix E for the proof. The mean embeddings are the same as in the main text. They encode the reweighting distributions as elements in the RKHS such that the counterfactual distribution embeddings can be expressed as evaluations of $(E_8^*, E_9^*)$. As in the main text, these decoupled representations help to define estimators with closed form solutions that can be easily computed. For example, for $\tilde{\theta}_0^{DME}(d,d')$, our estimator will be

$$\hat{\theta}^{DGF}(d,d') = \hat{E}_9^* [\phi(d_1) \otimes \phi(d_2) \otimes \hat{\mu}_{x_1,x_2}(d_1)] = \hat{E}_9^* \left[ \phi(d_1) \otimes \phi(d_2) \otimes \frac{1}{n} \sum_{i=1}^{n} \{\phi(X_{1i}) \otimes \hat{\mu}_{X_2}(d_1, X_{1i})\} \right].$$

The estimators $\hat{E}_9$ and $\hat{\mu}_{x_2}(d_1, x_1)$ are generalized kernel ridge regressions.
Algorithm 5 (Nonparametric estimation of counterfactual distribution embeddings). Denote by $\odot$ the elementwise product. For mediation analysis denote the kernel matrices $K_{DD}, K_{MM}, K_{XX}, K_{YY} \in \mathbb{R}^{n \times n}$. Then

1. $\{\hat{\theta}^{DME}(d, d')\}(y) = \frac{1}{n} \sum_{i=1}^{n} K_{yY}(K_{DD} \odot K_{MM} \odot K_{XX} + n\lambda_8 I)^{-1}$
   \[K_{D'd'} \odot \{K_{MM}(K_{DD} \odot K_{XX} + n\lambda_1 I)^{-1}(K_{Dd} \odot K_{Xxi})\} \odot K_{Xxi}].

For dynamic treatment effects, denote the kernel matrices $K_{D_1D_1}, K_{D_2D_2}, K_{X_1X_1}, K_{X_2X_2} \in \mathbb{R}^{n \times n}$ calculated from observations drawn from $\mathbb{P}$. Denote the kernel matrices $K_{\tilde{D}_1\tilde{D}_1}, K_{\tilde{D}_2\tilde{D}_2}, K_{\tilde{X}_1\tilde{X}_1}, K_{\tilde{X}_2\tilde{X}_2} \in \mathbb{R}^{n \times \tilde{n}}$ calculated from observations drawn from $\tilde{\mathbb{P}}$. Then

1. $\{\hat{\theta}^{DGF}(d_1, d_2)\}(y) = \frac{1}{n} \sum_{i=1}^{n} K_{yY}(K_{D_1D_1} \odot K_{D_2D_2} \odot K_{X_1X_1} \odot K_{X_2X_2} + n\lambda_9 I)^{-1}$
   \[K_{D_1d_1} \odot K_{D_2d_2} \odot K_{X_1x_1} \odot \{K_{X_2X_2}(K_{D_1D_1} \odot K_{X_1X_1} + n\lambda_4 I)^{-1}(K_{D_1d_1} \odot K_{X_1x_1})\}];

2. $\{\hat{\theta}^{DDS}(d_2, d_2; \tilde{\mathbb{P}})\}(y) = \frac{1}{\tilde{n}} \sum_{i=1}^{\tilde{n}} K_{yY}(K_{D_1D_1} \odot K_{D_2D_2} \odot K_{X_1X_1} \odot K_{X_2X_2} + n\lambda_9 I)^{-1}$
   \[K_{D_1d_1} \odot K_{D_2d_2} \odot K_{X_1\tilde{x}_1} \odot \{K_{X_2\tilde{x}_2}(K_{D_1D_1} \odot K_{X_1\tilde{x}_1} + \tilde{n}\lambda_5 I)^{-1}(K_{D_1d_1} \odot K_{X_1\tilde{x}_1})\}],

where $(\lambda_1, \lambda_4, \lambda_5, \lambda_8, \lambda_9)$ are ridge regression penalty hyperparameters.

We derive these algorithms in Appendix E. We give theoretical values for $(\lambda_1, \lambda_4, \lambda_5, \lambda_8, \lambda_9)$ that balance bias and variance in Theorem 41 below. Appendix H gives practical tuning procedures to empirically balance bias and variance. Note that $\hat{\theta}^{DDS}$ requires observations of treatments and covariates from the alternative population $\tilde{\mathbb{P}}$.

Importantly, Algorithm 5 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. The procedure is a variant of kernel herding [Welling, 2009; Muandet et al., 2021].

Algorithm 6 (Nonparametric estimation of counterfactual distributions). Recall that $\hat{\theta}^{DME}(d, d')$ is a mapping from $\mathcal{Y}$ to $\mathbb{R}$. Given $\hat{\theta}^{DME}(d, d')$, calculate

1. $\tilde{Y}_1 = \text{argmax}_{y \in \mathcal{Y}} \{\hat{\theta}^{DME}(d, d')(y)\},$

2. $\tilde{Y}_j = \text{argmax}_{y \in \mathcal{Y}} \{\hat{\theta}^{DME}(d, d')(y) - \frac{1}{j+1} \sum_{\ell=1}^{j-1} k_{\mathcal{Y}}(\tilde{Y}_\ell, y)\}$ for $j > 1$.

Likewise for the other counterfactual distributions, replacing $\hat{\theta}^{DME}(d, d')$ with the other quantities in Algorithm 5.
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 using samples \((\tilde{Y}_j)\).

### B.3 Guarantee

Towards a guarantee of uniform consistency, we place regularity conditions on the original spaces as in Assumption 3. Importantly, we relax the condition that \(Y \in \mathbb{R}\) and that it is bounded; instead, we assume \(Y \in \mathcal{Y}\), which is a Polish space. We place assumptions on the smoothness of the generalized regression \(\gamma_0\) and the effective dimension of its RKHS, expressed in terms of the conditional expectation operators \((E_8, E_9)\). Likewise, we place assumptions on the smoothness of the conditional mean embeddings and the effective dimensions of their RKHSs. With these assumptions, we arrive at our next main result.

**Theorem 11** (Nonparametric consistency of counterfactual distribution embeddings). Set \((\lambda_1, \lambda_4, \lambda_5, \lambda_8, \lambda_9) = (n^{-\frac{1}{c_1+1/c_1}}, n^{-\frac{1}{c_4+1/c_4}}, \tilde{n}^{-\frac{1}{c_5+1/c_5}}, n^{-\frac{1}{c_8+1/c_8}}, n^{-\frac{1}{c_9+1/c_9}})\), which is rate optimal regularization. For mediation analysis, suppose the conditions of Theorem 3 hold as well as Assumption 5 with \(A_8 = Y\) and \(B_8 = D \times M \times \mathcal{X}\). Then

\[
\sup_{d, d' \in D} \| \hat{\theta}^{DME}(d, d') - \hat{\theta}_0^{DME}(d, d') \|_{\mathcal{H}_Y} = O_p \left( n^{-\frac{1}{2(c_8+1/c_8)} + n^{-\frac{1}{2(c_1+1/c_1)}}} \right).
\]

For dynamic treatment effects, suppose the conditions of Theorem 7 hold as well as Assumption 5 with \(A_9 = Y\) and \(B_9 = D \times D \times \mathcal{X} \times \mathcal{X}\).

1. Then

\[
\sup_{d_1, d_2 \in D} \| \hat{\theta}^{DGF}(d_1, d_2) - \hat{\theta}_0^{DGF}(d_1, d_2) \|_{\mathcal{H}_Y} = O_p \left( n^{-\frac{1}{2(c_9+1/c_9)} + n^{-\frac{1}{2(c_4+1/c_4)}}} \right).
\]

2. If in addition Assumption 9 holds, then

\[
\sup_{d_1, d_2 \in D} \| \hat{\theta}^{DDS}(d_1, d_2; \tilde{P}) - \hat{\theta}_0^{DDS}(d_1, d_2; \tilde{P}) \|_{\mathcal{H}_Y} = O_p \left( n^{-\frac{1}{2(c_9+1/c_9)} + \tilde{n}^{-\frac{1}{2(c_5+1/c_5)}}} \right).
\]

Exact finite sample rates are given in Appendix F as well as the explicit specializations of Assumption 5. Again, these rates are at best \(n^{-\frac{1}{4}}\) when \((c_1, c_4, c_5, c_8, c_9) = 2\) and
(b_1, b_4, b_5, b_8, b_9) \to \infty. Finally, we state an additional regularity condition under which we can prove that the samples (\bar{Y}_j) calculated from the distribution embeddings weakly converge to the desired distribution.

**Assumption 12 (Additional regularity).** Assume

1. \( \mathcal{Y} \) is locally compact;
2. \( \mathcal{H}_\mathcal{Y} \subset \mathcal{C} \), where \( \mathcal{C} \) 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 imposes weak restrictions. In particular, if \( \mathcal{Y} \) is a Banach space, then to satisfy both conditions it must be finite dimensional. Trivially, \( \mathcal{Y} = \mathbb{R}^{\dim(\mathcal{Y})} \) satisfies both conditions. We arrive at our final result of this section.

**Corollary 1** (Convergence in distribution of counterfactual distributions; Theorem 5 of [Singh et al., 2020]). Suppose the conditions of Theorem 11 hold, as well as Assumption 12. Suppose samples (\bar{Y}_j) are calculated for \( \theta^{DME}_0(d, d') \) as described in Algorithm 6. Then (\bar{Y}_j) \overset{d}{\to} \theta^{DME}_0(d, d'). Likewise for the other counterfactual distributions, replacing \( \hat{\theta}^{DME}(d, d') \) with the other quantities in Algorithm 5.

Note that samples are drawn for given values \((d, d')\) or \((d_1, d_2)\). Though our nonparametric consistency result is uniform across treatment values, this weak convergence result is for fixed treatment values.

### C Dynamic dose response with longer horizons

In the main text, we focus on dynamic dose response curve with \( T = 2 \) time periods. In this appendix, we generalize our approach to \( T > 2 \) time periods. In doing so, we also clarify the role of auxiliary Markov assumptions that are common in the literature. In particular, we focus on the dynamic dose response \( \theta^{GF}_0(d_1:T) \) with and without Markov assumptions.
C.1 A generalized decoupling

Previously, Theorem 6 gave the RKHS representation for $T = 2$. In particular, if $\gamma_0 \in \mathcal{H} = \mathcal{H}_D \otimes \mathcal{H}_D \otimes \mathcal{H}_X \otimes \mathcal{H}_X$ and both Assumptions 2 and 8 hold then
\[
\theta_0^{GF}(d_1, d_2) = \langle \gamma_0, \phi(d_1) \otimes \phi(d_2) \otimes \int \{ \phi(x_1) \otimes \mu_{x_1}(d_1, x_1) \} dP(x_1) \rangle_{\mathcal{H}}
\]
\[
\mu_{x_2}(d_1, x_1) = \int \phi(x_2) dP(x_2 \mid d_1, x_1).
\]

Towards a more general result, define the notation $\mathcal{H}_T = \{ \otimes_{t=1}^T(\mathcal{H}_D) \} \otimes \{ \otimes_{t=1}^T(\mathcal{H}_X) \}$ where $\otimes_{t=1}^T(\mathcal{H}_D)$ means the $T$-times tensor product of $\mathcal{H}_D$. Also define the condensed notation $\phi(d_{1:T}) = \phi(d_1) \otimes \ldots \otimes \phi(d_T)$, so that the feature map of $\mathcal{H}_T$ is $\phi(d_{1:T}) \otimes \phi(x_{1:T})$.

Theorem 12 (Decoupling of dynamic dose response: $T > 2$). Suppose the conditions of Theorem 5 hold. Further suppose Assumption 2 holds and $\gamma_0 \in \mathcal{H}_T$. Then
\[
\theta_0^{GF}(d_{1:T}) = \langle \gamma_0, \phi(d_{1:T}) \otimes \mu_{1:T}\{d_{1:(T-1)}\} \rangle_{\mathcal{H}_T}
\]
\[
\mu_{1:T}\{d_{1:(T-1)}\} = \int \phi(x_{1:T}) dP(x_1) \prod_{t=2}^T dP(x_t \mid d_{1:(t-1)}, x_{1:(t-1)}).
\]

See Appendix 3 for the proof. $\mu_{1:T}\{d_{1:(T-1)}\}$ is the sequential mean embedding in $T$ time periods, generalizing $\mu_{1:2}(d_1) = \int \{ \phi(x_1) \otimes \mu_{x_2}(d_1, x_1) \} dP(x_1)$. What remains is an account of the structure of $\mu_{1:T}\{d_{1:(T-1)}\}$, which then implies an estimation procedure for $\hat{\mu}_{1:T}\{d_{1:(T-1)}\}$ and hence $\hat{\theta}^{GF}(d_{1:T}) = \langle \gamma_0, \phi(d_{1:T}) \otimes \hat{\mu}_{1:T}\{d_{1:(T-1)}\} \rangle_{\mathcal{H}_T}$, naturally generalizing Algorithm 3.

C.2 A generalized sequential mean embedding

Towards this end, we provide a recursive representation of the sequential mean embedding $\mu_{1:T}\{d_{1:(T-1)}\}$ that suggests a recursive estimator $\hat{\mu}_{1:T}\{d_{1:(T-1)}\}$. Write
\[
\mu_{1:T}\{d_{1:(T-1)}\}
\]
\[
= \int \{ \phi(x_1) \otimes \ldots \otimes \phi(x_{T-1}) \otimes \phi(x_T) \} dP(x_1) \prod_{t=2}^T dP(x_t \mid d_{1:(t-1)}, x_{1:(t-1)})
\]
\[
= \int [\phi(x_1) \otimes \ldots \otimes \phi(x_{T-1}) \otimes \mu_T\{d_{1:(T-1)}, x_{1:(T-1)}\}] dP(x_1) \prod_{t=2}^{T-1} dP(x_t \mid d_{1:(t-1)}, x_{1:(t-1)})
\]
\[
= \int [\phi(x_1) \otimes \ldots \otimes \mu_{(T-1):T}\{d_{1:(T-2)}, x_{1:(T-2)}\}] dP(x_1) \prod_{t=2}^{T-2} dP(x_t \mid d_{1:(t-1)}, x_{1:(t-1)}),
\]
\[ \mu_T \{ \mathbf{d}_{1:(T-1)}, \mathbf{x}_{1:(T-1)} \} = \int \phi(x_T) d\mathbb{P}\{x_T|\mathbf{d}_{1:(T-1)}, \mathbf{x}_{1:(T-1)}\}, \]
\[ \mu_{(T-1):T} \{ \mathbf{d}_{1:(T-1)}, \mathbf{x}_{1:(T-2)} \} = \int [\phi(x_{T-1}) \otimes \mu_T \{ \mathbf{d}_{1:(T-1)}, \mathbf{x}_{1:(T-1)} \}] d\mathbb{P}\{x_{T-1}|\mathbf{d}_{1:(T-2)}, \mathbf{x}_{1:(T-2)}\}. \]

Note that \( \mu_T \{ \mathbf{d}_{1:(T-1)}, \mathbf{x}_{1:(T-1)} \} \) is a conditional mean embedding as before, obtained by projecting \( \phi(x_T) \) onto \( \phi \{ \mathbf{d}_{1:(T-1)} \} \otimes \phi \{ \mathbf{x}_{1:(T-1)} \} \). Meanwhile, \( \mu_{(T-1):T} \{ \mathbf{d}_{1:(T-1)}, \mathbf{x}_{1:(T-2)} \} \) is a sequential mean embedding obtained by projecting \( [\phi(x_{T-1}) \otimes \mu_T \{ \mathbf{d}_{1:(T-1)}, \mathbf{x}_{1:(T-1)} \}] \) onto \( \phi \{ \mathbf{d}_{1:(T-2)} \} \otimes \phi \{ \mathbf{x}_{1:(T-2)} \} \).

One can continue recursively defining \( \mu_{t:T} \{ \mathbf{d}_{1:(T-1)}, \mathbf{x}_{1:(t-1)} \} \) all the way up to \( \mu_{1:T} \{ \mathbf{d}_{1:(T-1)} \} \). This recursive construction implies a recursive estimation procedure in which \( \hat{\mu}_{t:T} \{ \mathbf{d}_{1:(T-1)}, \mathbf{x}_{1:(t-1)} \} \) is estimated all the way up to \( \hat{\mu}_{1:T} \{ \mathbf{d}_{1:(T-1)} \} \). Altogether, estimating the sequential mean embedding in this way requires \( T - 1 \) kernel ridge regressions.

### C.3 Simplification via Markov assumptions

Next, we consider the setting where \( T > 2 \) and auxiliary Markov assumptions holds. We focus on the assumption that covariates \( X_t \) have the Markov property.

**Assumption 13 (Markov property).** Suppose \( \mathbb{P}\{x_t|\mathbf{d}_{1:(t-1)}, \mathbf{x}_{1:(t-1)}\} = \mathbb{P}(x_t|d_{t-1}, x_{t-1}) \) for \( t \in \{2, \ldots, T\} \).

In words, the distribution of \( X_t \) only depends on the immediate history \( (D_{t-1}, X_{t-1}) \); previous treatments and covariates are conditionally independent. Assumption 13 simplifies the representation of \( \theta_0^{GF} \).

**Theorem 13 (Decoupling of dynamic dose response: Markov).** Suppose the conditions of Theorem 5 hold. Further suppose Assumptions 2 and 13 hold, and \( \gamma_0 \in \mathcal{H}_T \). Then

\[ \theta_0^{GF} (\mathbf{d}_{1:T}) = \langle \gamma_0, \phi(\mathbf{d}_{1:T}) \otimes \mu_{1:T} \{ \mathbf{d}_{1:(T-1)} \} \rangle_{\mathcal{H}_T} \]
\[ \mu_{1:T} \{ \mathbf{d}_{1:(T-1)} \} = \int \phi(\mathbf{x}_{1:T}) d\mathbb{P}(x_1) \prod_{t=2}^{T} d\mathbb{P}(x_t|d_{t-1}, x_{t-1}). \]

See Appendix E for the proof. \( \mu_{1:T} \{ \mathbf{d}_{1:(T-1)} \} \) is the sequential mean embedding in \( T \) time periods, with limited dependence across time periods. Finally, we revisit the structure
of $\mu_{1:T}\{d_{1:(T-1)}\}$. Write
\[
\mu_{1:T}\{d_{1:(T-1)}\} = \int \{\phi(x_1) \otimes \cdots \otimes \phi(x_{T-1}) \otimes \phi(x_T)\} dP(x_1) \prod_{t=2}^{T} dP(x_t | d_{t-1}, x_{t-1})
\]
\[
= \int \{\phi(x_1) \otimes \cdots \otimes \phi(x_{T-1}) \otimes \mu_T(d_{T-1}, x_{T-1})\} dP(x_1) \prod_{t=2}^{T-1} dP(x_t | d_{t-1}, x_{t-1})
\]
\[
= \int [\phi(x_1) \otimes \cdots \otimes \mu_{(T-1):T}\{d_{(T-2):(T-1)}, x_{T-2}\}] dP(x_1) \prod_{t=2}^{T-2} dP(x_t | d_{t-1}, x_{t-1}),
\]
where
\[
\mu_T(d_{T-1}, x_{T-1}) = \int \phi(x_T) dP(x_T | d_{T-1}, x_{T-1}),
\]
\[
\mu_{(T-1):T}\{d_{(T-2):(T-1)}, x_{T-2}\} = \int \{\phi(x_{T-1}) \otimes \mu_T(d_{T-1}, x_{T-1})\} dP(x_{T-1} | d_{T-2}, x_{T-2}).
\]

Note that $\mu_T(d_{T-1}, x_{T-1})$ is a conditional mean embedding as before, obtained by projecting $\phi(x_T)$ onto $\phi(d_{T-1}) \otimes \phi(x_{T-1})$. Meanwhile, $\mu_{(T-1):T}\{d_{(T-2):(T-1)}, x_{T-2}\}$ is a sequential mean embedding obtained by projecting $[\phi(x_{T-1}) \otimes \mu_T(d_{T-1}, x_{T-1})]$ onto $\phi(d_{T-2}) \otimes \phi(x_{T-2})$.

One can continue recursively defining $\mu_{t:T}\{d_{(t-1):(T-1)}, x_{t-1}\}$ all the way up to $\mu_{1:T}\{d_{1:(T-1)}\}$. This recursive construction implies a recursive estimation procedure as before. Altogether, estimating the sequential mean embedding in this way requires $T-1$ kernel ridge regressions. Compared to the setting without Markov assumptions, each kernel ridge regression involves fewer regressors.

### D Identification

In this appendix, we prove identification of incremental response curves and effects.

#### D.1 Mediation analysis

**Proof of Theorem** The result for $\theta_0^{ME}$ is immediate from [Imai et al., 2010]. We generalize the argument to $\theta_0^{ME, \gamma}$. For the proof, we adopt nonseparable model notation $Y(d',m) = Y(d', m, \eta)$ and $M(d) = M(d, \eta)$, where $\eta$ is unobserved heterogeneity. Our innovation is to restructure the argument so that taking the derivative with respect to $d'$ does not lead to additional factors (as it otherwise would by chain rule). We proceed in steps.
1. Regression.

By definition
\[ \gamma_0(d', m, x) = \mathbb{E}(Y|D = d', M = m, X = x) = \int Y(d', m, \eta) d\mathbb{P}(\eta|d', m, x). \]

By the assumed conditional independences, \( \mathbb{P}(\eta|d', m, x) = \mathbb{P}(\eta|d', x) = \mathbb{P}(\eta|x) \). In summary,
\[ \gamma_0(d', m, x) = \int Y(d', m, \eta) d\mathbb{P}(\eta|x), \quad \nabla_{d'} \gamma_0(d', m, x) = \int \nabla_{d'} Y(d', m, \eta) d\mathbb{P}(\eta|x). \]

2. Target expression.

Beginning with the desired expression,
\[ RHS = \int \nabla_{d'} \gamma_0(d', m, x) d\mathbb{P}(m|d, x) d\mathbb{P}(x) \]
\[ = \int \nabla_{d'} Y(d', m, \eta) d\mathbb{P}(\eta|x) d\mathbb{P}(m|d, x) d\mathbb{P}(x). \]

Note that \( \mathbb{P}(m|d, x) = \mathbb{P}\{M(d, \eta)|d, x\} = \mathbb{P}\{M(d, \eta)|x\} \). Since \( \{M(d), Y^{(d,m)}\} \perp D|X \) implies \( (Y^{d,m}) \perp D|\{M(d)\}, X \)
\[ \mathbb{P}(\eta|x) = \mathbb{P}(\eta|d, x) = \mathbb{P}\{\eta|d, M(d, \eta), x\} = \mathbb{P}\{\eta|M(d, \eta), x\}. \]

In summary,
\[ RHS = \int \nabla_{d'} Y\{d', M(d, \eta), \eta\} d\mathbb{P}\{\eta|M(d, \eta), x\} d\mathbb{P}\{M(d, \eta)|x\} d\mathbb{P}(x). \]

Conveniently
\[ \int \mathbb{P}\{\eta|M(d, \eta), x\} d\mathbb{P}\{M(d, \eta)|x\} = \int \mathbb{P}\{\eta, M(d, \eta)|x\} d\{M(d, \eta)\} = \mathbb{P}(\eta|x) \]
\[ \mathbb{P}(\eta|x) \mathbb{P}(x) = \mathbb{P}(\eta, x). \]

Therefore
\[ RHS = \int \nabla_{d'} Y\{d', M(d, \eta), \eta\} d\mathbb{P}(\eta, x) = \int \nabla_{d'} Y\{d', M(d, \eta), \eta\} d\mathbb{P}(\eta) = LHS. \]

\[ \square \]
D.2 Dynamic response curves and effects

Proof of Theorem 5. The result for $\theta_0^{GF}$ is immediate from [Robins, 1986]. We generalize the argument to $\theta_0^{GF,\nabla}$. For clarity, we focus on the case with $T = 2$ and we adopt nonseparable model notation $Y^{(d_1,d_2)} = Y(d_1, d_2, \eta)$, where $\eta$ is unobserved heterogeneity. As before, our innovation is to restructure the argument so that taking the derivative with respect to $d_2$ does not lead to additional factors (as it otherwise would by chain rule). The argument for $\theta_0^{DS}$ is identical. We proceed in steps.

1. Regression.

By definition

$$\gamma_0(d_1, d_2, x_1, x_2) = \mathbb{E}(Y|D_1 = d_1, D_2 = d_2, X_1 = x_1, X_2 = x_2) = \int Y(d_1, d_2, \eta)d\mathbb{P}(\eta|d_1, d_2, x_1, x_2).$$

By the assumed conditional independences, $\mathbb{P}(\eta|d_1, d_2, x_1, x_2) = \mathbb{P}(\eta|d_1, x_1, x_2)$. In summary

$$\gamma_0(d_1, d_2, x_1, x_2) = \int Y(d_1, d_2, \eta)d\mathbb{P}(\eta|d_1, x_1, x_2)$$

$$\nabla_{d_2}\gamma_0(d_1, d_2, x_1, x_2) = \int \nabla_{d_2}Y(d_1, d_2, \eta)d\mathbb{P}(\eta|d_1, x_1, x_2).$$

2. Target expression.

Beginning with the desired expression,

$$RHS = \int \nabla_{d_2}\gamma_0(d_1, d_2, x_1, x_2)d\mathbb{P}(x_1)d\mathbb{P}(x_2|d_1, x_1)$$

$$= \int \nabla_{d_2}Y(d_1, d_2, \eta)d\mathbb{P}(\eta|d_1, x_1, x_2)d\mathbb{P}(x_1)d\mathbb{P}(x_2|d_1, x_1).$$

Conveniently

$$\int \mathbb{P}(\eta|d_1, x_1, x_2)d\mathbb{P}(x_2|d_1, x_1) = \int \mathbb{P}(x_2, \eta|d_1, x_1)dx_2 = \mathbb{P}(\eta|x_1)$$

$$\mathbb{P}(\eta|x_1)\mathbb{P}(x_1) = \mathbb{P}(\eta, x_1).$$

Therefore

$$RHS = \int \nabla_{d_2}Y(d_1, d_2, \eta)d\mathbb{P}(\eta, x_1) = \int \nabla_{d_2}Y(d_1, d_2, \eta)d\mathbb{P}(\eta) = LHS.$$
E  Algorithm derivation

In this appendix, we derive the closed form solutions for (i) mediation analysis, (ii) dynamic dose responses and treatment effects, and (iii) counterfactual distributions. We also provide alternative closed form expressions that run faster in statistical software.

E.1 Mediation analysis

Proof of Theorem 2. In Assumption 2, we impose that the scalar kernels are bounded. This assumption has several implications. First, the feature maps are Bochner integrable [Steinwart and Christmann, 2008, Definition A.5.20]. 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. Therefore

\[
\theta_0^{ME}(d, d') = \int \gamma_0(d', m, x)d\mathbb{P}(m|d, x)d\mathbb{P}(x)
\]

By [Steinwart and Christmann, 2008, Lemma 4.34], the derivative feature map \( \nabla_d \phi(d) \) exists, is continuous, and is Bochner integrable since \( \kappa'_d < \infty \). Therefore the derivation remains valid for incremental responses.

Derivation of Algorithm 1. By standard arguments [Kimeldorf and Wahba, 1971], write the conditional mean

\[
\hat{\gamma}(d, m, x) = \langle \gamma, \phi(d) \otimes \phi(m) \otimes \phi(x) \rangle_H
\]

\[
= \int \langle \gamma_0, \phi(d) \otimes \phi(m) \otimes \phi(x) \rangle_H d\mathbb{P}(m|d, x)d\mathbb{P}(x)
\]

\[
= \int \langle \gamma_0, \phi(d') \otimes \int \phi(m)d\mathbb{P}(m|d, x) \otimes \phi(x) \rangle_H d\mathbb{P}(x)
\]

\[
= \int \langle \gamma_0, \phi(d') \otimes \mu_m(d, x) \otimes \phi(x) \rangle_H d\mathbb{P}(x)
\]

\[
= \langle \gamma_0, \phi(d') \otimes \int \{ \mu_m(d, x) \otimes \phi(x) \} d\mathbb{P}(x) \rangle_H.
\]

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

\[
\hat{\mu}_m(d, x) = K_M(K_{DD} \otimes K_{MM} \otimes K_{XX} + n\lambda I)^{-1}(K_{Dd} \otimes K_Mm \otimes K_{Xx}).
\]
Therefore
\[ \frac{1}{n} \sum_{i=1}^{n} [\hat{\mu}_m(d, X_i) \otimes \phi(X_i)] = \frac{1}{n} \sum_{i=1}^{n} [(K_M(K_{DD} \otimes K_{XX} + n\lambda_1 I)^{-1}(K_{Dd} \otimes K_{Xx_i})) \otimes \phi(X_i)], \]
and
\[ \hat{\theta}^{ME}(d, d') = \langle \hat{\gamma}, \phi(d') \rangle \otimes \frac{1}{n} \sum_{i=1}^{n} [\hat{\mu}_m(d, X_i) \otimes \phi(X_i)] \rangle_H \]
\[ = \frac{1}{n} \sum_{i=1}^{n} Y^\top (K_{DD} \otimes K_{MM} \otimes K_{XX} + n\lambda I)^{-1} \]
\[ [K_{Dd} \otimes \{K_{MM}(K_{DD} \otimes K_{XX} + n\lambda I)^{-1}(K_{Dd} \otimes K_{Xx_i})\} \otimes K_{Xx_i}]. \]

For incremental responses, simply replace \( \hat{\gamma}(d, m, x) \) with
\[ \nabla_d \hat{\gamma}(d, m, x) = \langle \hat{\gamma}, \nabla_d \phi(d) \otimes \phi(m) \otimes \phi(x) \rangle_H \]
\[ = Y^\top (K_{DD} \otimes K_{MM} \otimes K_{XX} + n\lambda I)^{-1}(\nabla_d K_{Dd} \otimes K_{Mm} \otimes K_{Xx}). \]

\[ \square \]

**Algorithm 7** (Details for Algorithm 2). For simplicity, we abstract from sample splitting. Denote the kernel matrices \( K_{DD}, K_{MM}, K_{XX} \in \mathbb{R}^{n \times n} \).

1. \( \hat{\gamma}(d, m, x) = Y^\top (K_{DD} \otimes K_{MM} \otimes K_{XX} + n\lambda I)^{-1}(K_{Dd} \otimes K_{Mm} \otimes K_{Xx}), \)
2. \( \hat{\pi}(x) = D^\top (K_{XX} + n\lambda_2 I)^{-1}K_{Xx}, \)
3. \( \hat{\rho}(m, x) = D^\top (K_{MM} \otimes K_{XX} + n\lambda_3 I)^{-1}(K_{Mm} \otimes K_{Xx}). \)

**E.2 Dynamic dose response curves**

*Proof of Theorem 4.* Assumption 2 implies Bochner integrability, which permits us to interchange expectation and inner product. Therefore
\[ \theta_0^{GF}(d_1, d_2) = \int \gamma_0(d_1, d_2, x_1, x_2) d\mathbb{P}(x_2|d_1, x_1) d\mathbb{P}(x_1) \]
\[ = \int \langle \gamma_0, \phi(d_1) \otimes \phi(d_2) \otimes \phi(x_1) \otimes \phi(x_2) \rangle_H d\mathbb{P}(x_2|d_1, x_1) d\mathbb{P}(x_1) \]
\[ = \int \langle \gamma_0, \phi(d_1) \otimes \phi(d_2) \otimes \phi(x_1) \otimes \int \phi(x_2) d\mathbb{P}(x_2|d_1, x_1) \rangle_H d\mathbb{P}(x_1) \]
\[ = \int \langle \gamma_0, \phi(d_1) \otimes \phi(d_2) \otimes \phi(x_1) \otimes \mu_{x_2}(d_1, x_1) \rangle_H d\mathbb{P}(x_1) \]
\[ = \langle \gamma_0, \phi(d_1) \otimes \phi(d_2) \otimes \int \{\phi(x_1) \otimes \mu_{x_2}(d_1, x_1)\} d\mathbb{P}(x_1) \rangle_H. \]
The argument for $\theta_0^{DS}$ is identical.  

Proof of Theorem 12. Assumption 2 implies Bochner integrability, which permits us to interchange expectation and inner product. Therefore

$$\theta_0^{GF}(d_{1:T}) = \int \gamma_0(d_{1:T}, x_{1:T}) d\mathbb{P}(x_1) \prod_{t=2}^{T} d\mathbb{P}\{x_t|d_{1:(t-1)}, x_{1:(t-1)}\}$$

$$= \int \langle \gamma_0, \phi(d_{1:T}) \otimes \phi(x_{1:T}) \rangle_{\mathcal{H}} d\mathbb{P}(x_1) \prod_{t=2}^{T} d\mathbb{P}\{x_t|d_{1:(t-1)}, x_{1:(t-1)}\}$$

$$= \langle \gamma_0, \phi(d_{1:T}) \otimes \mathbb{E}_{t=1}^{T}\{d_{1:(T-1)}\} \rangle_{\mathcal{H}}.$$

Proof of Theorem 13. Immediate from Theorem 12 and Assumption 13.

Derivation of Algorithm 3. By standard arguments [Kimeldorf and Wahba, 1971]

$$\hat{\gamma}(d_1, d_2, x_1, x_2) = \langle \hat{\gamma}, \phi(d_1) \otimes \phi(d_2) \otimes \phi(x_1) \otimes \phi(x_2) \rangle_{\mathcal{H}}$$

$$= \langle \hat{\gamma}, \phi(d_1) \otimes \phi(d_2) \otimes \phi(x_1) \otimes \phi(x_2) \rangle_{\mathcal{H}}$$

$$= \mathbf{Y}^\top (K_{D_1D_1} \odot K_{D_2D_2} \odot K_{X_1X_1} \odot K_{X_2X_2} + n\lambda I)^{-1}(K_{D_1d_1} \odot K_{D_2d_2} \odot K_{X_1x_1} \odot K_{X_2x_2}).$$

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

$$\hat{\mu}_{x_2}(d_1, x_1) = K_{X_2}(K_{D_1D_1} \odot K_{X_1X_1} + n\lambda I)^{-1}(K_{D_1d_1} \odot K_{X_1x_1}).$$

Therefore

$$\frac{1}{n} \sum_{i=1}^{n} [\phi(X_{1i}) \otimes \hat{\mu}_{x_2}(d_1, X_{1i})]$$

$$= \frac{1}{n} \sum_{i=1}^{n} [\phi(X_{1i}) \otimes \{K_{X_2}(K_{D_1D_1} \odot K_{X_1X_1} + n\lambda I)^{-1}(K_{D_1d_1} \odot K_{X_1x_1})\}]$$

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and

\[
\hat{\theta}^{GF}(d_1, d_2) = \langle \hat{\gamma}, \phi(d_1) \otimes \phi(d_2) \otimes \frac{1}{n} \sum_{i=1}^{n} [\phi(X_{1i}) \otimes \hat{\mu}_{x_2}(d_1, X_{1i})] \rangle_H
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} Y^T(K_{D_1D_1} \circ K_{D_2D_2} \circ K_{X_1X_1} \circ K_{X_2X_2} + n\lambda I)^{-1}
\]

\[
[K_{D_1d_1} \circ K_{D_2d_2} \circ K_{X_1x_1i} \circ \{K_{X_2X_2}(K_{D_1D_1} \circ K_{X_1X_1} + n\lambda_i I)^{-1}(K_{D_1d_1} \circ K_{X_1x_1i})\}].
\]

The argument for \(\theta_0^{DS}\) is identical.

**Algorithm 8** (Details for Algorithm 4). For simplicity, we abstract from sample splitting. Denote the kernel matrices \(K_{D_1D_1}, K_{D_2D_2}, K_{X_1X_1}, K_{X_2X_2} \in \mathbb{R}^{n \times n}\) calculated from observations drawn from population \(P\).

1. \(\hat{\gamma}(d_1, d_2, x_1, x_2) = Y^T(K_{D_1D_1} \circ K_{D_2D_2} \circ K_{X_1X_1} \circ K_{X_2X_2} + n\lambda I)^{-1}(K_{D_1d_1} \circ K_{D_2d_2} \circ K_{X_1x_1} \circ K_{X_2x_2}),\)

2. \(\hat{\pi}(x_1) = D_1^T(K_{X_1X_1} + n\lambda_6 I)^{-1}K_{X_1x_1},\)

3. \(\hat{\rho}(d_1, x_1, x_2) = D_2^T(K_{D_1D_1} \circ K_{X_1X_1} \circ K_{X_2X_2} + n\lambda_7 I)^{-1}(K_{D_1d_1} \circ K_{X_1x_1} \circ K_{X_2x_2}).\)

**E.3 Counterfactual distributions**

**Proof of Theorem 10.** The argument is analogous to Theorems 2 and 6, recognizing that in the distributional setting

\[
\gamma_0(d, m, x) = E_0^*\{\phi(d) \otimes \phi(m) \otimes \phi(x)\},
\]

\[
\gamma_0(d_1, d_2, x_1, x_2) = E_0^*\{\phi(d_1) \otimes \phi(d_2) \otimes \phi(x_1) \otimes \phi(x_2)\}.
\]

**Derivation of Algorithm 5.** The argument is analogous to Algorithms 1 and 3 appealing to
Algorithm 1], which gives
\[ \hat{\gamma}(d, m, x) = \hat{E}^*_8[\phi(d) \otimes \phi(m) \otimes \phi(x)] \]
\[ = K_Y(K_{DD} \odot K_{MM} \odot K_{XX} + n\lambda_8 I)^{-1}(K_{Dd} \odot K_{Mm} \odot K_{Xx}), \]

\[ \hat{\gamma}(d_1, d_2, x_1, x_2) = \hat{E}^*_9\{\phi(d_1) \otimes \phi(d_2) \otimes \phi(x_1) \otimes \phi(x_2)\} \]
\[ = K_Y(K_{D_1D_1} \odot K_{D_2D_2} \odot K_{X_1X_1} \odot K_{X_2X_2} + n\lambda_9 I)^{-1} \]
\[ (K_{D_1D_1} \odot K_{D_2D_2} \odot K_{X_1X_1} \odot K_{X_2X_2}). \]

\[ \square \]

E.4 Alternative closed form

Although the closed form expressions above are intuitive, alternative closed form expressions may run faster in statistical software. Specifically, the original expressions for \( \hat{\theta}^{ME} \) in Algorithm \[1\] and for \( \hat{\theta}^{GF} \) and \( \hat{\theta}^{DS} \) in Algorithm \[3\] require the summation over \( n \) terms, each of which is a vector in \( \mathbb{R}^n \). This step is a computational bottleneck since looping is much slower than matrix multiplication in many modern programming languages such as MATLAB and Python. Here, we present alternative closed form expressions which replace the summations with matrix multiplications. In experiments, these alternative expressions run about 100 times faster. Although both the original and alternative expressions involve \( O(n^3) \) computations, the alternative expression runs faster in numerical packages due to efficient implementation of matrix multiplication.

We present a technical lemma to derive the alternative expressions. Let \( \mathbf{1}_n \in \mathbb{R}^n \) be vector of ones.

**Lemma 3.** If \( \mathbf{A} \in \mathbb{R}^{n \times n} \) and \( \mathbf{a}, \mathbf{b} \in \mathbb{R}^n \) then
\[ \mathbf{A}(\mathbf{a} \odot \mathbf{b}) = \{\mathbf{A} \odot (\mathbf{1}_n \mathbf{a}^\top)\}\mathbf{b}, \quad (\mathbf{Aa}) \odot \mathbf{b} = \{\mathbf{A} \odot (\mathbf{b}\mathbf{1}_n^\top)\}\mathbf{a}. \]

**Proof.** Immediate from the definitions of matrix product and elementwise product. \( \square \)

Equipped with Lemma \[3\] we provide alternative expressions for \( \hat{\theta}^{ME}, \hat{\theta}^{GF}, \) and \( \hat{\theta}^{DS}. \)

**Algorithm 9** (Alternative estimation of mediated response curves). Denote the kernel matrices \( K_{DD}, K_{MM}, K_{XX} \in \mathbb{R}^{n \times n} \). Mediated response estimators have closed form solutions
Algorithm 10 (Alternative estimation of dynamic response curves). Denote the kernel matrices $\mathbf{K}_{D_1D_1}$, $\mathbf{K}_{D_2D_2}$, $\mathbf{K}_{X_1X_1}$, $\mathbf{K}_{X_2X_2} \in \mathbb{R}^{n \times n}$ calculated from observations drawn from population $\mathbb{P}$. Denote the kernel matrices $\mathbf{K}_{\tilde{D}_1\tilde{D}_1}$, $\mathbf{K}_{\tilde{D}_2\tilde{D}_2}$, $\mathbf{K}_{\tilde{X}_1\tilde{X}_1}$, $\mathbf{K}_{\tilde{X}_2\tilde{X}_2} \in \mathbb{R}^{n \times n}$ calculated from observations drawn from population $\tilde{\mathbb{P}}$. Dynamic response curve estimators have closed form solutions

1. $\hat{\theta}^{GF} = \mathbf{Y}^\top (\mathbf{K}_{D_1D_1} \odot \mathbf{K}_{D_2D_2} \odot \mathbf{K}_{X_1X_1} \odot \mathbf{K}_{X_2X_2} + n\lambda_4 \mathbf{I})^{-1}$

   
   $$
   [\mathbf{K}_{D_1d_1} \odot \mathbf{K}_{D_2d_2} \odot \{\mathbf{K}_{X_2X_2}(\mathbf{K}_{D_1D_1} \odot \mathbf{K}_{X_1X_1} + n\lambda_4 \mathbf{I})^{-1} \odot \frac{1}{n}\mathbf{K}_{X_1X_1}^2\} \mathbf{K}_{D_1d_1}],
   $$

2. $\hat{\theta}^{DS} = \mathbf{Y}^\top (\mathbf{K}_{D_1D_1} \odot \mathbf{K}_{D_2D_2} \odot \mathbf{K}_{X_1X_1} \odot \mathbf{K}_{X_2X_2} + n\lambda_5 \mathbf{I})^{-1}$

   
   $$
   [\mathbf{K}_{D_1d_1} \odot \mathbf{K}_{D_2d_2} \odot \{\mathbf{K}_{X_2X_2}(\mathbf{K}_{D_1D_1} \odot \mathbf{K}_{X_1X_1} + n\lambda_5 \mathbf{I})^{-1} \odot \frac{1}{n}\mathbf{K}_{X_1X_1}\} \mathbf{K}_{D_1d_1}],
   $$

where $(\lambda, \lambda_4, \lambda_5)$ are ridge regression penalty parameters.

Derivation. The argument is analogous to the derivation of Algorithm 9.

Note that we use the identity $\mathbf{1}_n \mathbf{K}_{X_2X_2}^\top \mathbf{K}_{X_2X_2} \mathbf{1}_n = \mathbf{K}_{X_2X_2}^\top \mathbf{K}_{X_2X_2}$. \hfill $\square$
F Nonparametric consistency proofs

In this appendix, we (i) present an equivalent definition of smoothness and specialize the smoothness condition in various settings; (ii) present technical lemmas for regression, unconditional mean embeddings, and conditional mean embeddings; (iii) appeal to these lemmas to prove uniform consistency for mediation analysis and dynamic dose response curves as well as convergence in distribution for counterfactual distributions.

F.1 Representations of smoothness

F.1.1 Alternative representations

**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 smoothness conditions in Assumptions 4 and 5.

1. Smoothness in Assumption 4 holds if and only if the regression $\gamma_0$ is a particularly smooth element of $H$. Formally, define the covariance operator $T$ for $H$. We assume there exists $g \in H$ such that $\gamma_0 = T^{c-1} g, c \in (1, 2]$, and $\|g\|_H^2 \leq \zeta$.

2. Smoothness in Assumption 5 holds if and only if the conditional expectation operator $E_\ell$ is a particularly smooth element of $L_2(H_{A_\ell}, H_{B_\ell})$. Formally, define the covariance operator $T_\ell := E \{ \phi(B_\ell) \otimes \phi(B_\ell) \}$ for $L_2(H_{A_\ell}, H_{B_\ell})$. We assume there exists $G_\ell \in L_2(H_{A_\ell}, H_{B_\ell})$ such that $E_\ell = (T_\ell)^{c_\ell-1} \circ G_\ell, c_\ell \in (1, 2]$, and $\|G_\ell\|_{L_2(H_{A_\ell}, H_{B_\ell})} \leq \zeta_\ell$.

**Remark 1.** In Assumption 4, the covariance operator $T$ for the RKHS $H$ depends on the setting.

1. Mediation analysis: $T = \mathbb{E}\{[\phi(D) \otimes \phi(M) \otimes \phi(X)] \otimes [\phi(D) \otimes \phi(M) \otimes \phi(X)]\}$.

2. Dynamic response: $T = \mathbb{E}\{[\phi(D_1) \otimes \phi(D_2) \otimes \phi(X_1) \otimes \phi(X_2)] \otimes [\phi(D_1) \otimes \phi(D_2) \otimes \phi(X_1) \otimes \phi(X_2)]\}$.

See [Singh et al., 2019] for the proof that $T_\ell$ and its powers are well defined under Assumption 2.
Remark 2. In Assumption 5, the spaces $A_\ell$ and $B_\ell$ depend on the setting.

1. Mediation analysis

(a) Mean embedding $\mu_m(d, x): A_1 = \mathcal{M}$ and $B_1 = \mathcal{D} \times \mathcal{X}$.

(b) Regression operator $E_8$: $A_8 = \mathcal{Y}$ and $B_8 = \mathcal{D} \times \mathcal{M} \times \mathcal{X}$.

2. Dynamic response

(a) Mean embedding $\mu_{x2}(d_1, x_1): A_4 = \mathcal{X}$ and $B_4 = \mathcal{D} \times \mathcal{X}$.

(b) Mean embedding $\nu_{x2}(d_1, x_1): A_5 = \mathcal{X}$ and $B_5 = \mathcal{D} \times \mathcal{X}$.

(c) Regression operator $E_9$: $A_9 = \mathcal{Y}$ and $B_9 = \mathcal{D} \times \mathcal{D} \times \mathcal{X} \times \mathcal{X}$.

F.1.2 Explicit specializations

Assumption 14 (Smoothness of mean embedding $\mu_m(d, x)$). Assume

1. The conditional expectation operator $E_1$ is well specified as a Hilbert-Schmidt operator between RKHSs, i.e. $E_1 \in \mathcal{L}_2(\mathcal{H}_M, \mathcal{H}_D \otimes \mathcal{H}_X)$, where $E_1 : \mathcal{H}_M \to \mathcal{H}_D \otimes \mathcal{H}_X$, $f(\cdot) \mapsto \mathbb{E}\{f(M) | D = \cdot, X = \cdot\}$.

2. The conditional expectation operator is a particularly smooth element of $\mathcal{L}_2(\mathcal{H}_M, \mathcal{H}_D \otimes \mathcal{H}_X)$. Formally, define the covariance operator $T_1 := \mathbb{E}\{\phi(D) \otimes \phi(X)\} \otimes \{\phi(D) \otimes \phi(X)\}$ for $\mathcal{L}_2(\mathcal{H}_M, \mathcal{H}_D \otimes \mathcal{H}_X)$. We assume there exists $G_1 \in \mathcal{L}_2(\mathcal{H}_M, \mathcal{H}_D \otimes \mathcal{H}_X)$ such that $E_1 = (T_1)^{c_1^{-1}} \circ G_1$, $c_1 \in (1, 2]$, and $\|G_1\|^2_{\mathcal{L}_2(\mathcal{H}_M, \mathcal{H}_D \otimes \mathcal{H}_X)} \leq \zeta_1$.

Assumption 15 (Smoothness of mean embedding $\mu_{x2}(d_1, x_1)$). Assume

1. The conditional expectation operator $E_4$ is well specified as a Hilbert-Schmidt operator between RKHSs, i.e. $E_4 \in \mathcal{L}_2(\mathcal{H}_X, \mathcal{H}_D \otimes \mathcal{H}_X)$, where $E_4 : \mathcal{H}_X \to \mathcal{H}_D \otimes \mathcal{H}_X$, $f(\cdot) \mapsto \mathbb{E}\{f(X_2) | D_1 = \cdot, X_1 = \cdot\}$.

2. The conditional expectation operator is a particularly smooth element of $\mathcal{L}_2(\mathcal{H}_X, \mathcal{H}_D \otimes \mathcal{H}_X)$. Formally, define the covariance operator $T_4 := \mathbb{E}\{\phi(D_1) \otimes \phi(X_1)\} \otimes \{\phi(D_1) \otimes \phi(X_1)\}$ for $\mathcal{L}_2(\mathcal{H}_X, \mathcal{H}_D \otimes \mathcal{H}_X)$. We assume there exists $G_4 \in \mathcal{L}_2(\mathcal{H}_X, \mathcal{H}_D \otimes \mathcal{H}_X)$ such that $E_4 = (T_4)^{c_4^{-1}} \circ G_4$, $c_4 \in (1, 2]$, and $\|G_4\|^2_{\mathcal{L}_2(\mathcal{H}_X, \mathcal{H}_D \otimes \mathcal{H}_X)} \leq \zeta_4$. 56
**Assumption 16** (Smoothness of mean embedding $\nu_{x_2}(d_1, x_1)$). Assume

1. The conditional expectation operator $E_5$ is well specified as a Hilbert-Schmidt operator between RKHSs, i.e. $E_5 \in \mathcal{L}_2(\mathcal{H}_X, \mathcal{H}_D \otimes \mathcal{H}_X)$, where $E_5 : \mathcal{H}_X \to \mathcal{H}_D \otimes \mathcal{H}_X$, $f(\cdot) \mapsto \mathbb{E}_\varphi\{f(X_2)|D_1 = \cdot, X_1 = \cdot\}$. 

2. The conditional expectation operator is a particularly smooth element of $\mathcal{L}_2(\mathcal{H}_X, \mathcal{H}_D \otimes \mathcal{H}_X)$. Formally, define the covariance operator $T_5 := \mathbb{E}[\{\phi(D_1) \otimes \phi(X_1)\} \otimes \{\phi(D_1) \otimes \phi(X_1)\}]$ for $\mathcal{L}_2(\mathcal{H}_X, \mathcal{H}_D \otimes \mathcal{H}_X)$. We assume there exists $G_5 \in \mathcal{L}_2(\mathcal{H}_X, \mathcal{H}_D \otimes \mathcal{H}_X)$ such that $E_5 = (T_5)^{\frac{\alpha_5}{2}} \circ G_5$, $c_5 \in (1, 2]$, and $\|G_5\|_{\mathcal{L}_2(\mathcal{H}_X, \mathcal{H}_D \otimes \mathcal{H}_X)}^2 \leq \zeta_5$.

**Assumption 17** (Smoothness of regression operator $E_8$). Assume

1. The conditional expectation operator $E_8$ is well specified as a Hilbert-Schmidt operator between RKHSs, i.e. $E_8 \in \mathcal{L}_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_M \otimes \mathcal{H}_X)$, where $E_8 : \mathcal{H}_Y \to \mathcal{H}_D \otimes \mathcal{H}_M \otimes \mathcal{H}_X$, $f(\cdot) \mapsto \mathbb{E}\{f(Y)|D = \cdot, M = \cdot, X = \cdot\}$. 

2. The conditional expectation operator is a particularly smooth element of $\mathcal{L}_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_M \otimes \mathcal{H}_X)$. Formally, define the covariance operator $T_8 := \mathbb{E}[\{\phi(D) \otimes \phi(M) \otimes \phi(X)\} \otimes \{\phi(D) \otimes \phi(M) \otimes \phi(X)\}]$ for $\mathcal{L}_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_M \otimes \mathcal{H}_X)$. We assume there exists $G_8 \in \mathcal{L}_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_M \otimes \mathcal{H}_X)$ such that $E_8 = (T_8)^{\frac{\alpha_8}{2}} \circ G_8$, $c_8 \in (1, 2]$, and $\|G_8\|_{\mathcal{L}_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_M \otimes \mathcal{H}_X)}^2 \leq \zeta_8$.

**Assumption 18** (Smoothness of regression operator $E_9$). Assume

1. The conditional expectation operator $E_9$ is well specified as a Hilbert-Schmidt operator between RKHSs, i.e. $E_9 \in \mathcal{L}_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_X \otimes \mathcal{H}_X)$, where $E_9 : \mathcal{H}_Y \to \mathcal{H}_D \otimes \mathcal{H}_D \otimes \mathcal{H}_X \otimes \mathcal{H}_X$, $f(\cdot) \mapsto \mathbb{E}\{f(Y)|D_1 = \cdot, D_2 = \cdot, X_1 = \cdot, X_2 = \cdot\}$. 

2. The conditional expectation operator is a particularly smooth element of $\mathcal{L}_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_X \otimes \mathcal{H}_X)$. Formally, define the covariance operator $T_9 := \mathbb{E}[\{\phi(D_1) \otimes \phi(D_2) \otimes \phi(X_1) \otimes \phi(X_2)\} \otimes \{\phi(D_1) \otimes \phi(D_2) \otimes \phi(X_1) \otimes \phi(X_2)\}]$ for $\mathcal{L}_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_D \otimes \mathcal{H}_X \otimes \mathcal{H}_X)$. We assume there exists $G_9 \in \mathcal{L}_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_D \otimes \mathcal{H}_X \otimes \mathcal{H}_X)$ such that $E_9 = (T_9)^{\frac{\alpha_9}{2}} \circ G_9$, $c_9 \in (1, 2]$, and $\|G_9\|_{\mathcal{L}_2(\mathcal{H}_Y, \mathcal{H}_D \otimes \mathcal{H}_D \otimes \mathcal{H}_X \otimes \mathcal{H}_X)}^2 \leq \zeta_9$. 

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F.1.3 Interpreting smoothness for tensor products

Another way to interpret the smoothness assumption for a tensor product RKHS follows from manipulation of the product kernel. For simplicity, consider $k(w, w') = k_1(w_1, w_1')k_2(w_2, w_2')$ where $k_1$ and $k_2$ are exponentiated quadratic kernels over $W \subset \mathbb{R}$. Define the vector of differences $v = w - w'$. Then

$$k(w, w') = \exp\left(-\frac{1}{2}v_1^2\right)\exp\left(-\frac{1}{2}v_2^2\right) = \exp\left\{-\frac{1}{2}v^\top \begin{pmatrix} \iota_1^{-2} & 0 \\ 0 & \iota_2^{-2} \end{pmatrix} v\right\}.$$

In summary, the product of exponentiated quadratic kernels over scalars is an exponentiated quadratic kernel over vectors. Therefore a tensor product of exponentiated quadratic RKHSs $\mathcal{H}_1$ and $\mathcal{H}_2$ begets an exponentiated quadratic RKHS $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, for which the smoothness and spectral decay conditions admit their usual interpretation. The same is true anytime that products of kernels beget a recognizable kernel.

F.2 Lemmas

F.2.1 Regression

For expositional purposes, we summarize classic results for the kernel ridge regression estimator $\hat{\gamma}$ for $\gamma_0(w) := \mathbb{E}(Y|W = w)$. As in Section 2, we denote the concatenation of regressors by $W$. For mediation analysis, $W = (D, M, X)$; for dynamic responses, $W = (D_1, D_2, X_1, X_2)$. Consider the following notation:

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

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

**Lemma 5** (Regression rate; Proposition 1 of [Singh et al., 2020]). Suppose Assumptions 2, 3, and 4 hold. Set $\lambda = n^{-1/(c+1/b)}$. Then with probability $1 - \delta$, for $n$ sufficiently large,

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

where $C$ is a constant independent of $n$ and $\delta$. 58
F.2.2 Unconditional mean embedding

For expositional purposes, we summarize classic results for the unconditional mean embedding estimator $\hat{\mu}_w$ for $\mu_w := \mathbb{E}\{\phi(W)\}$. We let $W$ be a generic random variable which we instantiate differently for different causal parameters.

**Lemma 6** (Mean embedding rate; Proposition 2 of [Singh et al., 2020]). Suppose Assumptions 2 and 3 hold. Then with probability $1 - \delta$,

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

We quote a result that appeals to Bennett inequality. [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.** Note that in various applications, $\kappa_w$ varies.

1. Mediation analysis: with probability $1 - \delta$, $\forall d \in \mathcal{D}$

$$\left\| \frac{1}{n} \sum_{i=1}^{n} \{\mu_m(d, X_i) \otimes \phi(X_i)\} - \int \{\mu_m(d, x) \otimes \phi(x)\}d\mathbb{P}(x) \right\|_{\mathcal{H}_m \otimes \mathcal{H}_X} \leq r_{\mu}^{ME}(n, \delta) := \frac{4\kappa_m \kappa_x \ln(2/\delta)}{\sqrt{n}}.$$  

2. Dynamic response

   (a) $\theta_0^{GF}$: with probability $1 - \delta$, $\forall d_1 \in \mathcal{D}$

$$\left\| \frac{1}{n} \sum_{i=1}^{n} \{\phi(X_{1i}) \otimes \mu_{x_2}(d_1, X_{1i})\} - \int \{\phi(x_1) \otimes \mu_{x_2}(d_1, x_1)\}d\mathbb{P}(x_1) \right\|_{\mathcal{H}_x \otimes \mathcal{H}_x} \leq r_{\mu}^{GF}(n, \delta) := \frac{4\kappa_x^2 \ln(2/\delta)}{\sqrt{n}}.$$  

   (b) $\theta_0^{DS}$: with probability $1 - \delta$, $\forall d_1 \in \mathcal{D}$

$$\left\| \frac{1}{n} \sum_{i=1}^{n} \{\phi(\tilde{X}_{1i}) \otimes \mu_{x_2}(d_1, \tilde{X}_{1i})\} - \int \{\phi(x_1) \otimes \mu_{x_2}(d_1, x_1)\}d\mathbb{P}(x_1) \right\|_{\mathcal{H}_x \otimes \mathcal{H}_x} \leq r_{\nu}^{DS}(\tilde{n}, \delta) := \frac{4\kappa_x^2 \ln(2/\delta)}{\sqrt{\tilde{n}}}.$$  

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F.2.3 Conditional expectation operator and conditional mean embedding

As in Sections 3 and 4 as well as Appendix B, we consider the abstract operator \( E_\ell \in L_2(\mathcal{H}_A, \mathcal{H}_B) \), where \( \mathcal{A}_\ell \) and \( \mathcal{B}_\ell \) are spaces that can be instantiated for different causal parameters.

Consider the definitions

\[
E_\ell = \text{argmin}_{E \in L_2(\mathcal{H}_A, \mathcal{H}_B)} \mathcal{E}(E), \quad \mathcal{E}(E) = \mathbb{E}\{[\phi(A_\ell) - E^\ast \phi(B_\ell)]^2\};
\]

\[
\hat{E}_\ell = \text{argmin}_{E \in L_2(\mathcal{H}_A, \mathcal{H}_B)} \hat{\mathcal{E}}(E), \quad \hat{\mathcal{E}}(E) = \frac{1}{n} \sum_{i=1}^{n} [\phi(A_{\ell i}) - E^\ast \phi(B_{\ell i})]^2 + \lambda_\ell \|E\|_{L_2(\mathcal{H}_A, \mathcal{H}_B)}^2.
\]

Lemma 7 (Conditional mean embedding rate; Proposition 3 of [Singh et al., 2020]). Suppose Assumptions 2, 3, and 5 hold. Set \( \lambda_\ell = n^{-1/(c_\ell + 1/b_\ell)} \). Then with probability \( 1 - \delta \), for \( n \) sufficiently large,

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

Moreover, \( \forall b \in \mathcal{B}_\ell \)

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

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

1. Mediation analysis: \( \kappa_a = \kappa_m, \ k_b = \kappa_d \kappa_x \).

2. Dynamic response: \( \kappa_a = \kappa_x, \ k_b = \kappa_d \kappa_x \).

3. Counterfactual distributions
   
   (a) Mediation analysis: \( \kappa_a = \kappa_y, \ k_b = \kappa_d \kappa_m \kappa_x \).
   
   (b) Dynamic response: \( \kappa_a = \kappa_y, \ k_b = \kappa_d^2 \kappa_x^2 \).

F.3 Main results

Appealing to Lemmas 5, 6 and 7 we now prove consistency for (i) mediated responses, (ii) dynamic responses, and (iii) counterfactual distributions.
F.3.1 Mediation analysis

To lighten notation, define $\Delta_m := \frac{1}{n} \sum_{i=1}^{n} \{ \hat{\mu}_m(d, X_i) \otimes \phi(X_i) \} - \int \{ \mu_m(d, x) \otimes \phi(x) \} d\mathbb{P}(x)$.

**Proposition 2.** Suppose Assumptions 2, 3, and 14 hold. Then with probability $1 - 2\delta$,

$$\| \Delta_m \|_{H_M \otimes H_X} \leq \kappa_x \cdot r^M_M(n, \delta, b_1, c_1) + r^M_M(n, \delta).$$

**Proof.** By triangle inequality,

$$\| \Delta_m \|_{H_M \otimes H_X} \leq \left\| \frac{1}{n} \sum_{i=1}^{n} \{ \hat{\mu}_m(d, X_i) \otimes \phi(X_i) \} - \{ \mu_m(d, X_i) \otimes \phi(X_i) \} \right\|_{H_M \otimes H_X}$$

$$+ \left\| \frac{1}{n} \sum_{i=1}^{n} \{ \mu_m(d, X_i) \otimes \phi(X_i) \} - \int \{ \mu_m(d, x) \otimes \phi(x) \} d\mathbb{P}(x) \right\|_{H_M \otimes H_X}.$$ 

Focusing on the former term, by Lemma 7

$$\left\| \frac{1}{n} \sum_{i=1}^{n} \{ \hat{\mu}_m(d, X_i) \otimes \phi(X_i) \} - \{ \mu_m(d, X_i) \otimes \phi(X_i) \} \right\|_{H_M \otimes H_X}$$

$$= \left\| \frac{1}{n} \sum_{i=1}^{n} \{ \hat{\mu}_m(d, X_i) - \mu_m(d, X_i) \} \otimes \phi(X_i) \right\|_{H_M \otimes H_X}$$

$$\leq \kappa_x \cdot \sup_{x \in \mathcal{X}} \| \hat{\mu}_m(d, x) - \mu_m(d, x) \|_{H_M}$$

$$\leq \kappa_x \cdot r^M_M(n, \delta, b_1, c_1).$$

Focusing on the latter term, by Lemma 6

$$\left\| \frac{1}{n} \sum_{i=1}^{n} \{ \mu_m(d, X_i) \otimes \phi(X_i) \} - \int \{ \mu_m(d, x) \otimes \phi(x) \} d\mathbb{P}(x) \right\|_{H_M \otimes H_X} \leq r^M_M(n, \delta).$$

**Proof of Theorem 3** Observe that

$$\hat{\theta}^M_M(d, d') - \theta_0^M_M(d, d')$$

$$= \langle \hat{\gamma}, \phi(d') \otimes \frac{1}{n} \sum_{i=1}^{n} \{ \hat{\mu}_m(d, X_i) \otimes \phi(X_i) \} \rangle_{H} - \langle \gamma_0, \phi(d') \otimes \int \{ \mu_m(d, x) \otimes \phi(x) \} d\mathbb{P}(x) \rangle_{H}$$

$$= \langle \hat{\gamma}, \phi(d') \otimes \Delta_m \rangle_{H} + \langle (\hat{\gamma} - \gamma_0), \phi(d') \otimes \int \{ \mu_m(d, x) \otimes \phi(x) \} d\mathbb{P}(x) \rangle_{H}$$

$$= \langle (\hat{\gamma} - \gamma_0), \phi(d') \otimes \Delta_m \rangle_{H}$$

$$+ \langle \gamma_0, \phi(d') \otimes \Delta_m \rangle_{H} + \langle (\hat{\gamma} - \gamma_0), \phi(d') \otimes \int \{ \mu_m(d, x) \otimes \phi(x) \} d\mathbb{P}(x) \rangle_{H}.$$
Therefore by Lemmas 5, 6, and 7 as well as Proposition 2 with probability $1 - 3\delta$

$$|\hat{\theta}^{ME}(d, d') - \theta_0^{ME}(d, d')|$$

$$\leq \|\hat{\gamma} - \gamma_0\|_{\mathcal{H}} \|\phi(d')\|_{\mathcal{H}_P} \|\Delta_m\|_{\mathcal{H}_M \otimes \mathcal{H}_x}$$

$$+ \|\gamma_0\|_{\mathcal{H}} \|\phi(d')\|_{\mathcal{H}_P} \|\Delta_m\|_{\mathcal{H}_M \otimes \mathcal{H}_x}$$

$$+ \|\hat{\gamma} - \gamma_0\|_{\mathcal{H}} \|\phi(d')\|_{\mathcal{H}_P} \left\| \int \{\mu_m(d, x) \otimes \phi(x)\} dP(x) \right\|_{\mathcal{H}_M \otimes \mathcal{H}_x}$$

$$\leq \kappa_d \cdot r_\gamma(n, \delta, b, c) \cdot \{\kappa_x \cdot r_\mu^{ME}(n, \delta, b_1, c_1) + r_\mu^{ME}(n, \delta)\}$$

$$+ \kappa_d \cdot \|\gamma_0\|_{\mathcal{H}} \cdot \{\kappa_x \cdot r_\mu^{ME}(n, \delta, b_1, c_1) + r_\mu^{ME}(n, \delta)\}$$

$$+ \kappa_m \kappa_d \kappa_x \cdot r_\gamma(n, \delta, b, c)$$

$$= O\left(n^{-\frac{3}{2} \epsilon^{-1}} + n^{-\frac{3}{2} \gamma_{3/4}}\right).$$

Likewise for the incremental responses. \qed

F.3.2 Dynamic responses

To lighten notation, define

$$\Delta_p := \frac{1}{n} \sum_{i=1}^{n} \{\phi(X_{1i}) \otimes \hat{\mu}_x(d_1, X_{1i})\} - \int \{\phi(x_1) \otimes \mu_x(d_1, x_1)\} dP(x_1),$$

$$\Delta_q := \frac{1}{n} \sum_{i=1}^{n} \{\phi(X_{1i}) \otimes \hat{\nu}_x(d_1, X_{1i})\} - \int \{\phi(x_1) \otimes \nu_x(d_1, x_1)\} d\tilde{P}(x_1).$$

**Proposition 3.** Suppose Assumptions 2 and 3 hold.

1. If in addition Assumption 15 holds then with probability $1 - 2\delta$

$$\|\Delta_p\|_{\mathcal{H}_X \otimes \mathcal{H}_x} \leq \kappa_x \cdot r_{\mu}^{GF}(n, \delta, b_4, c_4) + r_\mu^{GF}(n, \delta).$$

2. If in addition Assumption 16 holds then with probability $1 - 2\delta$

$$\|\Delta_q\|_{\mathcal{H}_X \otimes \mathcal{H}_x} \leq \kappa_x \cdot r_{\nu}^{DS}(\bar{n}, \delta, c_5) + r_\nu^{DS}(\bar{n}, \delta).$$

**Proof.** We prove the result for $\theta_0^{GF}$. The argument for $\theta_0^{DS}$ is identical. By triangle inequality,

$$\|\Delta_p\|_{\mathcal{H}_X \otimes \mathcal{H}_x} \leq \left\| \frac{1}{n} \sum_{i=1}^{n} \{\phi(X_{1i}) \otimes \hat{\mu}_x(d_1, X_{1i})\} - \{\phi(X_{1i}) \otimes \mu_x(d_1, X_{1i})\} \right\|_{\mathcal{H}_X \otimes \mathcal{H}_x}$$

$$+ \left\| \frac{1}{n} \sum_{i=1}^{n} \{\phi(X_{1i}) \otimes \mu_x(d_1, X_{1i})\} - \int \{\phi(x_1) \otimes \mu_x(d_1, x_1)\} dP(x_1) \right\|_{\mathcal{H}_X \otimes \mathcal{H}_x}.\]
Focusing on the former term, by Lemma 7
\[
\frac{1}{n} \sum_{i=1}^{n} \left\{ \phi(X_{1i}) \otimes \hat{\mu}_x (d_1, X_{1i}) \right\} - \left\{ \phi(X_{1i}) \otimes \mu_x (d_1, X_{1i}) \right\} \\
= \frac{1}{n} \sum_{i=1}^{n} \left\{ \phi(X_{1i}) \otimes \{ \hat{\mu}_x (d_1, X_{1i}) - \mu_x (d_1, X_{1i}) \} \right\} \\
\leq \kappa_x \cdot \sup_{x_1 \in X} \| \hat{\mu}_x (d_1, x_1) - \mu_x (d_1, x_1) \|_{\mathcal{H}_X} \\
\leq \kappa_x \cdot \tau^{GF}_\mu (n, \delta, b_4, c_4).
\]

Focusing on the latter term, by Lemma 6
\[
\frac{1}{n} \sum_{i=1}^{n} \left\{ \phi(X_{1i}) \otimes \mu_x (d_1, X_{1i}) \right\} - \int \left\{ \phi(x_1) \otimes \mu_x (d_1, x_1) \right\} dP(x_1) \\
\leq \tau^{GF}_\mu (n, \delta).
\]

Proof of Theorem 7. We consider each dynamic response parameter.

1. $\theta_0^{GF}$. Observe that
\[
\hat{\theta}^{GF}(d_1, d_2) - \theta_0^{GF}(d_1, d_2) \\
= \langle \hat{\gamma}, \phi(d_1) \otimes \phi(d_2) \otimes \frac{1}{n} \sum_{i=1}^{n} \{ \phi(X_{1i}) \otimes \hat{\mu}_x (d_1, X_{1i}) \} \rangle_{\mathcal{H}} \\
- \langle \gamma_0, \phi(d_1) \otimes \phi(d_2) \otimes \int \phi(x_1) \otimes \mu_x (d_1, x_1) dP(x_1) \rangle_{\mathcal{H}} \\
= \langle \hat{\gamma}, \phi(d_1) \otimes \phi(d_2) \otimes \Delta_p \rangle_{\mathcal{H}} \\
+ \langle (\hat{\gamma} - \gamma_0), \phi(d_1) \otimes \phi(d_2) \otimes \int \phi(x_1) \otimes \mu_x (d_1, x_1) dP(x_1) \rangle_{\mathcal{H}} \\
= \langle (\hat{\gamma} - \gamma_0), \phi(d_1) \otimes \phi(d_2) \otimes \Delta_p \rangle_{\mathcal{H}} \\
+ \langle \gamma_0, \phi(d_1) \otimes \phi(d_2) \otimes \Delta_p \rangle_{\mathcal{H}} \\
+ \langle (\hat{\gamma} - \gamma_0), \phi(d_1) \otimes \phi(d_2) \otimes \int \phi(x_1) \otimes \mu_x (d_1, x_1) dP(x_1) \rangle_{\mathcal{H}}.
Therefore by Lemmas 5, 6, and 7 as well as Proposition 3 with probability $1 - 3\delta$

\[
|\hat{\theta}^{GF}(d_1, d_2) - \theta_0^{GF}(d_1, d_2)| \\
\leq \|\hat{\gamma} - \gamma_0\|_H \Phi(d_1) \|\phi(d_2)\| \Delta_p \|\mathcal{H}_x \otimes \mathcal{H}_x \\
+ \|\gamma_0\|_H \Phi(d_1) \|\phi(d_2)\| \Delta_p \|\mathcal{H}_x \otimes \mathcal{H}_x \\
+ \|\hat{\gamma} - \gamma_0\|_H \Phi(d_1) \|\phi(d_2)\| \Delta_p \times \left\|\int \{\phi(x_1) \otimes \mu_{x_2}(d_1, x_1)\} d\mathbb{P}(x_1)\right\|_{\mathcal{H}_x \otimes \mathcal{H}_x} \\
\leq \kappa_d \cdot r_\gamma(n, \delta, b, c) \cdot \{\kappa_x \cdot r_{\mu}^{GF}(n, \delta, b_4, c_4) + r_{\mu}^{GF}(n, \delta)\} \\
+ \kappa_d^2 \cdot \|\gamma_0\|_H \cdot \{\kappa_x \cdot r_{\mu}^{GF}(n, \delta, b_4, c_4) + r_{\mu}^{GF}(n, \delta)\} \\
+ \kappa_d^2 \cdot \|\gamma_0\|_H \cdot \{\kappa_x \cdot r_{\mu}^{DS}(\tilde{n}, \delta, c_5) + r_{\mu}^{DS}(\tilde{n}, \delta)\} \\
+ \kappa_d^2 \cdot \|\gamma_0\|_H \cdot \{\kappa_x \cdot r_{\mu}^{DS}(\tilde{n}, \delta, c_5) + r_{\mu}^{DS}(\tilde{n}, \delta)\} \\
+ \kappa_d^2 \kappa_x^2 \cdot r_\gamma(n, \delta, b, c) \\
= O\left(n^{-\frac{1}{2}} + \tilde{n}^{-\frac{1}{2} - \frac{1}{2} c_4^{-1} + \frac{1}{4} b c_4^2} + \tilde{n}^{-\frac{1}{2}} + \tilde{n}^{-\frac{1}{2} - \frac{1}{2} c_4^{-1} + \frac{1}{4} b c_4^2}\right).
\]

2. $\theta_0^{DS}$. By the same argument

\[
|\hat{\theta}^{DS}(d_1, d_2) - \theta_0^{DS}(d_1, d_2)| \\
\leq \kappa_d^2 \cdot r_\gamma(n, \delta, b, c) \cdot \{\kappa_x \cdot r_{\mu}^{DS}(\tilde{n}, \delta, c_5) + r_{\mu}^{DS}(\tilde{n}, \delta)\} \\
+ \kappa_d^2 \cdot \|\gamma_0\|_H \cdot \{\kappa_x \cdot r_{\mu}^{DS}(\tilde{n}, \delta, c_5) + r_{\mu}^{DS}(\tilde{n}, \delta)\} \\
+ \kappa_d^2 \kappa_x^2 \cdot r_\gamma(n, \delta, b, c) \\
= O\left(n^{-\frac{1}{2}} + \tilde{n}^{-\frac{1}{2} - \frac{1}{2} c_5^{-1} + \frac{1}{4} b c_5^2}\right).
\]

Likewise for the incremental effects.

F.3.3 Counterfactual distributions

Proof of Theorem 11. The argument is analogous to Theorems 3 and 7 replacing $\|\gamma_0\|_H$ with $\|E_8\|_{L_2}$ or $\|E_9\|_{L_2}$ and replacing $r_\gamma(n, \delta, b, c)$ with $r_E(n, \delta, b_8, c_8)$ or $r_E(n, \delta, b_9, c_9)$.

G Semiparametric inference proofs

In this appendix, we (i) present technical lemmas for regression; (ii) appeal to these lemmas to prove $n^{-1/2}$ consistency, finite sample Gaussian approximation, and semiparametric efficiency of mediation analysis and dynamic treatment effects.
G.1 Lemmas

Recall the various nonparametric objects required for inference. For mediation analysis,

\[ \gamma_0(d, m, x) = \mathbb{E}(Y | D = d, M = m, X = x), \]
\[ \pi_0(d; x) = \mathbb{P}(D = d | X = x), \]
\[ \rho_0(d; m, x) = \mathbb{P}(D = d | M = m, X = x), \]
\[ \omega_0(d, d'; x) = \int \gamma_0(d', m, x) d\mathbb{P}(m | d, x). \]

For dynamic treatment effects,

\[ \gamma_0(d_1, d_2, x_1, x_2) = \mathbb{E}(Y | D_1 = d_1, D_2 = d_2, X_1 = x_1, X_2 = x_2), \]
\[ \pi_0(d_1; x_1) = \mathbb{P}(D_1 = d_1 | X_1 = x_1), \]
\[ \rho_0(d_2; d_1, x_1, x_2) = \mathbb{P}(D_2 = d_2 | D_1 = d_1, X_1 = x_1, X_2 = x_2), \]
\[ \omega_0(d_1, d_2; x_1) = \int \gamma_0(d_1, d_2, x_2) d\mathbb{P}(x_2 | d_1, x_1). \]

We begin by summarizing rates for these various quantities.

G.1.1 Response curve rate

To being, we provide a uniform rate for \( \omega_0 \), using nonparametric techniques developed in Appendix \( \text{F} \).

**Proposition 4** (Uniform \( \omega \) rate). Suppose Assumptions \([2,3,4]\) hold.

1. If in addition Assumption \([14]\) holds then for mediation analysis, with probability \( 1 - 2\delta \),

\[ \| \hat{\omega} - \omega_0 \|_{\infty} \leq r^M_{\omega}(n, \delta, b, c, b_1, c_1) \]
\[ := \kappa_d \kappa_{m} \cdot r_\gamma(n, \delta, b, c) \cdot r^M_\mu(n, \delta, b_1, c_1) + \kappa_d \kappa_{x} \cdot \| \gamma_0 \|_{\mathcal{H}} \cdot r^M_\mu(n, \delta, b_1, c_1) \]
\[ + \kappa_d \kappa_{m} \kappa_{x} \cdot r_\gamma(n, \delta, b, c). \]

We summarize the rate as \( r^M_{\omega}(n, b, c, b_1, c_1) = O \left( n^{-\frac{1}{2} \frac{c-1}{c+1}b_1} + n^{-\frac{1}{2} \frac{c_1-1}{c_1+1}b_1} \right). \)

2. If in addition Assumption \([15]\) holds then for dynamic treatment effects, with probability
\[1 - 2\delta\]

\[
\|\hat{\omega} - \omega_0\|_\infty \leq r^{GF}_\omega(n, \delta, b, c, b_4, c_4) \\
:= \kappa^2_d\kappa_x \cdot r_\gamma(n, \delta, b, c) \cdot r^{GF}_\mu(n, \delta, b_4, c_4) + \kappa^2_d\kappa_x \cdot \|\gamma_0\|_\mathcal{H} \cdot r^{GF}_\mu(n, \delta, b_4, c_4) \\
+ \kappa^2_d\kappa_x^2 \cdot r_\gamma(n, \delta, b, c).
\]

We summarize the rate as \(r^{GF}(n, b, c, b_4, c_4) = O\left(n^{-\frac{1}{2} + \frac{1}{2\epsilon + 1/8}} + n^{-\frac{1}{2} + 1/3\epsilon + 1/8}\right)\).

**Proof.** We prove each result.

1. Mediation analysis. Fix \((d, d', x)\). Then

\[
\hat{\omega}(d, d'; x) - \omega_0(d, d'; x) \\
= \langle \hat{\gamma}, \phi(d') \otimes \hat{\mu}_m(d, x) \otimes \phi(x) \rangle_{\mathcal{H}} - \langle \gamma_0, \phi(d') \otimes \mu_m(d, x) \otimes \phi(x) \rangle_{\mathcal{H}} \\
= \langle \hat{\gamma}, \phi(d') \otimes \{\hat{\mu}_m(d, x) - \mu_m(d, x)\} \otimes \phi(x) \rangle_{\mathcal{H}} + \langle (\hat{\gamma} - \gamma_0), \phi(d') \otimes \mu_m(d, x) \otimes \phi(x) \rangle_{\mathcal{H}} \\
= \langle (\hat{\gamma} - \gamma_0), \phi(d') \otimes \{\hat{\mu}_m(d, x) - \mu_m(d, x)\} \otimes \phi(x) \rangle_{\mathcal{H}} \\
+ \langle (\hat{\gamma} - \gamma_0), \phi(d') \otimes \mu_m(d, x) \otimes \phi(x) \rangle_{\mathcal{H}}.
\]

Therefore by Lemmas 5 and 7 with probability \(1 - 2\delta\)

\[
|\hat{\omega}(d, d'; x) - \omega_0(d, d'; x)| \\
\leq \|\hat{\gamma} - \gamma_0\|_{\mathcal{H}} \|\phi(d')\|_{\mathcal{H}} \|\hat{\mu}_m(d, x) - \mu_m(d, x)\|_{\mathcal{H}_m} \|\phi(x)\|_{\mathcal{H}_x} \\
+ \|\gamma_0\|_{\mathcal{H}} \|\phi(d')\|_{\mathcal{H}} \|\hat{\mu}_m(d, x) - \mu_m(d, x)\|_{\mathcal{H}_m} \|\phi(x)\|_{\mathcal{H}_x} \\
+ \|\hat{\gamma} - \gamma_0\|_{\mathcal{H}} \|\phi(d')\|_{\mathcal{H}} \|\mu_m(d, x)\|_{\mathcal{H}_m} \|\phi(x)\|_{\mathcal{H}_x} \\
\leq \kappa_d\kappa_x \cdot r_\gamma(n, \delta, b, c) \cdot r_{ME}^{\mu}(n, \delta, b_1, c_1) + \kappa_d\kappa_x \cdot \|\gamma_0\|_{\mathcal{H}} \cdot r_{ME}^{\mu}(n, \delta, b_1, c_1) \\
+ \kappa_d\kappa_m\kappa_x \cdot r_\gamma(n, \delta, b, c) \\
= O\left(n^{-\frac{1}{2} + \frac{1}{2\epsilon + 1/8}} + n^{-\frac{1}{2} + 1/3\epsilon + 1/8}\right).
\]
2. Dynamic treatment effect. Fix $(d_1, d_2, x_1)$. Then

$$
\hat{\omega}(d_1, d_2; x_1) - \omega_0(d, d'; x_1)
= \langle \dot{\gamma}, \phi(d_1) \otimes \phi(d_2) \otimes \phi(x_1) \otimes \hat{\mu}_{x_2}(d_1, x_1) \rangle_{\mathcal{H}}
- \langle \gamma_0, \phi(d_1) \otimes \phi(d_2) \otimes \phi(x_1) \otimes \mu_{x_2}(d_1, x_1) \rangle_{\mathcal{H}}
= \langle \dot{\gamma}, \phi(d_1) \otimes \phi(d_2) \otimes \phi(x_1) \otimes \{\hat{\mu}_{x_2}(d_1, x_1) - \mu_{x_2}(d_1, x_1)\} \rangle_{\mathcal{H}}
+ \langle (\dot{\gamma} - \gamma_0), \phi(d_1) \otimes \phi(d_2) \otimes \phi(x_1) \otimes \mu_{x_2}(d_1, x_1) \rangle_{\mathcal{H}}
+ \langle (\dot{\gamma} - \gamma_0), \phi(d_1) \otimes \phi(d_2) \otimes \phi(x_1) \otimes \mu_{x_2}(d_1, x_1) \rangle_{\mathcal{H}}.
$$

Therefore by Lemmas [5] and [7] with probability $1 - 2\delta$

$$
|\hat{\omega}(d, d'; x) - \omega_0(d, d'; x)|
\leq \|\dot{\gamma} - \gamma_0\|_{\mathcal{H}} \|\phi(d_1)\|_{\mathcal{H}_D} \|\phi(d_2)\|_{\mathcal{H}_D} \|\phi(x_1)\|_{\mathcal{H}_X} \|\hat{\mu}_{x_2}(d_1, x_1) - \mu_{x_2}(d_1, x_1)\|_{\mathcal{H}_X}
+ \|\gamma_0\|_{\mathcal{H}} \|\phi(d_1)\|_{\mathcal{H}_D} \|\phi(d_2)\|_{\mathcal{H}_D} \|\phi(x_1)\|_{\mathcal{H}_X} \|\hat{\mu}_{x_2}(d_1, x_1) - \mu_{x_2}(d_1, x_1)\|_{\mathcal{H}_X}
+ \|\dot{\gamma} - \gamma_0\|_{\mathcal{H}} \|\phi(d_1)\|_{\mathcal{H}_D} \|\phi(d_2)\|_{\mathcal{H}_D} \|\phi(x_1)\|_{\mathcal{H}_X} \|\mu_{x_2}(d_1, x_1)\|_{\mathcal{H}_X}
\leq \kappa_\delta \kappa_x \cdot r_\gamma(n, \delta, b, c) \cdot r_\mu^{GF}(n, \delta, b_4, c_4) + \kappa_\delta^2 \kappa_x \cdot \|\gamma_0\|_{\mathcal{H}} \cdot r_\mu^{GF}(n, \delta, b_4, c_4)
+ \kappa_\delta^2 \kappa_x \cdot r_\gamma(n, \delta, b, c)
= O\left(n^{-\frac{1}{2}} \frac{c-1}{c+1} + n^{-\frac{1}{2}} \frac{c_4-1}{c_4+1} \frac{1}{\sqrt{q_i}} \right).
$$

G.1.2 Mean square rate

Observe that $(\gamma_0, \pi_0, \rho_0)$ can be estimated by nonparametric regressions. We write an abstract result for kernel ridge regression then specialize it for these various nonparametric regressions. For the abstract result, write

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

$$
\hat{\gamma} = \arg\min_{\gamma \in \mathcal{H}} \hat{\mathcal{E}}(\gamma), \quad \hat{\mathcal{E}}(\gamma) = \frac{1}{n} \sum_{i=1}^{n} \{Y_i - \gamma(W_i)\}^2 + \lambda \|\gamma\|_{\mathcal{H}}^2.
$$
Define the mean square learning rate $\mathcal{R}(\hat{\gamma}_\ell)$ of $\hat{\gamma}_\ell$ trained on observations indexed by $I_\ell^c$ as

$$\mathcal{R}(\hat{\gamma}_\ell) = \mathbb{E}[(\hat{\gamma}_\ell(W) - \gamma_0(W))^2 | I_\ell^c].$$

**Lemma 8** (Regression mean square rate). Suppose Assumptions 2, 3, and 4 hold. Set $\lambda = n^{-1/(c+1/b)}$. Then with probability $1 - \delta$, for $n$ sufficiently large,

$$\{\mathcal{R}(\hat{\gamma}_\ell)\}^{1/2} \leq s_\gamma(n, \delta, b, c) := C \ln(4/\delta) \cdot n^{-\frac{1}{2 + c + 1/b}}.$$

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

**Proof.** The proof is identical to the proof of [Singh et al., 2020, Proposition 1], changing the Hilbert scale from one to zero. \qed

**Remark 5.** Note that in various applications, $(b, c)$ vary.

1. Mediation analysis
   
   (a) $\{\mathcal{R}(\hat{\gamma}_\ell)\}^{1/2} \leq s_{\gamma}^{ME}(n, b, c)$.
   
   (b) $\{\mathcal{R}(\hat{\pi}_\ell)\}^{1/2} \leq s_{\pi}^{ME}(n, b_2, c_2)$.
   
   (c) $\{\mathcal{R}(\hat{\rho}_\ell)\}^{1/2} \leq s_{\rho}^{ME}(n, b_3, c_3)$.

2. Dynamic treatment effects
   
   (a) $\{\mathcal{R}(\hat{\gamma}_\ell)\}^{1/2} \leq s_{\gamma}^{GF}(n, b, c)$.
   
   (b) $\{\mathcal{R}(\hat{\pi}_\ell)\}^{1/2} \leq s_{\pi}^{GF}(n, b_6, c_6)$.
   
   (c) $\{\mathcal{R}(\hat{\rho}_\ell)\}^{1/2} \leq s_{\rho}^{GF}(n, b_7, c_7)$.

**G.2 Gaussian approximation**

We quote an abstract result for semiparametric inference in longitudinal settings. The result concerns a causal parameter $\theta_0 = \mathbb{E}[\psi(\delta_0, \nu_0, \alpha_0, \eta_0; W)]$ whose multiply robust moment function is of the form

$$\psi(\delta, \nu, \alpha, \eta; W) = \nu(W) + \alpha(W)\{Y - \delta(W)\} + \eta(W)\{\delta(W) - \nu(W)\}.$$ 

To lighten notation, we write $\psi_0(W) = \psi(\delta_0, \nu_0, \alpha_0, \eta_0; W)$ and define the oracle moments

$$0 = \mathbb{E}\{\psi_0(W) - \theta_0\}, \quad \sigma^2 = \mathbb{E}[\{\psi_0(W) - \theta_0\}^2], \quad \xi^3 = \mathbb{E}\{|\psi_0(W) - \theta_0|^3\}, \quad \chi^4 = \mathbb{E}\{|\psi_0(W) - \theta_0|^4\}.$$ 

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Lemma 9 (Semiparametric inference; Corollary 6.1 of [Singh, 2021b]). Suppose the following conditions hold:

1. Neyman orthogonal moment function $\psi$;

2. Bounded residual variances: $\mathbb{E}[(Y - \delta_0(W))^2 \mid W] \leq \bar{\sigma}_1^2$ and $\mathbb{E}[(\delta_0(W) - \nu_0(W_1))^2 \mid W_1] \leq \bar{\sigma}_2^2$, where $W_1 \subset W$ is the argument of $\nu_0$;

3. Bounded balancing weights: $\|\alpha_0\|_{\infty} \leq \bar{\alpha}$ and $\|\eta_0\|_{\infty} \leq \bar{\eta}$;

4. Censored balancing weight estimators: $\|\hat{\alpha}_\ell\|_{\infty} \leq \bar{\alpha}'$ and $\|\hat{\eta}_\ell\|_{\infty} \leq \bar{\eta}'$.

Next assume the regularity condition on moments $\{(\xi/\sigma)^3 + \chi^2\} n^{-1/2} \rightarrow 0$. Finally assume the learning rate conditions

1. $(1 + \bar{\eta}/\sigma + \bar{\eta}'/\sigma) \{\mathcal{R}(\hat{\nu}_\ell)\}^{1/2} \rightarrow 0$;

2. $(\bar{\alpha}/\sigma + \bar{\alpha}' + \bar{\eta}/\sigma + \bar{\eta}') \{\mathcal{R}(\hat{\delta}_\ell)\}^{1/2} \rightarrow 0$;

3. $(\bar{\eta}' + \bar{\sigma}_1)\{\mathcal{R}(\hat{\alpha}_\ell)\}^{1/2} \rightarrow 0$;

4. $\bar{\sigma}_2\{\mathcal{R}(\hat{\eta}_\ell)\}^{1/2} \rightarrow 0$;

5. $[\{n\mathcal{R}(\hat{\nu}_\ell)\mathcal{R}(\hat{\eta}_\ell)\}^{1/2}] / \sigma \rightarrow 0$.

6. $[\{n\mathcal{R}(\hat{\delta}_\ell)\mathcal{R}(\hat{\alpha}_\ell)\}^{1/2}] / \sigma \rightarrow 0$.

7. $[\{n\mathcal{R}(\hat{\delta}_\ell)\mathcal{R}(\hat{\eta}_\ell)\}^{1/2}] / \sigma \rightarrow 0$.

Then

$$\hat{\theta} \xrightarrow{p} \theta_0, \quad \frac{\sqrt{n}}{\sigma} (\hat{\theta} - \theta_0) \xrightarrow{d} \mathcal{N}(0, 1), \quad \mathbb{P}\left\{\theta_0 \in \left(\hat{\theta} \pm \zeta_\alpha \hat{\sigma} n^{-1/2}\right)\right\} \rightarrow 1 - a.$$

Moreover, the finite sample rate of Gaussian approximation can expressed in terms of the learning rates above.

We will match symbols to appeal to this result.

G.3 Main results

Appealing to Proposition 4, Lemma 8 and Lemma 9, we now prove inference for (i) mediation analysis and (ii) dynamic treatment effects.
G.3.1 Mediation analysis

Recall

\[ \gamma_0(d, m, x) = \mathbb{E}(Y | D = d, M = m, X = x), \]
\[ \omega_0(d, d'; x) = \int \gamma_0(d', m, x) d \mathbb{P}(m | d, x), \]
\[ \pi_0(d; x) = \mathbb{P}(D = d | X = x), \]
\[ \rho_0(d; m, x) = \mathbb{P}(D = d | M = m, X = x). \]

Fix \((d, d')\). Matching symbols with the abstract Gaussian approximation,

\[ \delta_0(W) = \gamma_0(d', M, X), \]
\[ \nu_0(W) = \int \gamma_0(d', m, X) d \mathbb{P}(m | d, X) = \omega_0(d, d'; X) \]
\[ \alpha_0(W) = \frac{1_{D = d'}}{\rho_0(d'; M, X)} \frac{\rho_0(d; M, X)}{\pi_0(d; X)} \]
\[ \eta_0(W) = \frac{1_{D = d}}{\pi_0(d; X)}. \]

Proof of Theorem 4. We proceed in steps, verifying the conditions of Lemma 9.

1. Neyman orthogonal moment function. By [Singh, 2021b, Proposition A.2], it suffices to show the following four equalities.

\[ \mathbb{E}[\nu(W) \{1 - \eta_0(W)\}] = 0 \]
\[ \mathbb{E}[\delta(W) \{\eta_0(W) - \alpha_0(W)\}] = 0 \]
\[ \mathbb{E}[\alpha(W) \{Y - \delta_0(W)\}] = 0 \]
\[ \mathbb{E}[\eta(W) \{\delta_0(W) - \nu_0(W)\}] = 0. \]

We verify each one.
(a) First, write

\[ \mathbb{E}[\nu(W)\{1 - \eta_0(W)\}] = \mathbb{E}\left[ \omega_0(d, d'; X) \left\{ 1 - \frac{\mathbb{I}_{D=d}}{\pi_0(d; X)} \right\} \right] \]

\[ = \mathbb{E}\left[ \omega_0(d, d'; X) \left\{ 1 - \frac{\mathbb{E}(\mathbb{I}_{D=d}|X)}{\pi_0(d; X)} \right\} \right] \]

\[ = \mathbb{E}\left[ \omega_0(d, d'; X) \left\{ 1 - \frac{\pi_0(d; X)}{\pi_0(d; X)} \right\} \right] \]

\[ = 0. \]

(b) Second, write

\[ \mathbb{E}[\delta(W)\{\eta_0(W) - \alpha_0(W)\}] \]

\[ = \mathbb{E}\left[ \gamma(d', M, X) \left\{ \frac{\mathbb{I}_{D=d}}{\pi_0(d; X)} - \frac{\mathbb{I}_{D=d'}}{\rho_0(d'; M, X)} \frac{\rho_0(d; M, X)}{\pi_0(d; X)} \right\} \right] \]

\[ = \mathbb{E}\left[ \gamma(d', M, X) \left\{ \frac{E(\mathbb{I}_{D=d}|M, X)}{\pi_0(d; X)} - \frac{E(\mathbb{I}_{D=d'}|M, X)}{\rho_0(d'; M, X)} \frac{\rho_0(d; M, X)}{\pi_0(d; X)} \right\} \right] \]

\[ = \mathbb{E}\left[ \gamma(d', M, X) \left\{ \frac{\rho_0(d; M, X)}{\pi_0(d; X)} - \frac{\rho_0(d'; M, X)}{\rho_0(d'; M, X) \pi_0(d; X)} \right\} \right] \]

\[ = 0. \]

(c) Third, write

\[ \mathbb{E}[\alpha(W)\{Y - \delta_0(W)\}] \]

\[ = \mathbb{E}\left[ \frac{1}{\rho(d'; M, X)} \frac{\rho(d; M, X)}{\pi(d; X)} \{Y - \gamma_0(d', M, X)\} \right] \]

\[ = \mathbb{E}\left[ \frac{\mathbb{I}_{D=d'}}{\rho(d'; M, X)} \frac{\rho(d; M, X)}{\pi(d; X)} \{\gamma_0(D, M, X) - \gamma_0(d', M, X)\} \right] \]

\[ = \mathbb{E}\left( \frac{1}{\rho(d'; M, X)} \frac{\rho(d; M, X)}{\pi(d; X)} \mathbb{E}[\mathbb{I}_{D=d'} \{\gamma_0(D, M, X) - \gamma_0(d', M, X)\} | M, X] \right). \]

Focusing on the inner expectation,

\[ \mathbb{E}[\mathbb{I}_{D=d'} \{\gamma_0(D, M, X) - \gamma_0(d', M, X)\} | M, X] \]

\[ = \mathbb{E}[\mathbb{I}_{D=d'} \{\gamma_0(D, M, X) - \gamma_0(d', M, X)\} | D = d', M, X] \mathbb{P}(D = d'|M, X) \]

\[ = \mathbb{E}[\{\gamma_0(d', M, X) - \gamma_0(d', M, X)\} | D = d', M, X] \mathbb{P}(D = d'|M, X) \]

\[ = 0. \]
(d) Finally, write
\[
\mathbb{E}[\eta(W)\{\delta_0(W) - \nu_0(W)\}] = \mathbb{E}\left[\frac{1}{\pi(d; X)} \{\gamma_0(d', M, X) - \omega_0(d, d'; X)\}\right] = \mathbb{E}\left(\frac{1}{\pi(d; X)} \mathbb{E}[\mathbb{I}_{D=d}\{\gamma_0(d', M, X) - \omega_0(d, d'; X)\}|X]\right).
\]

Focusing on the inner expectation,
\[
\mathbb{E}[\mathbb{I}_{D=d}\{\gamma_0(d', M, X) - \omega_0(d, d'; X)\}|X] = \mathbb{E}[\mathbb{I}_{D=d}\{\gamma_0(d', M, X) - \omega_0(d, d'; X)\}|D = d, X]\mathbb{P}(d|X) = \mathbb{E}[\{\gamma_0(d', M, X) - \omega_0(d, d'; X)\}|D = d, X]\mathbb{P}(d|X) = 0.
\]

2. Bounded residual variances holds since \(Y\) is bounded.

3. Bounded balancing weights is immediate from the assumption of bounded propensity scores.

4. Censored balancing weight estimators is immediate from the assumption of censored propensity score estimators.

5. Regularity on moments holds by hypothesis.

6. Individual rate conditions. After bounding various quantities by constants, the rate conditions simplify as
   \[
   \{\mathcal{R}(\hat{\nu}_\ell)\}^{1/2} \to 0. \text{ By Proposition 4, } \{\mathcal{R}(\hat{\nu}_\ell)\}^{1/2} \leq \gamma_{ME}(n, b, c, b_1, c_1).
   \]
   \[
   \{\mathcal{R}(\hat{\delta}_\ell)\}^{1/2} \to 0. \text{ Write } \mathcal{R}(\hat{\delta}_\ell) = \mathbb{E}[\{\delta(W) - \delta_0(W)\}^2] = \mathbb{E}[\{\gamma(d', M, X) - \gamma_0(d', M, X)\}^2] = \mathbb{E}\left[\frac{\mathbb{I}_{D=d'}}{\rho_0(d'; M, X)}\{\gamma(D, M, X) - \gamma_0(D, M, X)\}^2\right] \leq C\mathbb{E}[\{\gamma(D, M, X) - \gamma_0(D, M, X)\}^2] = C\mathcal{R}(\gamma).
   \]

Using this result and Lemma 8, \(\{\mathcal{R}(\hat{\delta}_\ell)\}^{1/2} \leq C\{\mathcal{R}(\hat{\gamma}_\ell)\}^{1/2} \leq \gamma_{ME}(n, b, c)\).
(c) \( \{\mathcal{R}(\hat{\alpha})\}\)^{1/2} \to 0. Write

\[
\mathcal{R}(\alpha) = \mathbb{E}[\{\alpha(W) - \alpha_0(W)\}^2] = \mathbb{E} \left[ \left\{ \frac{1_{D=d'}}{\rho(d'; M, X)} - \frac{1_{D=d}}{\rho_0(d'; M, X)} \right\}^2 \right] \leq C \mathbb{E} \left[ \{\rho(d; M, X)\rho_0(d'; M, X)\pi_0(d; X) - \rho_0(d; M, X)\rho(d'; M, X)\pi(d; X)\}^2 \right].
\]

Focusing on the RHS, and using natural abbreviations

\[
\rho_0'\pi_0 - \rho_0\rho'\pi = \rho\rho_0'\pi_0 \pm \rho_0\rho_0'\pi_0 - \rho_0\rho'\pi = (\rho - \rho_0)\rho_0'\pi_0 + \rho_0(\rho' - \rho)\pi_0 + \rho_0\rho(\pi_0 - \pi).
\]

Therefore by triangle inequality,

\[
\mathcal{R}(\alpha) \leq C \mathbb{E} \left[ \{\rho(d; M, X) - \rho_0(d; M, X)\}^2 \right] + C \mathbb{E} \left[ \{\rho(d'; M, X) - \rho_0(d'; M, X)\}^2 \right] + C \mathbb{E} \left[ \{\pi(d; X) - \pi_0(d; X)\}^2 \right] = C \{\mathcal{R}(\rho) + \mathcal{R}(\pi)\}.
\]

Using this result and Lemma 8, \( \{\mathcal{R}(\hat{\eta})\}\)^{1/2} \leq C \{\mathcal{R}(\hat{\pi}) + \mathcal{R}(\hat{\rho})\}^{1/2} \leq s^{ME}_\pi(n, b_2, c_2) + s^{ME}_\rho(n, b_3, c_3).

(d) \( \{\mathcal{R}(\hat{\eta})\}\)^{1/2} \to 0. Write

\[
\mathcal{R}(\eta) = \mathbb{E}[\{\eta(W) - \eta_0(W)\}^2] = \mathbb{E} \left[ \left\{ \frac{1_{D=d}}{\pi(d; X)} - \frac{1_{D=d}}{\pi_0(d; X)} \right\}^2 \right] \leq C \mathbb{E} \left[ \{\pi_0(d; X) - \pi(d; X)\}^2 \right] = C \mathcal{R}(\pi).
\]

Using this result and Lemma 8, \( \{\mathcal{R}(\hat{\eta})\}\)^{1/2} \leq C \{\mathcal{R}(\hat{\pi})\}^{1/2} \leq s^{ME}_\pi(n, b_2, c_2).

7. Product rate conditions. After bounding various quantities by constants, the rate conditions simplify as
(a) \( \{ n\mathcal{R}(\hat{\nu}_t)\mathcal{R}(\hat{\eta}_t) \}^{1/2} \to 0 \). As in the argument for individual rate conditions,

\[
\{ n\mathcal{R}(\hat{\nu}_t)\mathcal{R}(\hat{\eta}_t) \}^{1/2} \leq n^{1/2}\omega(t) \leq n^{1/2} ME(n, b, c, b_1, c_1) s_{\pi}^M (n, b_2, c_2)
\]

\[
= n^{1/2} \left( n^{-\frac{1}{2}} \frac{c_1 - 1}{c_1 + 1/b_1} + n^{-\frac{1}{2}} \frac{c_2 - 1}{c_2 + 1/b_2} \right) n^{-\frac{1}{2}} \frac{c_2}{c_2 + 1/b_2} .
\]

A sufficient condition is that

\[
1 - \frac{c - 1}{c + 1/b} - \frac{c_2}{c_2 + 1/b_2} > 0, \quad 1 - \frac{c_1 - 1}{c_1 + 1/b} - \frac{c_2}{c_2 + 1/b_2} > 0,
\]

i.e.

\[
\min \left( \frac{c - 1}{c + 1/b}, \frac{c_1 - 1}{c_1 + 1/b_1} \right) + \frac{c_2}{c_2 + 1/b_2} > 1.
\]

(b) \( \{ n\mathcal{R}(\hat{\delta}_t)\mathcal{R}(\hat{\alpha}_t) \}^{1/2} \to 0 \). As in the argument for individual rate conditions,

\[
\{ n\mathcal{R}(\hat{\delta}_t)\mathcal{R}(\hat{\alpha}_t) \}^{1/2} \leq n^{1/2} s_{\gamma}^M (n, b, c) \{ s_{\pi}^M (n, b_2, c_2) + s_{\rho}^M (n, b_3, c_3) \}
\]

\[
= n^{1/2} n^{-\frac{1}{2}} \frac{c_2 - 1}{c_2 + 1/b_2} + n^{-\frac{1}{2}} \frac{c_3 - 1}{c_3 + 1/b_3} .
\]

A sufficient condition is that

\[
1 - \frac{c_2}{c_2 + 1/b_2} > 0, \quad 1 - \frac{c_3}{c_3 + 1/b_3} > 0,
\]

i.e.

\[
\min \left( \frac{c_2}{c_2 + 1/b_2}, \frac{c_3}{c_3 + 1/b_3} \right) + \frac{c}{c + 1/b} > 1.
\]

Since we have assumed bounded kernels, \( b, b_2, b_3 \geq 1 \). By correct specification, \( c, c_2, c_3 \geq 1 \). Finally, we have already assumed \( c > 1 \). These conditions imply the desired inequality.

(c) \( \{ n\mathcal{R}(\hat{\delta}_t)\mathcal{R}(\hat{\eta}_t) \}^{1/2} \to 0 \). As in the argument for individual rate conditions,

\[
\{ n\mathcal{R}(\hat{\delta}_t)\mathcal{R}(\hat{\eta}_t) \}^{1/2} \leq n^{1/2} s_{\gamma}^M (n, b, c) s_{\pi}^M (n, b_2, c_2),
\]

which is dominated by the previous product rate condition.
G.3.2 Dynamic treatment effects

Recall
\[ \gamma_0(d_1, d_2, x_1, x_2) = \mathbb{E}(Y|D_1 = d_1, D_2 = d_2, X_1 = x_1, X_2 = x_2), \]
\[ \omega_0(d_1, d_2; x_1) = \int \gamma_0(d_1, d_2, x_1, x_2) d\mathbb{P}(x_2|d_1, x_1), \]
\[ \pi_0(d_1; x_1) = \mathbb{P}(D_1 = d_1|X_1 = x_1), \]
\[ \rho_0(d_2; d_1, x_1, x_2) = \mathbb{P}(D_2 = d_2|D_1 = d_1, X_1 = x_1, X_2 = x_2) d\mathbb{P}(x_2|d_1, x_1). \]

Fix \((d_1, d_2)\). Matching symbols with the abstract Gaussian approximation,
\[ \delta_0(W) = \gamma_0(d_1, d_2, X_1, X_2), \]
\[ \nu_0(W) = \int \gamma_0(d_1, d_2, X_1, x_2) d\mathbb{P}(x_2|d_1, X_1) = \omega_0(d_1, d_2; X_1) \]
\[ \alpha_0(W) = \frac{1_{D_1 = d_1}}{\pi_0(d_1; X_1)} \frac{1_{D_2 = d_2}}{\rho_0(d_2; d_1, X_1, X_2)} \]
\[ \eta_0(W) = \frac{1_{D_1 = d_1}}{\pi_0(d_1; X_1)} \]

Proof of Theorem 8 We proceed in steps, verifying the conditions of Lemma 9

1. Neyman orthogonal moment function follows from [Singh, 2021b, Proposition 4.1].
2. Bounded residual variances holds since \(Y\) is bounded.
3. Bounded balancing weights is immediate from the assumption of bounded propensity scores.
4. Censored balancing weight estimators is immediate from the assumption of censored propensity score estimators.
5. Regularity on moments holds by hypothesis.
6. Individual rate conditions. After bounding various quantities by constants, the rate conditions simplify as
   \[ (a) \ \{R(\hat{\nu}_\ell)\}^{1/2} \to 0. \] By Proposition 4 \( \{R(\hat{\nu}_\ell)\}^{1/2} \leq s_\omega^{GF}(n, b, c_4, c_4) \).
   \[ (b) \ \{R(\hat{\delta}_\ell)\}^{1/2} \to 0. \] By [Singh, 2021b, Proposition 6.2] and Lemma 8 \( \{R(\hat{\delta}_\ell)\}^{1/2} \leq C\{R(\hat{\gamma}_\ell)\}^{1/2} \leq s_\gamma^{GF}(n, b, c). \)
7. Product rate conditions. After bounding various quantities by constants, the rate conditions simplify as

(a) \( \{n \mathcal{R}(\hat{v}_\ell) \mathcal{R}(\hat{\eta}_\ell)\}^{1/2} \to 0 \). As in the argument for individual rate conditions,

\[
\{n \mathcal{R}(\hat{v}_\ell) \mathcal{R}(\hat{\eta}_\ell)\}^{1/2} \leq n^{1/2} s^{GF}_\omega(n, b, c, d, e) s^{GF}_\pi(n, b, c) + \mathcal{R}(\hat{\rho}_\ell) \]

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

A sufficient condition is that

\[ 1 - \frac{c - 1}{c + 1/b} - \frac{c_6}{c_6 + 1/b_6} > 0, \quad 1 - \frac{c_4 - 1}{c_4 + 1/b} - \frac{c_6}{c_6 + 1/b_6} > 0, \]

i.e.

\[ \min \left( \frac{c - 1}{c + 1/b}, \frac{c_4 - 1}{c_4 + 1/b}, \frac{c_6}{c_6 + 1/b_6} \right) > 1. \]

(b) \( \{n \mathcal{R}(\hat{\delta}_\ell) \mathcal{R}(\hat{\eta}_\ell)\}^{1/2} \to 0 \). As in the argument for individual rate conditions,

\[
\{n \mathcal{R}(\hat{\delta}_\ell) \mathcal{R}(\hat{\eta}_\ell)\}^{1/2} \leq n^{1/2} s^{GF}_\omega(n, b, c) \{s^{GF}_\pi(n, b, c) + s^{GF}_\rho(n, b, c)\}
\]

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

A sufficient condition is that

\[ 1 - \frac{c}{c + 1/b} - \frac{c_6}{c_6 + 1/b_6} > 0, \quad 1 - \frac{c}{c + 1/b} - \frac{c_7}{c_7 + 1/b_7} > 0, \]

i.e.

\[ \min \left( \frac{c_6}{c_6 + 1/b_6}, \frac{c_7}{c_7 + 1/b_7} \right) + \frac{c}{c + 1/b} > 1. \]

Since we have assumed bounded kernels, \( (b, b_6, b_7) \geq 1 \). By correct specification, \( (c, c_6, c_7) \geq 1 \). Finally, we have already assumed \( c > 1 \). These conditions imply the desired inequality.

(c) \( \{n \mathcal{R}(\hat{\delta}_\ell) \mathcal{R}(\hat{\eta}_\ell)\}^{1/2} \to 0 \). As in the argument for individual rate conditions,

\[
\{n \mathcal{R}(\hat{\delta}_\ell) \mathcal{R}(\hat{\eta}_\ell)\}^{1/2} \leq n^{1/2} s^{GF}_\omega(n, b, c) s^{GF}_\pi(n, b, c),
\]

which is dominated by the previous product rate condition.
H Tuning

In this appendix, we present tuning procedures for the ridge regularization and kernel hyperparameters.

H.1 Simplified setting

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

H.2 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 a closed form solutions. The latter is asymptotically optimal in the $L^2$ sense [Craven and Wahba, 1978, Li, 1986]. In our main results, we require theoretical regularization that is optimal for both $L^2$ norm and RKHS norm. As such, GCV should lead to the theoretically required regularization for both nonparametric consistency and semiparametric inference. In practice, LOOCV and GCV lead to nearly identical tuning.

Algorithm 11 (Ridge penalty tuning by LOOCV; Algorithm 5 of [Singh et al., 2020]). Construct the matrices

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

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

$$\lambda^* = \arg\min_{\lambda \in \Lambda} \frac{1}{n} \|\tilde{H}_\lambda^{-1}H_\lambda Y\|_2^2, \quad \Lambda \subset \mathbb{R}.$$
Algorithm 12 (Ridge penalty tuning by GCV; Algorithm 6 of [Singh et al., 2020]). Construct the matrix
\[ H_\lambda := I - K_{WW}(K_{WW} + n\lambda I)^{-1} \in \mathbb{R}^{n \times n}. \]
Then set
\[ \lambda^* = \arg\min_{\lambda \in \Lambda} \frac{1}{n} \| \{\text{Tr}(H_\lambda)\}^{-1} \cdot H_\lambda Y \|_2^2, \quad \Lambda \subset \mathbb{R}. \]

H.3 Kernel

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

[Rasmussen and Williams, 2006, Section 4.3] characterize the exponentiated quadratic RKHS as an attenuated series of the form
\[ \mathcal{H} = \left( f = \sum_{j=1}^{\infty} f_j \varphi_j : \sum_{j=1}^{\infty} \frac{f_j^2}{\eta_j} < \infty \right), \quad \langle f, g \rangle_{\mathcal{H}} = \sum_{j=1}^{\infty} \frac{f_j g_j}{\eta_j}. \]
For simplicity, take \( W = \mathbb{R} \) and take the measure \( \nu \) to be the standard Gaussian distribution (more generally, it can be the population distribution \( \mathbb{P} \)). A generalization of Mercer’s Theorem permits \( W \) to be separable. Then the induced RKHS is characterized by
\[ \eta_j = \sqrt{\frac{2a}{A}} B^j, \quad \varphi_j(w) = \exp\{-(c-a)w^2\} H_j(w\sqrt{2c}), \]
where \( H_j \) is the \( j \)-th Hermite polynomial, and the constants \( (a, b, c, A, B) > 0 \) are
\[ a = \frac{1}{4}, \quad b = \frac{1}{2\iota^2}, \quad c = \sqrt{a^2 + 2ab}, \quad A = a + b + c, \quad B = \frac{b}{A} < 1. \]
In summary, 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.

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 \( (W_i)_{i=1}^n \), 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

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

Each lengthscale $\nu_j$ is set according to the median interpoint distance for that input dimension.

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

I Simulation details

In this appendix, we provide additional details for various simulations: mediated response curves, mediated effects, dynamic response curves, and dynamic effects.

I.1 Nonparametric mediated response

A single observation consists of the tuple $(Y, D, M, X)$ for outcome, treatment, mediator, and covariates where $Y, D, M, X \in \mathbb{R}$. A single observation is generated is as follows. Draw unobserved noise as $u, v, w \overset{	ext{i.i.d.}}{\sim} \mathcal{U}(-2, 2)$. Draw the covariate as $X \sim \mathcal{U}(-1.5, 1.5)$. Then set

$$D = 0.3X + w,$$
$$M = 0.3D + 0.3X + v,$$
$$Y = 0.3D + 0.3M + 0.5DM + 0.3X + 0.25D^3 + u.$$ 

Note that [Huber et al., 2020] also present a simpler version of this design.

We implement our nonparametric estimator $\hat{\theta}^{ME}(d, d')$ (RKHS) described in Section 3 with the tuning procedure described in Appendix H. 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 \cite{Huber2020} (IPW) using the default settings of the command \texttt{medweightcont} in the R package \texttt{causalweight}.

### I.2 Semiparametric mediated effect

A single observation consists of the tuple $(Y, D, M, X)$ for outcome, treatment, mediator, and covariates where $Y, M, X \in \mathbb{R}$ and $D \in \{0, 1\}$. A single observation is generated is as follows. Draw unobserved noise as $u, v, w \overset{i.i.d.}\sim \mathcal{U}(-2, 2)$. Draw the covariate as $X \sim \mathcal{U}(-1.5, 1.5)$. Then set

\begin{align*}
D &= 1(0.3X + w > 0), \\
M &= 0.3D + 0.3X + v, \\
Y &= 0.3D + 0.3M + 0.5DM + 0.3X + 0.25D^3 + u.
\end{align*}

Note that

\begin{align*}
\mathbb{E}\{M(d)\} &= 0.3d, \\
\mathbb{E}[Y^{(d'),M(d)}] &= 0.55d' + 0.09d + 0.15d'd.
\end{align*}

Hence \{\theta_{ME}^{0}(0, 0), \theta_{ME}^{0}(1, 0), \theta_{ME}^{0}(0, 1), \theta_{ME}^{0}(1, 1)\} = (0, 0.09, 0.55, 0.79).

We implement our semiparametric estimator $\hat{\theta}_{ME}(d, d')$ (RKHS) described in Section 3 with $L = 5$ folds and the tuning procedure described in Appendix H. Specifically, we use ridge penalties determined by leave-one-out cross validation. For continuous variables, we use product exponentiated quadratic kernel with lengthscales set by the median heuristic. For discrete variables, we use the indicator kernel.
Table 4: Semiparametric mediated effect coverage simulations

| Sample size | Mean  | S.E.  | Coverage |
|-------------|-------|-------|----------|
| 500         | 0.004 | 0.008 | 94%      |
| 1000        | 0.000 | 0.005 | 97%      |
| 5000        | 0.000 | 0.002 | 99%      |

| Sample size | Mean  | S.E.  | Coverage |
|-------------|-------|-------|----------|
| 500         | 0.077 | 0.011 | 98%      |
| 1000        | 0.085 | 0.007 | 98%      |
| 5000        | 0.083 | 0.002 | 98%      |

| Sample size | Mean  | S.E.  | Coverage |
|-------------|-------|-------|----------|
| 500         | 0.575 | 0.013 | 93%      |
| 1000        | 0.583 | 0.009 | 93%      |
| 5000        | 0.571 | 0.003 | 87%      |

| Sample size | Mean  | S.E.  | Coverage |
|-------------|-------|-------|----------|
| 500         | 0.792 | 0.010 | 94%      |
| 1000        | 0.796 | 0.007 | 96%      |
| 5000        | 0.793 | 0.003 | 99%      |

I.3 Nonparametric dynamic response

This design extends the one-stage dose response design of [Colangelo and Lee, 2020] to a multistage setting. Set the number of periods to be $T = 2$. A single observation consists of the tuple $(Y, D_{1:2}, X_{1:2})$ for outcome, treatments, and covariates. $Y, D_t \in \mathbb{R}$ and $X_t \in \mathbb{R}^p$.

A single observation is generated as follows. Draw unobserved noise as $\epsilon_t \sim \mathcal{N}(0, 1)$.

Define the vector $\beta \in \mathbb{R}^p$ by $\beta_j = j^{-2}$. Define the matrix $\Sigma \in \mathbb{R}^{p \times p}$ such that $\Sigma_{ii} = 1$ and $\Sigma_{ij} = \frac{1}{2} \cdot 1\{|i - j| = 1\}$ for $i \neq j$. Then draw $W_t \sim \mathcal{N}(0, \Sigma)$ and set

\begin{align*}
X_1 &= W_1, \\
D_1 &= \Lambda(X_1^T \beta) + 0.75 \nu_1, \\
X_2 &= 0.5(1 - D_1)X_1 + 0.5W_2, \\
D_2 &= \Lambda(0.5X_1^T \beta + X_2^T \beta - 0.2D_1) + 0.75 \nu_2, \\
Y &= 0.5\{1.2D_1 + 1.2X_1^T \beta + D_1^2 + D_1(X_1)\} + \{1.2D_2 + 1.2X_2^T \beta + D_2^2 + D_2(X_2)\} + \epsilon,
\end{align*}

where we use the truncated logistic link function

\[ \Lambda(t) = (0.9 - 0.1) \frac{\exp(t)}{1 + \exp(t)} + 0.1. \]
It follows that \( \theta^{GF}_0(d_1, d_2) = 0.6d_1 + 0.5d_1^2 + 1.2d_2 + d_2^2 \).

Clinical intuition guides simulation design. At \( t = 1 \), the patient experiences correlated symptoms \( X_1 \). Based on the symptom index \( X_1^\top \beta \) as well as unobserved considerations \( \nu_1 \), the doctor administers the first dose \( D_1 \). At \( t = 2 \), the patient experiences new symptoms \( X_2 \) which are the average of attenuated original symptoms \( (1 - D_1)X_1 \) and new developments \( W_2 \). The first dose \( D_1 \) has an expectation between zero and one, so a higher dose tends to attenuate original symptoms \( X_1 \) more. The doctor administers a second dose \( D_2 \) based on the initial symptom index \( X_1^\top \beta \), the new symptom index \( X_2^\top \beta \), the initial dose \( D_1 \), and unobserved considerations \( \nu_2 \). The patient’s health outcome \( Y \) depends on the history of symptoms \( X_{1:2} \) and treatments \( D_{1:2} \) as well as chance \( \epsilon \). Specifically, the health outcome depends on treatment levels quadratically, symptom indices linearly, and an interaction between treatment level and the primary symptom linearly. More weight is given to the recent history.

![Figure 4: Nonparametric dynamic response simulations](image)

We implement our nonparametric estimator \( \hat{\theta}^{GF}_0(d_1, d_2) \) \{RKHS(GF)\} described in Section 4 with the tuning procedure described in Appendix H. 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 use the same tuning procedures when implementing the one-stage dose response \{RKHS(ATE)\} and heterogeneous dose response \{RKHS(CATE)\} estimators of [Singh et al., 2020]. Finally, we implement the estimator of [Lewis and Syrgkanis, 2020] (SNMM) using the flexible heterogeneous setting in Python code shared by the authors, though their algorithm is designed for linear Markov models without effect modification.
Figure 4 presents results for different choices of $p = \text{dim}(X_t) \in \{1, 10, 100\}$, corresponding to low, moderate, and high dimensional settings. Across choices of $\text{dim}(X_t)$, RKHS(GF) significantly outperforms alternatives at sample size 5000. In particular, RKHS(GF) outperforms SNMM with p-value < 0.001 by the Wilcoxon rank sum test for $\text{dim}(X_t) \in \{1, 10, 100\}$.

I.4 Semiparametric dynamic treatment effect

A single observation consists of the tuple $(Y, D_{1:2}, X_{1:2})$ for outcome, treatments, and covariates. $Y \in \mathbb{R}$, $D_t \in \{0, 1\}$, and $X_t \in \mathbb{R}^p$. A single observation is generated as follows. Draw unobserved noise as $\epsilon_t \sim \mathcal{N}(0, 1)$. Define the vector $\beta \in \mathbb{R}^p$ by $\beta_j = j - 2$. Define the matrix $\Sigma \in \mathbb{R}^{p \times p}$ such that $\Sigma_{ii} = 1$ and $\Sigma_{ij} = \frac{1}{2} \cdot 1\{|i - j| = 1\}$ for $i \neq j$. Then draw $W_t \sim \mathcal{N}(0, \Sigma)$ and set

\[
X_1 = W_1, \\
D_1 \sim \text{Bernoulli}\left\{\Lambda(X_1^\top \beta)\right\}, \\
X_2 = 0.5(1 - D_1)X_1 + 0.5W_2, \\
D_2 \sim \text{Bernoulli}\left\{\Lambda(0.5X_1^\top \beta + X_2^\top \beta - 0.2D_1)\right\}, \\
Y = 0.5\{1.2D_1 + 1.2X_1^\top \beta + D_2^2 + D_1(X_1)\} + \{1.2D_2 + 1.2X_2^\top \beta + D_2^2 + D_2(X_2)\} \\
\quad + 0.5D_1D_2 + \epsilon,
\]

where we use the truncated logistic link function $\Lambda(t) = (0.9 - 0.1) \frac{\exp(t)}{1 + \exp(t)} + 0.1$.

Note that

\[
\mathbb{E}\{Y^{(d_1, d_2)}\} = 0.5(1.2d_1 + d_1) + (1.2d_2 + d_2) + 0.5d_1d_2 = 1.1d_1 + 2.2d_2 + 0.5d_1d_2.
\]

Hence $\{\theta^{GF}_0(0, 0), \theta^{GF}_0(1, 0), \theta^{GF}_0(0, 1), \theta^{GF}_0(1, 1)\} = (0, 1.1, 2.2, 3.8)$.

We implement our semiparametric estimator $\hat{\theta}^{GF}(d_1, d_2) \{\text{RKHS(GF)}\}$ described in Section 8, with $L = 5$ folds and the tuning procedure described in Appendix III. Specifically, we use ridge penalties determined by leave-one-out cross validation. For continuous variables, we use product exponentiated quadratic kernel with lengthscales set by the median heuristic. For discrete variables, we use the indicator kernel.
Table 5: Semiparametric dynamic treatment effect coverage simulations

| Sample size | Mean   | S.E.  | Coverage |
|-------------|--------|-------|----------|
| 500         | 0.079  | 0.048 | 95%      |
| 1000        | 0.034  | 0.029 | 96%      |
| 5000        | 0.013  | 0.007 | 98%      |

J Application details

In this appendix, we provide implementation details and robustness checks for our real world program evaluation.

J.1 Mediation analysis

We implement our nonparametric estimator \( \hat{\theta}^{ME}(d, d') \) described in Section 3. We use the tuning procedure described in Appendix H. Specifically, we use ridge penalties determined by leave-one-out cross validation. For continuous variables, we use product exponentiated quadratic kernel with lengthscales set by the median heuristic. For discrete variables, we use the indicator kernel. We use the covariates \( X \in \mathbb{R}^{40} \) of [Colangelo and Lee, 2020].

In the main text, we focus on the \( n = 2,913 \) observations for which \( D \geq 40 \) and \( M > 0 \), i.e. individuals who completed at least one week of training and who found employment. This choice follows [Colangelo and Lee, 2020, Singh et al., 2020]. We now verify that our results are robust to the choice of sample. Specifically, we consider the \( n = 3,906 \) observations with \( D \geq 40 \).
For each sample, we visualize class-hours $D$ with a histogram in Figure 5. The class-hour distribution in the sample with $D \geq 40$ is similar to the class-hour distribution in the sample with $D \geq 40$ and $M > 0$ that we use in the main text.

![Histograms of class-hours](image)

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

Figure 5: Class-hours for different samples

Next, we estimate total, direct, and indirect responses for the new sample choice. Figure 6 visualizes results. For the sample with $D \geq 40$, the mediated responses are essentially identical to the mediated responses of the sample with $D \geq 40$ and $M > 0$ presented in the main text. These results confirm the robustness of the results we present in the main text.

![Dose response surfaces](image)

(a) Total response  
(b) Direct response  
(c) Indirect response

Figure 6: Total, direct, and indirect dose responses of job training on arrests: $D \geq 40$

### J.2 Dynamic responses

We implement our nonparametric estimators $\hat{\theta}_{GF}(d_1, d_2)$ and $\theta^*_{GF, V}(d_1, d_2)$ described in Section 4 as well as our semiparametric estimator $\hat{\theta}_{GF}(d_1, d_2)$ described in Section 4. We
use the tuning procedure described in Appendix H. Specifically, we use ridge penalties
determined by leave-one-out cross validation. For continuous variables, we use product
exponentiated quadratic kernel with lengthscales set by the median heuristic. For discrete
variables, we use the indicator kernel. For the semiparametric case, we truncate extreme
propensity scores to lie in the interval $[0.05, 0.95]$ consistent with Assumption 10.

We extract relevant covariates $X_1 \in \mathbb{R}^{65}$ from the baseline survey and $X_2 \in \mathbb{R}^{30}$ from the
one year follow-up interview raw files provided by [Schochet et al., 2008, Section III.A]. The
covariates $X_1$ are a superset of the $X \in \mathbb{R}^{40}$ chosen by [Colangelo and Lee, 2020], and they
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. We enlarge the set of covariates to include additional variables that may
vary from one year to the next, e.g. extra variables concerning health and health related
behavior. When a variable never varies over time, e.g. race, we include it in $X_1$ but not $X_2$
so as not to clash with the characteristic property in our RKHS approach. The follow up
interview was also less extensive than the baseline interview. These two reasons explain
why $X_1 \in \mathbb{R}^{65}$ yet $X_2 \in \mathbb{R}^{30}$.

In the main text, we focus on the $n = 3,141$ observations for which $D_1 + D_2 \geq 40$
and $Y > 0$, i.e. individuals who completed at least one week of training and who found
employment. This choice generalizes our previous rule. We now verify that our results are
robust to the choice of sample. Specifically, we consider the $n = 3,710$ observations with
$D_1 + D_2 \geq 40$.

For each sample, we visualize total class-hours $D_1 + D_2$ with a histogram in Figure 7.
The class-hour distribution in the sample with $D_1 + D_2 \geq 40$ is similar to the class-hour
distribution in the sample with $D_1 + D_2 \geq 40$ and $Y > 0$ that we use in the main text.
Next, we estimate dynamic responses for the new sample choice. Figure 8 visualizes results. For the sample with $D_1 + D_2 \geq 40$, the dynamic responses are similar to the dynamic responses of the sample with $D_1 + D_2 \geq 40$ and $Y > 0$ presented in the main text, albeit with a lower plateau and overall lower levels of counterfactual employment. These results confirm the robustness of the results we present in the main text.

Figure 7: Class-hours for different samples

(a) $D_1 + D_2 \geq 40$ and $Y > 0$

(b) $D_1 + D_2 \geq 40$

Figure 8: Dynamic and incremental response of job training on employment: $D_1 + D_2 \geq 40$

(a) Dynamic response

(b) Incremental response