

TRANSFER ESTIMATES FOR CAUSAL EFFECTS ACROSS HETEROGENEOUS SITES

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ABSTRACT. We consider the problem of extrapolating treatment effects across heterogeneous populations (“sites”/“contexts”). We consider an idealized scenario in which the researcher observes cross-sectional data for a large number of units across several “experimental” sites in which an intervention has already been implemented to a new “target” site for which a baseline survey of unit-specific, pre-treatment outcomes and relevant attributes is available. Our approach treats the baseline as functional data, and this choice is motivated by the observation that unobserved site-specific confounders manifest themselves not only in average levels of outcomes, but also how these interact with observed unit-specific attributes. We consider the problem of determining the optimal finite-dimensional feature space in which to solve that prediction problem. Our approach is design-based in the sense that the performance of the predictor is evaluated given the specific, finite selection of experimental and target sites. Our approach is nonparametric, and our formal results concern the construction of an optimal basis of predictors as well as convergence rates for the estimated conditional average treatment effect relative to the constrained-optimal population predictor for the target site. We quantify the potential gains from adapting experimental estimates to a target location in an application to conditional cash transfer (CCT) programs using a combined data set from five multi-site randomized controlled trials.

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1. INTRODUCTION

When scaling up an intervention or planning an implementation at a new location, it is often necessary to extrapolate experimental evidence to new sites or contexts, knowing that average causal effects are likely heterogeneous across sites. We consider a problem in which cross-sectional information on outcomes and covariates is available for both experimental

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and target sites, and we formalize a process of predicting a causal response that uses pre-intervention (baseline) outcome data from the target location to obtain a forecast that is responsive to site-specific heterogeneity. The underlying premise of such an approach is that the data-generating processes for potential outcomes for pre- and post-intervention outcomes are likely similar, and depend on the same unit- and site specific factors, so that baseline outcomes are in fact predictive for treatment effects. Such an assumption may be particularly plausible when the effect of the intervention is expected to be only incremental rather than fundamentally altering the relationship between unit or site characteristics and the outcome of interest.

In principle, the relevant baseline information for a given site consists of the full conditional distribution of pre-intervention outcomes given unit covariates, that is we view the baseline as functional data. This choice is motivated by the observation that unobserved site-specific confounders may generally manifest themselves not only in average levels of outcomes, but also how these interact with observed unit-specific attributes. However, in most practically relevant settings, the number of observed sites is not large, forcing the researcher to make pragmatic decisions on how flexibly to model the observable data.¹ The corresponding problem of predicting conditional average treatment effects from baseline outcome data can be viewed as functional regression where a realistic implementation can at best achieve a highly regularized solution. Moreover these data constraints also make it all the more important to choose a procedure that makes statistically efficient use of the available data.

Our approach corresponds to a finite-dimensional approximation to that problem, where we determine the optimal feature space in which to solve a linear version of the prediction problem. In our leading application, cross-validation suggests that the optimal number of features for prediction is $K = 2$. Compared to alternative regularization schemes, one advantage of this particular approach is interpretability, where the resulting transfer estimate is the best linear predictor given those constructed site-specific features. Furthermore, the proposed approximation is chosen optimally for prediction of conditional average treatment effects. We can furthermore assess whether there exist sites in the experimental population that are similar to a target location in terms of these site characteristics that were determined to be most predictive of conditional average treatment effects. Similar techniques could in principle be developed to predict conditional treatment effects for sites within the experimental sample when treatment assignment was randomized at the site level.

Conditioning on baseline data requires the definition of a joint distribution for pre- and post-intervention outcomes across sites. We choose a design-based approach that regards

¹Allcott (2015) considers a setting in which a policy was initially evaluated at 10 sites and eventually scaled up to 111 separate sites. Dehejia, Pop-Eleches, and Samii (2021) use 142 year/country samples from 61 different countries. The PROGRESA study of conditional cash transfers in Mexico was initially conducted in 506 rural communities across 7 states in Mexico (see Todd and Wolpin (2006)). Meager (2022) aggregates across seven different RCTs for micro-credit interventions published in 2015.

the combined (finite) population of experimental and target sites as fixed, but assumes that the number of cross-sectional units within each cluster is large. Statistical properties of extrapolation estimators are then evaluated under a randomization protocol that assigns experimental versus target status at random among those clusters. In analogy with the literature on conformal prediction, the constructed statistical experiment treats experimental and target locations as finitely exchangeable. We do not necessarily regard this assignment mechanism as factually accurate - e.g. the observed assignment may likely exhibit site-selection effects of the kind documented by Allcott (2015). Rather, this data generating process can alternatively be viewed a device to define a pseudo-true treatment parameter that incorporates the available information on average effects and between cluster heterogeneity. A transfer estimate of this kind would summarize the relevant evidence from the available experimental data and could be subject to additional (qualitative or quantitative) sensitivity analysis with respect to potential violations of the exchangeability assumption.

Notice also that rather than imposing strong assumptions necessary for identification of counterfactuals in a target location, our focus is on prediction. That said, in Section 2.3 we also discuss some conditions under which the bias from linear interpolation vanishes, in which case the predictor could be interpreted as asymptotically unbiased estimator for a version of the problem in which sites are drawn at random from an infinite superpopulation.

The empirical application in this paper concerns the effect of conditional cash transfers (CCT) to households on children’s school attendance. The effect of CCTs was first evaluated in a large multi-site trial of the PROGRESA/OPORTUNIDADES program in Mexico, which was followed by implementations and additional RCTs in many developing and middle-income countries, often modeled after the PROGRESA study. After applying selection criteria we construct a data set of 640 sites, combining data from five studies in Mexico, Morocco, Indonesia, Kenya, and Ecuador to illustrate our approach. One non-technical contribution of this paper is to exploit cross-site variation within and across studies for extrapolation across populations, where we find that site heterogeneity at baseline predicts cross-study differences in post-intervention responses and conditional average treatment effects.

The problem of adapting empirical findings to new contexts allowing for unobserved heterogeneity is certainly not limited to estimation of discrete treatment contrasts but is also relevant to make more model-based estimates generalizable or comparable across settings. A fully nonparametric approach appears to be well-suited for the particular problem of a binary policy intervention, but can be seen as a stand-in for a more pragmatic estimation approach based on a more explicit model for the outcome of interest. For more “structural” approaches, it may be preferable to choose low-dimensional models of site heterogeneity that can be directly incorporated into the model, possibly motivated by economic theory or empirical regularities.

The remainder of the paper is organized as follows: we first give a formal characterization of transfer estimation as a statistical problem. We then determine the optimal finite-dimensional subspace of features of the baseline data, and propose nonparametric estimators based on the experimental sample. Asymptotic properties of those estimators, assuming the number of experimental sites grows large, are given in Appendix A. The approach is then illustrated using an application to predicting the causal effect of conditional cash transfer programs to new locations.

2. PROBLEM DESCRIPTION

The population of interest consists of G sites (“clusters”/“contexts”), where the g th site consists of N_g units. For the purposes of this paper, we focus on the case in which there is a single target site g^* in addition to $G - 1$ experimental sites $g \in \{1, \dots, G\} \setminus \{g^*\}$. We also use the dummy variable $R_g \in \{0, 1\}$ to indicate whether g is an experimental location ($R_g = 1$), or a target site ($R_g = 0$).

There is a binary policy variable (“treatment”) $D_{gi} \in \{0, 1\}$ which acts at the level of the unit i at site g , where we assume that the outcome of interest is determined only by the unit’s own treatment status. Specifically, the unit is associated with potential outcomes $Y_{gi}(0), Y_{gi}(1)$, where the realized outcome is given by $Y_{gi} := Y_{gi}(D_{gi})$. Furthermore, each unit is associated with a finite-dimensional vector X_{gi} of attributes whose distribution is given by the p.d.f. $f_g(x)$ for cluster g , where we assume that the support \mathcal{X} of X_{gi} is a compact subset of \mathbb{R}^d . For the purposes of this paper N_g will be treated as infinite, but the researcher only observes a finite random sample of units for each cluster.

Adapting notation from Nie, Imbens, and Wager (2021), we can without loss of generality characterize potential outcomes as

$$Y_{gi}(d) \equiv y(d; X_{gi}, U_{gi}, V_g), \quad d = 0, 1 \tag{2.1}$$

for some unspecified mapping $y(\cdot)$ and potentially multi-dimensional unobserved individual and site-specific heterogeneity U_{gi} and V_g . Previous work by Gechter (2023) and Nie, Imbens, and Wager (2021) proposed strategies to address cross-site differences in the conditional distribution of individual heterogeneity U_{gi} , whereas our focus is on site-specific heterogeneity V_g . While V_g could be included with the vector U_{gi} as a matter of notation, the approaches in Gechter (2023) and Nie, Imbens, and Wager (2021) require U_{gi} to have the same support across sites, which can’t be satisfied by variables V_g that are shared by all units at the site. We therefore prefer to keep site-specific heterogeneity explicit in our notation.

Using this notation we can write the conditional means of post-intervention outcomes at site g

$$\mu_g(x; 1) \equiv \mu(x; 1, V_g) := \mathbb{E}[Y_{gi}(1) | X_{gi} = x, V_g]$$

or conditional average treatment effects

$$\tau_g(x) \equiv \tau(x; V_g) := \mathbb{E}[Y_{gi}(1) - Y_{gi}(0) | X_{gi} = x, V_g]$$

For a given superpopulation $V_g \sim F_V$, we can also define the cross-site averages $\mu(x; 1) := \mathbb{E}_{F_V}[\mu(x; 1, V_g)]$ and $\tau(x) := \mathbb{E}_{F_V}[\tau(x; V_g)]$ of the CATE.

Our goal is to use the site-specific distribution of pre-intervention outcomes, $Y_{gi}(0) | X_{gi}$ to predict $\tau_g(x)$ and $\mu_g(x; 1)$ given the conditional distribution of pre-intervention outcomes $Y_{gi}(0) | X_{gi}$. In particular, we aim to use baseline outcome data to predict model shifts $\Delta\tau_g(x) := \tau_g(x) - \tau(x)$ and $\Delta\mu_g(x; 1) := \mu_g(x; 1) - \mu(x; 1)$. While other moments of the conditional distribution of baseline outcomes may reveal additional information regarding V_g , in this paper we restrict our attention to the problem of using only the conditional first moment of baseline outcomes

$$\mu_g(x; 0) \equiv \mu(x; 0, V_g) := \mathbb{E}[Y_{gi}(0) | X_{gi} = x, V_g]$$

as a predictor of $\Delta\tau_g(x)$.

In our application, the outcome of interest Y_{gi} is a binary indicator whether a school-age child attends school, so that all higher moments of potential outcomes are known functions of the conditional expectation $\mu_g(x; 0)$, but in general higher-order conditional moments of $Y_{gi}(0)$ given X_{gi} may also be predictive of the CATE at the target site. We also do not consider the use potentially predictive information from the marginal distribution of covariates $f_{X_g|V_g}(x|V_g)$. We also discuss how to incorporate observable site-specific covariates into our approach in Section 3.4 below, however the main focus is on prediction using $\mu_g(\cdot; 0)$ alone.²

By focusing on the conditional average treatment effects (CATE), *covariate shifts* across sites are already accounted for. Prediction of site-specific CATE therefore seeks to account for *model shifts* $\Delta\tau_g(x)$. Our method aggregates information on the first two moments of the distribution of conditional expectation functions (pre- and post-intervention) across sites and does not require that we can estimate either conditional mean function consistently for any individual site. In particular, we also discuss a version of our approach for the case in which treatment assignment was randomized at the site level. In principle, the arguments behind our method can therefore also be extended to imputation of site-specific CATE for *experimental* sites when treatment was randomized at the site level, or the researcher only observes a moderate number of units for each site.

²For our empirical application to conditional cash transfer (CCT) programs, the main outcome of interest is whether a school age child regularly attends school, which is binary so that higher-order moments do not provide additional information. The main individual attributes in our empirical analysis are gender, age, and per capita household income, where the distribution of age and gender does not vary substantially across sites.

2.1. Stylized Example. The problem of adapting an estimate to a target location using baseline data can be illustrated using the following idealized example: Suppose that sites are sampled i.i.d. from a superpopulation according to $V_g \sim F_V(v)$ for some distribution F_V , and for each site we observe an i.i.d. sample $(Y_{gi}(0), X_{gi})_{i=1}^{n_g}$ from the p.d.f. $f_{X_g Y_g(0)|V_g}(x, y|V_g)$.

If in addition all variables are discrete with $Y_{gi}(0) \in \{0, 1\}$ and $X_{gi} \in \{x_1, x_2\}$, the p.d.f. of the baseline sample can be written as the probability mass function

$$f_{X_g Y_g(0)|V_g}(x, y|V_g) = f_{Y_g(0)|X_g V_g}(y|x) f_{X_g|V_g}(x|V_g) \equiv \mu_g(x; 0) f_{X_g}(x|V_g).$$

If we also assume for simplicity that $X_{gi} \perp\!\!\!\perp V_g$, we have $f_{X_g}(x|V_g) \equiv f_{X_g}(x)$ a.s., so that the only predictive information for potential outcomes at site g corresponds to the two conditional means $\mu_g(x_1; 0), \mu_g(x_2; 0)$.

In this stylized setting, the best predictor (in the usual sense) for the model shift relative to the cross-site CATE given baseline data is then given by the conditional expectation

$$\Delta \tilde{\tau}_g(x) := \mathbb{E}[Y_{gi}(1) - Y_{gi}(0)|X_{gi}, \mu_g(x_1; 0), \mu_g(x_2; 0)] - \tau(x) \quad (2.2)$$

Hence, the predicted model shift in this simple example amounts to a regression adjustment over $\tau(x)$, where we condition on the two scalar variables $\mu_g(x_1; 0), \mu_g(x_2; 0) \in [0, 1]$. In more realistic settings, implementation is more challenging:

- (1) For one, a typical application may combine data from separate studies that were planned and conducted independently, so that observed sites do not represent a random sample from a well-defined superpopulation $F_V(\cdot)$. We therefore cast the transfer problem as prediction, where we optimize predictive performance within the *fixed* population of sites included in the sample.
- (2) Since the dimension of $(\mu_g(x; 0))_{x \in \mathcal{X}}$ corresponds to the cardinality of \mathcal{X} (potentially infinite), we typically need to restrict the conditioning set in (2.2) to a smaller number of variates. The focus of this paper is therefore on how to represent the space of cross-site predictors and systematically determine the most relevant features for prediction of the model shift. In our particular application, cross-validation recommends an approximation using a subspace of dimension as low as $K = 2$.

The remainder of this section discusses each of these aspects in more detail.

2.2. Fixed-Population Approach. The first problem consists in determining the relevant superpopulation for the prediction problem, when the researcher wishes to extrapolate from existing experimental data and therefore has limited control or knowledge on how those sites had been selected. In such a scenario, it is generally implausible to assume a well defined sampling mechanism from a particular population, however defined. Instead, we

follow a fixed-population (design-based) approach to the problem of extrapolating from experimental to target sites, where our statistical theory will regard the combined population of experimental and target clusters as fixed.

We consider a **transfer estimate** $\hat{\tau}_{g^*,1,\dots,G}(x)$ for extrapolating from the sites $\{1, \dots, G\} \setminus \{g^*\}$ to g^* . Such a transfer estimate combines information on covariates and outcomes from the G experimental and target sites to predict the CATE for the target site, g^* . Specifically, when treatment is assigned at random within each experimental site, the site-specific conditional average treatment effect $\tau_g(x) := \mu_g(x; 1) - \mu_g(x; 0)$ is identified for each $g \in \{1, \dots, G\} \setminus \{g^*\}$ under standard conditions on the assignment mechanism, whereas for the target site, only the conditional distribution of $Y_{g^*i}(0)$ given X_{g^*i} is identified from a pre-intervention baseline sample.

The key structure we impose on this problem is that we treat the combined experimental and target sites as finitely exchangeable (see Assumption 2.2 below), in close analogy with the literature on conformal prediction (see e.g. Vovk, Gammerman, and Shafer (2005) and Lei, G’Sell, Rinaldo, Tibshirani, and Wasserman (2018)). This exchangeability condition requires that the researcher “curate” a sample of experimental sites from available data that is generally comparable *ex ante* to the target site, and potentially discard sites or studies that are known to differ systematically from that site. The resulting prediction may also be interpreted *ex post* in light of possible departures from exchangeability.³

Under this fixed-population approach, the cluster-specific conditional average treatment effects $\tau_1(x), \dots, \tau_G(x)$ are viewed as deterministic, however the assignment R_g of sites to the experimental population as well as the selection D_{gi} of treated units within each experimental cluster are random. In particular, the cross-cluster average and empirical covariance of the functions $\mu_g(x; d)$ can only be estimated with error since even for units included in the sample, only one of the two potential outcomes $Y_{gi}(0), Y_{gi}(1)$ is observed. For the remainder of the paper we only consider the case in which there is a single target cluster in addition to $G - 1$ experimental clusters.

We then evaluate the statistical performance of such a transfer estimate $\hat{\tau}_{g,1,\dots,G}(x)$ in terms of the integrated mean-squared error (IMSE) under the resulting statistical experiment,

$$IMSE := \frac{1}{G} \sum_{g=1}^G \mathbb{E} \left[(1 - R_g) \int (\hat{\tau}_{g,1,\dots,G}(x) - \tau_g(x))^2 f_0(x) dx \right] \quad (2.3)$$

with a weight function $f_0(x)$ that has the properties of a p.d.f. and is chosen by the researcher. The finite population approach is used as a way of formalizing the researcher’s problem who aims to produce a forecast that performs as well as possible *on average* for prediction *among*

³In the literature on conformal prediction such a sensitivity analysis was formally proposed by Barber, Candès, Ramdas, and Tibshirani (2023).

this fixed population of sites. The best feasible prediction under those circumstances is a parameter that is specific to the set of observable experimental and target sites.

The resulting transfer estimator represents a summary of site-specific unobserved model heterogeneity that can be quantified based on the experimental sample and used to predict the treatment effect at the target site. This is analogous to a situation that would arise when the sample average treatment effect (SATE) is used to predict the treatment effect for an individual participant in an experimental trial on subjects that were not sampled at random from a well-defined population.

Our approach could also be directly implemented in a sampling based framework by replacing sample with superpopulation moments. However we do not evaluate prediction errors with respect to a (“natural” or constructed) superpopulation, but define transfer estimate as fixed-population, design-based analogs instead. This design-based interpretation of transfer estimation therefore keeps any potential caveats about non-representative sampling of sites explicit. There are in fact some scenarios in which the experimental clusters were in fact chosen at random from the relevant superpopulation, allowing for an alternative, sampling based interpretation. For example, for several of the studies of conditional cash transfers the study population consisted of randomly selected villages or schools in a subset of major administrative regions (states, provinces) of the country in which the study was conducted. In such a setting, a sampling-based approach is well-suited to estimating the anticipated effect of scaling the policy to the remaining sites in those regions.

2.3. Functional Predictors. The premise of our approach is that baseline (pre-intervention) outcome data is predictive of post-intervention outcomes, both at the level of the site and the individual unit. This may be particularly plausible when the effect of the intervention is expected to be only incremental so that pre- and post-intervention outcomes behave similarly and depend on the same unit- and site-specific factors. Under this view of the DGP, unobserved site-specific heterogeneity V_g is not necessarily separable, but site effects will often manifest themselves in interactions between attributes and outcome variables. Hence there is generally relevant predictive information regarding V_g from the **conditional** moments of baseline outcomes in addition to unconditional moments of $Y_{gi}(0)$.

For example in the study of conditional cash transfers, school attendance may differ across sites according to whether there is a secondary school in close proximity to the community. If the closest secondary school is difficult to reach, then older age groups will likely have substantially lower attendance at baseline, but also be less responsive to a cash incentive. Also, local price levels may differ across communities, causing shifts between sites in the relationship between attendance and nominal measures of income. Sites may also differ e.g. in terms of how well the site is connected to urban centers, or whether the language of instruction is widely spoken within the community. For the CCT data one might expect that

there is a substantial amount of heterogeneity of sites within each study country regarding these aspects, and that these site-specific factors may have similar effects on the outcome of interest across these countries. In practice, the researcher may in addition directly observe site-specific measures e.g. of price variables or the cost of attending school, and our approach could then be viewed as addressing residual site-specific heterogeneity after practically feasible adjustments for observable covariates. We discuss this further in Section 3.4 below.

To frame thoughts, consider first the case in which sites are random draws from an abstract superpopulation, $V_g \sim F_V$. For a target site g^* drawn from such a superpopulation the best (lowest variance) predictor of $\tau_{g^*}(x)$ given $\mu_{g^*}(\cdot; 0)$ is then given by the conditional expectation function,

$$\mathbb{E}[\tau(x; V_{g^*}) | \mu(\cdot; 0, V_{g^*})] = \mathbb{E}[\mu(x; 1, V_{g^*}) - \mu(x; 0, V_{g^*}) | \mu(\cdot; 0, V_{g^*})] \quad (2.4)$$

For the fixed-population problem discussed before, sites are not i.i.d. draws from a distribution, but instead drawn without replacement from the finite set $\{V_1, \dots, V_G\}$. Since $\mu(\cdot; 0, V_{g^*})$ is generally infinite-dimensional (unless all attributes X_{gi} are discrete), completely flexible interpolation between sites is generally not feasible as a practical matter.

Instead, we restrict our attention to predictors that are *linear* in $\mu_{g^*}(x)$, i.e. that can be expressed in terms of a linear operator B acting on μ_{g^*} ,

$$\Pi[\tau(x, V_{g^*}) | \mu(\cdot; 0, V_{g^*})] := \tau(x) + \int \mu(x_1; 0, V_{g^*}) \beta(x_1, x) f_0(x_1) dx_1 =: (B\mu_{g^*}(\cdot; 0))(x) \quad (2.5)$$

where $\beta(x_1, x_2)$ is a square integrable function. That is, we can view a linear predictor as a regression adjustment over the unconditional CATE $\tau(x)$, corresponding to a Hilbert-Schmidt integral operator acting on $\mu(\cdot; 0, V_{g^*})$ with kernel function $\beta(x_1, x_2)$.

Finding the kernel $\beta(x_1, x_2)$ corresponding to the best linear predictor corresponds to functional linear regression (see Ramsay and Silverman (2005), He, Müller, Wang, and Yang (2010), and Benatia, Carrasco, and Florens (2017)). Our approach approximates that kernel in terms of K basis function pairs $\{\phi_k(\cdot), \psi_k(\cdot)\}_{k=1}^K$, that is we solve the linear problem (2.5) after projecting into a finite-dimensional subspace of L_2 . Our main technical contribution concerns the optimal choice of such a finite-dimensional subspace at any order of approximation. In the fixed-population setting of interest for this paper, the relevant superpopulation is finite, so that the conditional expectation (2.4) is generally degenerate and not identified. A finite-dimensional approximation to the problem (2.5) therefore works not only as a regularization device in the usual statistical sense but also ensures that the prediction problem is well-defined without having to invoke an abstract infinite superpopulation.

Our choice of restricting the problem to linear predictors also allows us to use modeling techniques from the literature on functional data analysis. In general, there is no guarantee

that a linear projection (2.5) can extract all relevant information on site heterogeneity from $\mu_g(\cdot; 0)$ but will in general result in an interpolation error $e_g(x) := \mathbb{E}[\tau(x; V_g) | \mu(\cdot; 0, V_g)] - \Pi[\tau(x; V_g) | \mu(\cdot; 0, V_g)]$. While the assumption of linearity is fairly well understood in the finite-dimensional case, we next illustrate the possibilities and limitations of this approach using a few stylized examples for the functional prediction case that are motivated by our leading application.

Example 2.1. Location-Scale Model. $\mu_g(x) = v_{g11} + v_{g12}m(x)$ and $\tau_g(x) = v_{g21} + v_{g22}t(x)$ for functions $m(x), t(x)$, where $m(x)$ takes at least two different values in the support of X_{g_i} for all g , and the conditional expectations $\mathbb{E}[v_{g2s} | v_{g11}, v_{g12}]$ are linear in v_{g11}, v_{g12} for $s = 1, 2$. Then $\mathbb{E}[\tau_g(x) | \mu_g(\cdot; 0)]$ is linear in $\mu_g(\cdot; 0)$, so that in particular the interpolation error $e_g(x) \equiv 0$.

Specifically, without loss of generality assume that the support of X_{g_i} equals $[0, 1]$, and that there exists $0 < \kappa < 1$ such that $w_0 \equiv \frac{1}{\kappa} \int_0^\kappa m(s) ds \neq \frac{1}{1-\kappa} \int_\kappa^1 m(s) ds \equiv w_1$. Then, for $w_{g0} := \frac{1}{\kappa} \int_0^\kappa \mu_g(s) ds$ and $w_{g1} := \frac{1}{1-\kappa} \int_\kappa^1 \mu_g(s) ds$ we can write $v_{g12} = \frac{w_{g1} - w_{g0}}{w_1 - w_0}$ and $v_{g11} = \int_0^1 \mu_g(s) ds - v_{g12} \int_0^1 \mu(s) ds$. Moreover,

$$\mathbb{E}[\tau_g(x) | \mu_g(\cdot)] = \mathbb{E}[\tau_g(x) | v_{g11}, v_{g12}] = \mathbb{E}[v_{g21} | v_{g11}, v_{g12}] + \mathbb{E}[v_{g22} | v_{g11}, v_{g12}] t(x)$$

is linear in v_{g11}, v_{g12} by assumption, and therefore also linear in $\mu_g(x)$, so that recursive substitution yields a bounded expression for the kernel $\beta(x_1, x_2)$ in (2.5) as long as κ is bounded from zero and one, and $t(x)$ and the conditional expectations of v_{g2s} are bounded.

We next give an example where the distribution of the outcome variable is discontinuous at a known value of a covariate. The main empirical motivation for this setting concerns school attendance according to the child's age, where the cost of attending secondary school at age 12 or above may be different from that for primary school, and both costs may also vary across sites. For example, many sites may have access to a primary school in close proximity, but the nearest secondary school may be more difficult to reach at some sites, leading to lower attendance pre- and post-intervention.

Example 2.2. Common Structural Break. Suppose that $\mu_g(x) = v_{g11}\underline{m}(x)\mathbb{1}\{x \leq x_0\} + v_{g12}\bar{m}(x)\mathbb{1}\{x > x_0\}$ and $\tau_g(x) = v_{g21}\underline{t}(x)\mathbb{1}\{x \leq x_0\} + v_{g22}\bar{t}(x)\mathbb{1}\{x > x_0\}$, where the conditional expectations $\mathbb{E}[v_{g2s} | v_{g11}, v_{g12}]$ are linear in v_{g11}, v_{g12} for $s = 1, 2$. Then $\mathbb{E}[\tau_g(x) | \mu_g(\cdot; 0)]$ is linear in $\mu_g(\cdot; 0)$ and $e_g(x) \equiv 0$. The structure of this example closely parallels the previous one, we therefore omit a separate proof.

The following example concerns the case in which a covariate may be measured at different units at each site. For example, agents choices may be determined by income and costs in terms of site-specific purchasing power, whereas recorded amounts are in terms local currency

units, typically expressed in US Dollar equivalents according to purchasing power parity at the national level.

Example 2.3. Heterogeneous Measurement Units I Suppose that sites are heterogeneous with respect to the scale at which a characteristic is measured, where $\mu_g(x) = m(v_g x)$ and $\tau_g(x) = t(v_g x)$, and that v_g only takes finitely many values v_1, \dots, v_J . If for some collection of intervals I_1, \dots, I_J , the matrix $M := \left(\int_{I_i} m(v_j s) f_0(s) ds \right)_{i,j}$ has full rank then $\tau_g(x) \equiv \int \mu_g(s) \beta(s, x) f_0(s) ds$ where $\beta(s, x) := (\mathbb{1}\{s \in I_j\})_{j=1}^J M^{-1} (t(v_j x))_{j=1}^J$ and we take $(c_j)_{j=1}^J$ to be a column vector with entries c_1, \dots, c_J . In particular, the resulting interpolation error is zero, $e_g(x) \equiv 0$.

Alternatively, under global smoothness of $m(x)$, the relevant information on v_g may be recovered as a limit of linear functionals in $\mu_g(\cdot)$ even when the site-specific scaling factor may take infinitely many values.

Example 2.4. Heterogeneous Measurement Units II Consider again the setting from the previous example, where this time, v_g may be continuously supported but $m(x)$ is differentiable at any order at $x = 0$, and $[0, \varepsilon)$ is contained in the support of X_{g_i} . Furthermore suppose that $t(x)$ is the limit of a convergent power series on the support of X_{g_i} where the polynomial coefficients k_1, k_2, \dots are nonzero. Also, Then, if the corresponding derivatives $m^{(k_s)}(0) := \left. \frac{d^{k_s}}{dx^{k_s}} m(x) \right|_{x=0}$ are all nonvanishing at zero, the linear projection of $\tau_g(x)$ on $\mu_g(x; 0)$ equals $\tau_g(x)$, in particular $\mathbb{E}[\tau_g(x) | \mu_g(\cdot; 0)]$ is linear in $\mu_g(\cdot; 0)$.

To see why this is the case, note first that the derivatives $\mu_g^{(k_s)}(0) := \frac{d^{k_s}}{dx^{k_s}} \mu_g(x; 0) \equiv v_g^{k_s} \frac{d^{k_s}}{dx^{k_s}} m(x)$ are limits of finite differences of $\mu_g(x; 0)$ and therefore linear in values of the function at points in the neighborhood of x . By assumption we can then represent

$$\tau_g(x) = \sum_{s \geq 1} v_g^{k_s} \frac{t^{(k_s)}(0) x^{k_s}}{k_s!} = \sum_{s \geq 1} \frac{\mu_g^{(k_s)}(0)}{m^{(k_s)}(0)} \frac{t^{(k_s)}(0) x^{k_s}}{k_s!}$$

which is linear in $\mu_g(\cdot, 0)$ since $m^{(k_s)}(0)$ and $t^{(k_s)}(0)$ are constant across sites.

Using this argument, $\tau_g(x)$ is recovered only in the limit along sequences of Hilbert-Schmidt operators acting on $\mu_g(\cdot)$. In particular there is no guarantee that the limit itself will be Hilbert-Schmidt, so the function $\tau_g(x)$ may only be recovered as an approximation.

The preceding examples suggest that even in the presence of interpolation error, linear projection can be responsive to the patterns of unobserved site heterogeneity used to motivate our approach although conditional expectations are linear only under admittedly fairly stylized assumptions. While our arguments are given in terms of $m(x), t(x)$, an implementation of linear projection obviously does not require knowledge of these functions.

Finally, even under linearity, there may still remain relevant site-specific unobserved heterogeneity that does not express itself in $\mu_g(\cdot; 0)$ and therefore cannot be predicted from

baseline outcomes. For example, modeling pre-intervention outcomes $\mu_g(x; 0)$ as a function of household income could help predict aggregate heterogeneity in income effects in the response to a conditional cash transfer program. At the same time, a predictor based on income alone may not be responsive to site-specific (rather than only individual-specific) heterogeneity in substitution effects which may manifest themselves more clearly if in addition some measure of the cost of school attendance were taken into account.

2.4. Assumptions. We next formalize the identifying conditions which are adapted from Hotz, Imbens, and Mortimer (2005). We depart from their main framework in two substantial ways: for one our design-based approach treats experimental and target sites as random draws from a finite population of sites. Moreover, we also consider a version of the problem in which baseline data on pre-treatment outcomes for the target site are available and are to be used to predict site-specific “macro” effects. We highlight how this affects the interpretation of the assumptions on the assignment mechanism. While our derivation of optimal predictors in section 3 is directly in terms of high-level properties of covariance operators, the following assumptions are maintained to establish asymptotic rates for estimates in Appendix A.

We assume throughout that for each cluster $g = 1, \dots, G$ the researcher observes a sample of n_g units that are drawn independently and uniformly at random from $\{1, \dots, N_g\}$, and also independently of potential values and unit attributes. For notational convenience our results will be stated for the case that the observed number of units is the same for each site, $n_g \equiv n$ for $g = 1, \dots, G$. For each experimental site, we assume that selection of units into treatment is based only on observables X_{gi} ,

Assumption 2.1. (*Unconfounded Assignment*) For all g with $R_g = 1$,

$$D_{gi} \perp\!\!\!\perp (Y_{gi}(0), Y_{gi}(1)) | X_{gi}, R_g = 1$$

where D_{g1}, \dots, D_{gN_g} are also conditionally independent across units and clusters given attributes and R_1, \dots, R_G .

This condition is met if D_{gi} was assigned at random as part of a randomized controlled trial (RCT) at each experimental site, and it captures the idea of extrapolating from a collection of internally valid estimates of site-specific causal effects to a new site. In a practical application the set of confounders X_{gi} may differ from the conditioning variables chosen by the researcher for define the relevant conditional average treatment effect, however for expositional clarity we only consider the case in which the conditioning variables are the same. It is also possible to adapt our approach to the case of randomization at the cluster level, $D_{gi} \equiv D_g$ for all $i = 1, \dots, n_g$, see Appendix A for a brief discussion.

Furthermore, we assume that among the G sites, the $G - 1$ experimental locations were selected independently of potential values, conditional on observable covariates:

Assumption 2.2. (*Unconfounded Location*) g^* is drawn uniformly at random from $\{1, \dots, G\}$ independently of $\{Y_{gi}(0), Y_{gi}(1), X_{gi} : g = 1, \dots, G, i = 1, \dots, N_g\}$.

This assumption is strengthened version of Assumption 2 in Hotz, Imbens, and Mortimer (2005) and describes an idealized observational protocol that rules out systematic ex-ante site selection bias. It can be seen immediately that under this condition, for a randomly selected experimental site \tilde{g} with $R_{\tilde{g}} = 1$, $(Y_{\tilde{g}i}(0), Y_{\tilde{g}i}(1), X_{\tilde{g}i}) \stackrel{d}{=} (Y_{g^*i}(0), Y_{g^*i}(1), X_{g^*i})$, where “ $\stackrel{d}{=}$ ” denotes equality in marginal distributions. Therefore, Assumption 2.2 implies that experimental and target sites are exchangeable, the fundamental assumption in the literature on conformal prediction (Vovk, Gammerman, and Shafer (2005) and Lei, G’Sell, Rinaldo, Tibshirani, and Wasserman (2018)).

In practice, we do not expect that assumption to be an accurate description on how experimental (study) and target sites were selected. Rather, in the absence of additional knowledge regarding site selection, this auxiliary assumption defines a pseudo-true parameter, which aggregates estimates from experimental sites into a “best” prediction for the target population. The resulting transfer estimate should therefore be interpreted as a summary of the directly quantifiable relevant information from previous experiments, which could be subject to additional (qualitative or quantitative) sensitivity analysis with respect to suspected violations of that exchangeability condition (see e.g. Barber, Candès, Ramdas, and Tibshirani (2023) for the problem of conformal prediction).

For the next assumption, we define the site-specific propensity score as

$$p_g(x) := \mathbb{P}(D_{gi} = 1 | X_{gi} = x)$$

We require that the supports of covariates overlap, both between treated and control units, as well as across the sites $g = 1, \dots, G$.

Assumption 2.3. (*Support Conditions*) There exists δ , $0 < \delta < 1$ such that

$$\delta < p_g(x) < 1 - \delta \quad \text{and} \quad \delta < f_g(x)/f_0(x) < 1/\delta$$

for all $g \in \{1, \dots, G\} \setminus \{g^*\}$ and x in the support of $f(x)$. Furthermore, the support \mathcal{X} of X_{gi} is a compact subset of \mathbb{R}^d , without loss of generality $\mathcal{X} = [0, 1]^d$, and we assume $\inf_{x \in [0, 1]^d} f_g(x) \geq \kappa > 0$ for all $g = 1, \dots, G$.

The role of this assumption is to ensure that conditional moments of either potential value are identified and can be estimated consistently across sites. While Assumption 2.2 does allow for experimental and target sites to differ in terms of the distribution of observables, we require that the site-specific supports overlap, potentially after trimming non-overlapping regions in the covariate space as suggested in Hotz, Imbens, and Mortimer (2005). This assumption also does not cover site-specific aggregate covariates that may serve as additional predictors as analyzed by Hotz, Imbens, and Mortimer (2005) and

Dehejia, Pop-Eleches, and Samii (2021). Randomization at the level of the site would not satisfy the support condition on the site-specific propensity score and therefore requires a different approach which is discussed in Appendix A. Additional adjustments for site-specific variables may be possible, but would also be severely constrained by the small number of observable sites. While our focus is on the optimal use of cross-sectional information for extrapolation, we briefly discuss how to incorporate site-level covariates in Section 3.4.

Nonparametric estimation of the first two conditional moments of potential values $Y_{gi}(d)$ given attributes X_{gi} requires additional moment and smoothness conditions, where we specifically assume the following:

Assumption 2.4. (*Distribution and Moments*) For $g = 1, \dots, G$, (a) X_{gi} is continuously distributed on $[0, 1]^d$ with marginal p.d.f. that is bounded from above $\sup_{x \in [0, 1]^d} f_g(x) \leq B_0 < \infty$. (b) The site-specific density $f_g(x)$, propensity score $p_g(x)$, and conditional mean functions $\mu_g(x; d)$ are twice continuously differentiable in x with uniformly bounded derivatives. We also assume that (c) potential outcomes have bounded moments $\mathbb{E}|Y_{gi}(d)|^s < \infty$ for $d = 0, 1$ and some $s > 3$, (d) there exist finite constants B_0, B_1 such that $\sup_x f(x) \leq B_0$ and $\sup_x \mathbb{E}[|Y_{gi}(d)|^s | X_{gi} = x] f_g(x) \leq B_1$ for all g .

To avoid additional notation, we do not explicitly discuss the case in which some components of X_{gi} may be discrete. With the exception of part (c), the conditions in Assumption 2.4 are commonly assumed for nonparametric estimation of conditional moments, see e.g. Hansen (2008). Notice also that we effectively need to be able to estimate conditional moments separately for each site, and therefore require these conditions to hold uniformly over g . In the absence of covariate shifts, i.e. if the distribution of covariates $f_g(x)$ or propensity score $p_g(x)$ did not vary over g , this issue could be avoided (see Yao, Müller, and Wang (2005a)), however we do not find such an assumption plausible for the problem considered here.

2.5. Literature. A conceptual framework for the problem of extrapolation of estimated treatment effects across heterogeneous sites was developed in the seminal article by Hotz, Imbens, and Mortimer (2005). Using their terminology, we assume unconfounded locations, but specifically want to allow for (site-specific) model shifts (“macro effects”), that is shared heterogeneity in potential outcomes and treatment effects within each cluster. We propose a mechanism to incorporate information on pre-treatment outcomes at the cluster/site level when no treated units are observed in the population of interest.

Extrapolation of treatment effects was considered by various studies, including Dehejia, Pop-Eleches, and Samii (2021), Gechter (2023), Meager (2022), Nie, Imbens, and Wager (2021), Adjaho and Christensen (2022), and Canen and Song (2023). Dehejia, Pop-Eleches, and Samii (2021) considered the problem of predicting treatment effects at target sites based

on observed site-specific covariates. Gechter (2023), Manski (2020), and Nie, Imbens, and Wager (2021) derive bounds that account for selection effects at the individual level, allowing individual heterogeneity to be distributed differently across sites. Our focus is on site-specific heterogeneity, in particular we do not require the support of unobservables $(U'_{ig}, V'_g)'$ to be shared across sites for the approach to be useful. Adjaho and Christensen (2022) consider robust extrapolation of treatment rules when there is no separate data on the target site, but the distribution of potential outcomes is in a neighborhood of that for the experimental population.

A separate question concerns the transfer performance of extrapolation methods. Gechter, Samii, Dehejia, and Pop-Eleches (2019) use data from two conditional cash transfer programs to evaluate extrapolation of empirical treatment rules. Kuang, Xiong, Cui, Athey, and Li (2018) identify attributes that exhibit a stable predictive relationship to the outcome of interest across environments. Andrews, Fudenberg, Liang, and Wu (2022) analyze the problem of assessing transfer performance, where model estimates from data in one domain are transferred to another, whereas this paper optimizes cross-domain model performance within the experimental sample. While our analysis is formally design-based conditional on the experimental sample (rather than assuming i.i.d. draws of contexts from a meta-population), a sampling-based interpretation similar to theirs is also possible. Gechter, Hirano, Lee, Mahmud, Mondal, Morduch, Ravindran, and Shonchoy (2023) discuss optimal selection of experimental locations for extrapolation to other sites.

The work closest to ours is Canen and Song (2023) who propose to use the distribution of pre-intervention outcomes for the target site together with post-intervention outcomes from the experimental locations to predict outcomes under a synthetic transferability condition. Their approach predicts policy effects based on the assumption that the policy shift affects outcomes through an index where the supports of pre- and post-intervention index values overlap in the target population. We consider a setting in which the policy intervention is binary and not equivalent to a shift in other observed covariates. Under that scenario the supports for pre- and post-intervention values for that index are disjoint, so that no subpopulation of the target site can be directly matched to post-intervention outcomes in the experimental sample. Our approach predicts counterfactuals conditional on pre-treatment outcomes alone, and is therefore complementary to theirs.

The working assumption of exchangeability between experimental and target sites is shared by conformal prediction methods (see Vovk, Gammerman, and Shafer (2005) and Lei, G'Sell, Rinaldo, Tibshirani, and Wasserman (2018)). The focus of the present paper is on a point estimate that is informed by the experimental sample rather than inference, however under an exchangeability assumption our approach could in principle be combined with classical or

conformal methods for inference with either asymptotic or finite-sample guarantees. Sensitivity of conformal inference with respect to departures from exchangeability was characterized by Barber, Candès, Ramdas, and Tibshirani (2023). We do not explore the problems of inference or sensitivity analysis in this paper but leave this for future research.

It is also worth comparing our approach to other conceptual frameworks for aggregation of causal estimates across different populations: Pearl and Bareinboim (2014) gave explicit conditions for transportability of causal estimates across populations in terms of selection diagrams. One interpretation of our approach is the construction of a site-level covariate from baseline outcome data conditional on which potential outcomes are, to an approximation, mean-independent of selection. This paper also differs in the interpretation of transfer estimates, where our focus is on cross-population prediction of causal effects, rather than assuming the idealized conditions that would guarantee transportability in the strict sense.

Conceptually, the extrapolation problem also has some resemblance with the method of synthetic controls (Abadie and Gardeazabal (2003), Abadie, Diamond, and Hainmueller (2010)). However our approach is developed with a setting in mind where we do not have (typically aggregate) time series information on a treated unit and the “donor pool” of potential controls. Rather we assume that each site/context provides rich cross-sectional information, where a fraction of units is treated in a study population of sites, and we then predict treatment effects for the (yet untreated) target cluster. For that problem, Gunsilius (2023) is most similar to our approach in that he proposes to use cross-sectional variation in micro-data to calibrate synthetic weights, however our approach differs in that rather than optimizing weights to match the distribution of baseline outcomes as closely as possible, we construct factors that are optimized to predict post-treatment outcomes based on the conditional distribution given unit-specific attributes. Shin (2022) uses a k-means algorithm to model unobserved heterogeneity in a problem with cluster dependence in treatment assignment.

In order to model site-specific conditional mean functions as random objects, we use tools from functional data analysis (Ramsay and Silverman (2005) for an overview), where function-to-function regression was analyzed by He, Müller, and Wang (2003) and He, Müller, Wang, and Yang (2010), Yang, Müller, and Stadtmüller (2011), and Benatia, Carrasco, and Florens (2017). Our approach is also related to functional principal components approaches for function completion/reconstruction based on partially observed functional data, where our setting corresponds more closely to that of sparsely sampled functions analyzed in Yao, Müller, and Wang (2005a), rather than the dense case considered by Kraus (2015) and Kneip and Liebl (2020), although we assume that the number of points sampled for each curve (site) grows large. Since our focus is on cases in which only a modest number of trajectories is observed, the basis functions for our approach is constructed in as to be

optimal for prediction, using both covariate and outcome data rather than separate principal components for covariate and outcome trajectories.

Generally our problem differs from function reconstruction in that our objective is to predict the *difference* between two curves, corresponding to conditional mean functions for either potential value, rather than the trajectory of the partially observed curve, so that the functional principal components of the conditional mean functions themselves do not generally have the best basis property for this particular task. Our problem differs from that of covariate adaptive reconstruction (Jiang and Wang (2010), Liebl (2019)) in that we consider unit-specific covariates which correspond to coordinates of the random trajectories, rather than site-specific covariates that shift the distribution of the random curve. Prediction of scalar outcomes based on functional principal components was analyzed by Cai and Hall (2006) and Hall and Horowitz (2007).

Our focus is on prediction of the conditional average treatment effect as a function of covariates, and we derive a choice of basis functions that is optimal for that prediction task in a sense to be made more specific below. We show that our solution bears some resemblance with, but is distinct from Hotelling (1936)’s classical problem of canonical correlation analysis. For functional data, functional canonical regression has first been proposed by He, Müller, Wang, and Yang (2010) whose approach differs from the present paper in terms of the approach to regularization. We derive our approach from optimality considerations and establish a (to our knowledge novel) formal optimality result.

Interpreting “locations” at which random trajectories are evaluated as covariates or causal variables also requires a few subtle adjustments relative to the classical literature on functional data analysis. In particular, the covariate distributions may differ across sites, so nonparametric estimation of moments of the distribution of the random function requires some local reweighting and support conditions.

3. ESTIMATION APPROACH

This section concerns the optimal choice of basis functions (features) for estimation of the linear projection problem (2.5). Our general approach is based on a representation of the random processes $\mu_{g^*}(x; 0)$ and $\tau_{g^*}(x)$ for the target site g^* in terms of orthogonal bases, ϕ_1, ϕ_2, \dots and ψ_1, ψ_2, \dots ,

$$\begin{aligned}\mu_{g^*}(x; 0) &= \mu(x; 0) + \sum_{k=1}^{\infty} m_{g^*k} \phi_k(x) \\ \tau_{g^*}(x) &= \tau(x) + \sum_{k=1}^{\infty} t_{g^*k} \psi_k(x)\end{aligned}\tag{3.1}$$

Note that $\mu_{g^*}(x; 0)$ and $\tau_{g^*}(x)$ are stochastic only due to the fact that the target site g^* is random draw from the population $\{1, \dots, G\}$.

Our approach then estimates a truncated version of this expansion,

$$\tau_{g^*}^K(x) := \tau(x) + \sum_{k=1}^K t_{g^*k} \psi_k(x) \quad (3.2)$$

to approximate the CATE at site g at a low order $K \ll G$. For the scenarios we are envisioning in this paper, the number of experimental clusters $\sum_{g=1}^G R_g$ is not very large, so K should be thought of as fairly small. In fact, for our empirical application, cross-validation (with respect to cross-site prediction) suggests a value of K equal to 2 or 3, depending on the exact specification. So rather than aiming for consistent estimation of $\tau_g(x)$, we view the use of the first few leading factors in the expansion (3.1) as a method of improving over an unconditional forecast $\tau(x)$ that doesn't account for site heterogeneity.

It is therefore all the more important to have theoretical guidance on how to choose the basis of that expansion optimally so as to prioritize those features in the data that will be most predictive for $\tau_{g^*}(x)$. The need to truncate the expansion for purposes of estimation stems from ill-posedness in the problem of predicting $\tau_{g^*}(x)$ based on trajectories $\mu_{g^*}(x; 0)$. While other continuous regularization methods are available (see Carrasco, Florens, and Renault (2007)), an advantage of this finite-dimensional approximation is that it can be interpreted as a linear prediction of the CATE based on the first K factors in an analogous expansion of the trajectory $\mu_{g^*}(x; 0)$ even for small values of K .

Our approach requires nonparametric estimation of the mean functions

$$\mu(x; d) := \mathbb{E}[\mu_{g^*}(x; d)] \equiv \frac{1}{G} \sum_{g=1}^G \mu_g(x; d), \quad d = 0, 1$$

and

$$\tau(x; d) := \mathbb{E}[\tau_{g^*}(x; d)] \equiv \frac{1}{G} \sum_{g=1}^G \tau_g(x; d), \quad d = 0, 1$$

as well as the covariance kernels

$$\begin{aligned} H_{\mu\mu}(x_1, x_2) &:= \text{Cov}(\mu_g(x_1; 0) - \mu(x_1; 0), \mu_g(x_2; 0) - \mu(x_2; 0)) \\ &= \frac{1}{G} \sum_{g=1}^G (\mu_g(x_1; 0) - \mu(x_1; 0))(\mu_g(x_2; 0) - \mu(x_2; 0)) \\ H_{\mu\tau}(x_1, x_2) &:= \text{Cov}(\mu_g(x_1; 0) - \mu(x_1; 0), \tau_g(x_2) - \tau(x_2)) \\ &= \frac{1}{G} \sum_{g=1}^G (\mu_g(x_1; 0) - \mu(x_1; 0))(\tau_g(x_2) - \tau(x_2)) \end{aligned}$$

$$\begin{aligned}
H_{\tau\tau}(x_1, x_2) &:= \text{Cov}(\tau_g(x_1; 0) - \tau(x_1; 0), \tau_g(x_2) - \tau(x_2)) \\
&= \frac{1}{G} \sum_{g=1}^G (\tau_g(x_1; 0) - \tau(x_1; 0))(\tau_g(x_2) - \tau(x_2))
\end{aligned}$$

where covariances are with respect to a random draw of a site g from the discrete uniform distribution over $\{1, \dots, G\}$.

A standard representation of the random processes $\mu_g(x; 0)$ and $\tau_g(x)$ in (3.1) is the Karhunen-Loève expansion, which chooses the basis functions ϕ_1, ϕ_2, \dots and ψ_1, ψ_2, \dots as eigenfunctions of the respective covariance operators $H_{\mu\mu}(\cdot), H_{\tau,\tau}(\cdot)$, see Ramsay and Silverman (2005) and Rasmussen and Williams (2006). These bases of eigenfunctions ordered by their associated eigenvalues are also known as the functional principal components (FPC) of the random functions $\mu_g(x; 0)$ and $\tau_g(x)$. At any finite order, an approximation of the function by its leading K FPC is known to be optimal with respect to the mean-square error of approximation. However, our goal is to extract those features of $\mu_g(x; 0)$ that are “most predictive” for the average of $\tau_g(X_{gi})$, which generally do not coincide with the FPC. We show that instead, that optimal choice can be described in terms of a singular value decomposition of an operator characterizing the covariance between $\mu_g(x; 0)$ and $\tau_g(x)$.

3.1. Optimal Basis Functions. Our main objective is to determine the optimal finite-dimensional feature space for the baseline data in which to solve the prediction problem (2.5). We regard the conditional mean functions $\mu_g(x; d)$ and $\tau_g(x)$ as random elements of the Hilbert space $L_2(\mathcal{X}, f_0)$ ($L_2(\mathcal{X})$ henceforth) of square integrable functions with norm induced by the scalar product

$$\langle \phi, \psi \rangle = \int \phi(x)\psi(x)f_0(x)dx$$

where $f_0(x)$ denotes the weighting function introduced in (2.3).

We also define integral operators $T_{\mu\mu}, T_{\mu\tau}$ associated with the covariance kernels

$$\begin{aligned}
(T_{\mu\mu}\varphi)(x) &:= \int H_{\mu\mu}(x_1, x)\varphi(x_1)f_0(x_1)dx_1 \\
(T_{\mu\tau}\varphi)(x) &:= \int H_{\mu\tau}(x_1, x)\varphi(x_1)f_0(x_1)dx_1 \\
(T_{\tau\tau}\varphi)(x) &:= \int H_{\tau\tau}(x_1, x)\varphi(x_1)f_0(x_1)dx_1
\end{aligned}$$

for any square integrable function φ . The operators $T_{\mu\mu}, T_{\tau\tau}$ are self-adjoint, whereas the adjoint of $T_{\mu\tau}$ is given by

$$(T_{\mu\tau}^*\varphi)(x) := \int H_{\mu\tau}(x, x_1)\varphi(x_1)f_0(x_1)dx_1.$$

We now turn to the construction of an optimal K -dimensional basis for predicting $\tau_g(x)$ based on $\mu_g(x; 0)$. For a collection $\phi_1(x), \dots, \phi_K(x)$ of K functions we let $P_K : L_2(\mathcal{X}) \rightarrow \mathcal{H}_K$ denote the operator associated with orthogonal projection onto the closed linear subspace

$$\mathcal{H}_K := \text{span}(\phi_1, \dots, \phi_K) := \left\{ \sum_{k=1}^K a_k \phi_k : a_1, \dots, a_K \in \mathbb{R} \right\}$$

By the classical projection theorem (Theorem 2 on p.51 in Luenberger (1969)) that projection is well-defined.

We then consider the predictors $BP_K \mu_g$ for τ_g on that subspace corresponding to linear operators $B : \mathcal{H}_K \rightarrow L_2(\mathcal{X})$. We then let

$$\begin{aligned} IMSE_K &\equiv IMSE_K[\phi_1, \dots, \phi_K] \\ &:= \int_{B \in \mathcal{H}_K \times L_2(\mathcal{X})} \min \mathbb{E} [(\Delta \tau_{g^*}(x) - BP_K \mu_{g^*}(x))^2] f_0(x) dx \end{aligned}$$

denote the integrated mean-square error of prediction, minimized over the set of linear predictors using those K functions. We restrict our attention to basis functions in the closed linear subspace \mathcal{N}^\perp , the orthogonal complement of the null space of $T_{\mu\mu}$, $\mathcal{N} := \ker(T_{\mu\mu})$. This restriction is of no practical consequence since for any function h in the null space of $T_{\mu\mu}$, $\text{Var}(\langle \mu_g, h \rangle) = \langle h, T_{\mu\mu} h \rangle = 0$. Considering any possible choices of $\phi_1, \dots, \phi_K \in L_2(\mathcal{X})$, we first give a lower bound on $IMSE_K$

Lemma 3.1. *Suppose that $T_{\mu\mu}, T_{\mu\tau}$ are compact operators, and define*

$$IMSE_K^* := \inf_{\phi_1, \dots, \phi_K} \left(\int \mathbb{E}[\Delta \tau_{g^*}(x)^2] f_0(x) dx - \sum_{k=1}^K \langle \phi_k, T_{\mu\tau} T_{\mu\tau}^* \phi_k \rangle \right) \quad (3.3)$$

where the infimum is taken over $\phi_1, \dots, \phi_K \in L_2(\mathcal{X})$ such that $\langle \phi_k, T_{\mu\mu} \phi_l \rangle = \delta_{kl}$ for all $k, l = 1, \dots, K$. Then for an arbitrary choice of $\phi_1(x), \dots, \phi_K(x)$ we have that $IMSE_K \geq IMSE_K^*$.

See the appendix for a proof. Since the operator $T_{\mu\mu}$ in the constraint is compact, there is no guarantee that the infimum will be attained by square integrable functions ϕ_1, \dots, ϕ_K . Intuitively, this ill-posedness stems from the fact that there may be functionals of $\mu_g(x; 0)$ that have small variance across sites but are highly predictive with respect to $\tau_{g^*}(x)$. This problem bears some resemblance with functional canonical analysis, where He, Müller, and Wang (2003) propose high-level conditions on the cross-correlation operator which would also be sufficient to guarantee that the infimum in (3.3) is in fact attained at elements in $L_2(\mathcal{X})$.

If such a solution exists, it can be easily seen from the expression for $IMSE_K^*$ that the optimal basis functions for linear prediction are given by the solutions to the generalized

eigenvalue problem

$$T_{\mu\tau}T_{\mu\tau}^*\phi_k^* = \lambda_k T_{\mu\mu}\phi_k^* \quad \text{for each } k = 1, \dots, K \quad (3.4)$$

where we select the eigenfunctions $\phi_1^*, \dots, \phi_K^*$ associated with the K leading eigenvalues $|\lambda_1| \geq |\lambda_2| \geq \dots$. Note that while the self-adjoint operators $T_{\mu\tau}T_{\mu\tau}^*$ and $T_{\mu\mu}$ are both non-negative, the generalized eigenvalue problem may have solutions associated with a negative eigenvalue.

Rather than imposing conditions for existence, we focus instead on a regularized version of the problem, where we then demonstrate that the solution to that problem is approximately optimal in the sense that they achieve an IMSE that can be arbitrarily close to $IMSE_K^*$ when the regularization parameter is sufficiently small. Specifically, we consider the following generalized eigenvalue problem

$$T_{\mu\tau}T_{\mu\tau}^*\phi_{ka}^* = \lambda_{ka}(T_{\mu\mu} + a\text{Id})\phi_{ka}^* \quad \text{for each } k = 1, \dots, K \quad (3.5)$$

where $a > 0$ is a regularization parameter. We then let $\phi_{1a}^*, \dots, \phi_{Ka}^*$ be the eigenvectors corresponding to the K largest eigenvalues (in absolute value), that is $|\lambda_{1a}| \geq |\lambda_{2a}| \geq \dots \geq |\lambda_{Ka}| \geq |\lambda_{K+sa}|$ for each $s \geq 1$, where we impose the normalization $\langle \phi_{ka}^*, T_{\mu\mu}\phi_{ka}^* \rangle = 1$ for each $k = 1, \dots, K$. In what follows, we also denote the operator $T_{\mu\mu a} := T_{\mu\mu} + a\text{Id}$.

We denote the integrated mean-square error of prediction using the basis from the regularized problem (3.5) with

$$IMSE_K^*(a) := \int \min_{B \in \mathcal{H}_K^* \times L_2(\mathcal{X})} \mathbb{E} [(\Delta\tau_{g^*}(x) - BP_K^*\mu_{g^*}(x))^2] f_0(x) dx$$

where P_K^* is the orthogonal projector onto $\mathcal{H}_K^* := \text{span}(\phi_{1a}^*, \dots, \phi_{Ka}^*)$. We show that the solutions to (3.5) corresponding to the K largest eigenvalues are approximately optimal as $a \rightarrow 0$:

Theorem 3.1. (Optimal Basis for $\mu_g(x; 0)$) *Suppose that $T_{\mu\mu}$ and $T_{\mu\tau}$ are compact operators. Then for any $a > 0$ and fixed K there exists a solution $\phi_{1a}^*, \dots, \phi_{Ka}^*$ the functions solving the generalized eigenvalue problem (3.5), and the resulting IMSE satisfies*

$$IMSE_K^*(a) \leq IMSE_K^* + o(1)$$

as $a \rightarrow 0$.

See the appendix for a proof. We can interpret this result as establishing an optimal finite-dimensional feature space for $\mu_g(\cdot; 0)$ for predicting the conditional average treatment effect, up to a regularization bias that can be made small in terms of its impact on the IMSE of prediction.

3.1.1. *Digression: Existence of Solution without Regularization.* We next give results on the behavior of $IMSE_K(a)$ under conditions for which a solution to the non-regularized problem (3.4) exists. Following He, Müller, Wang, and Yang (2010), we state those sufficient conditions in terms of separate Karhunen-Loève expansions for $\mu_g(x; 0)$ and $\tau_g(x; 0)$,

$$\begin{aligned}\mu_{g^*}(x; 0) &= \mu(x; 0) + \sum_{k=1}^{\infty} \alpha_{g^*k} \xi_k(x) \\ \tau_{g^*}(x) &= \tau(x) + \sum_{k=1}^{\infty} \beta_{g^*k} \zeta_k(x)\end{aligned}\tag{3.6}$$

where ξ_1, ξ_2, \dots and ζ_1, ζ_2, \dots are orthonormal systems corresponding to the eigenfunctions of the covariance operators for $\mu_{g^*}(\cdot; 0)$ and $\tau_{g^*}(\cdot)$ associated with eigenvalues $\mathbb{E}[\alpha_{g^*k}^2]$ and $\mathbb{E}[\beta_{g^*k}^2]$, respectively. By the usual properties of the Karhunen-Loève representation, the coefficients satisfy $\mathbb{E}[\alpha_{g^*k}] = \mathbb{E}[\beta_{g^*k}] = 0$ and $\mathbb{E}[\alpha_{g^*k} \alpha_{g^*l}] = \mathbb{E}[\beta_{g^*k} \beta_{g^*l}] = 0$ for all $k = 1, 2, \dots$, and $l \neq k$.

We then analyze regularization bias under the following condition:

$$\sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \frac{\mathbb{E}[\alpha_{g^*k} \beta_{g^*l}]^2}{\mathbb{E}[\alpha_{g^*k}^2]^{3/2}} < \infty\tag{3.7}$$

Note that by compactness of $T_{\mu\mu}$, $\mathbb{E}[\alpha_{g^*k}^2] \rightarrow 0$ as k grows, so that this condition is slightly weaker than the sufficient condition given by He, Müller, Wang, and Yang (2010) for the existence of a functional linear regression model representing the linear projection of τ_{g^*} on μ_{g^*} (see their Proposition 2.4).

While the squared correlation coefficient $r_{kl}^2 := \frac{\mathbb{E}[\alpha_{g^*k} \beta_{g^*l}]^2}{\mathbb{E}[\alpha_{g^*k}^2] \mathbb{E}[\beta_{g^*l}^2]}$ is bounded by 1 for any fixed k, l and $\mathbb{E}[\beta_{g^*l}^2]$ are square summable in l , (3.7) may fail when there are many features of the conditional mean of baseline outcomes $Y_{g^*i}(0)$ given X_{gi} that have low variability in α_{g^*k} but are highly predictive of τ_{g^*} .

Proposition 3.1. *Suppose that $T_{\mu\mu}$ and $T_{\mu\tau}$ are compact and that $\mu_{g^*}(x; 0)$ and $\tau_{g^*}(x)$ have a Karhunen-Loève representation (3.6) with coefficients satisfying (3.7). Then (a) the solutions to the problem (3.4) are well-defined, and the conclusion of Theorem 3.1 holds with*

$$IMSE_K^*(a) \leq IMSE_K^* + O(a)$$

See the appendix for a proof. This result establishes not only that the optimal IMSE can be achieved at a linear rate in a , but also that the condition (3.7) is sufficient to guarantee that the optimal predictors defined in (3.4) exist independently of a particular regularization scheme, and can also be estimated consistently under conditions given in the next section.

3.1.2. *Prediction of Model Shift.* Given the proposed choice of $\phi_1^*, \dots, \phi_K^*$, we also state the projection of τ_g onto the optimal basis:

Corollary 3.1. *Suppose the assumptions of Theorem 3.1 hold. Then for any $K = 1, \dots, K^*$, the projection based on the solution of (3.5) takes the form*

$$\tau_{g^*K}^*(x) := \tau(x) + \sum_{k=1}^K t_{g^*k} \psi_{ka}^*(x)$$

where $t_{g^*k} := \frac{1+a}{1-a} \langle \mu_{g^*}, \phi_{ka}^* \rangle$ and

$$\psi_{ka}^*(x) := (T_{\mu\tau}^* \phi_{ka}^*)(x) \quad (3.8)$$

See the appendix for a proof. In particular, given the operators $T_{\mu\mu}, T_{\mu\tau}$ defined at the population level, the optimal projection depends on the site-specific mean function $\mu_{g^*}(x, 0)$ only through K scalar features $(t_{g^*1}, \dots, t_{g^*K})$ that can be estimated consistently as the number n_{g^*} of observations in the target cluster grows large.

Incidentally, we can also confirm that each of the functions $\psi_{1a}^*, \dots, \phi_{Ka}^*$ is an eigenfunction of the operator $T_{\mu\tau}^* T_{\mu\mu a}^{-1} T_{\mu\tau}$ at the eigenvalue λ_{ka} :

$$\begin{aligned} T_{\mu\tau}^* T_{\mu\mu a}^{-1} T_{\mu\tau} \psi_{ka}^* &= T_{\mu\tau}^* T_{\mu\mu a}^{-1} T_{\mu\tau} T_{\mu\tau}^* \phi_{ka}^* \\ &= \lambda_k T_{\mu\tau}^* \phi_{ka}^* = \lambda_k \psi_{ka}^* \end{aligned}$$

Hence one interpretation of the approach is as an approximation based on the K leading components of a singular value decomposition of the operator $T_{\mu\mu a}^{-1/2} T_{\mu\tau}^*$ on a suitably chosen linear subspace of $L_2(\mathcal{X})$: Consider the eigensystem $\phi_{1a}^*, \phi_{2a}^*, \dots$ solving (3.5) at any nonzero value for the generalized eigenvalue λ_{ka} , and the corresponding functions $\psi_{1a}^*, \psi_{2a}^*, \dots$. By standard properties of eigenfunctions, these systems form a basis for the orthogonal complements of the null spaces $\ker(T_{\mu\tau} T_{\mu\mu a}^{-1/2})$ and $\ker(T_{\mu\mu a}^{-1/2} T_{\mu\tau}^*)$, respectively. Hence, using these bases as test functions, we can confirm that $\{\phi_{1a}^*, \phi_{2a}^*, \dots\}$, $\{\psi_{1a}^*, \psi_{2a}^*, \dots\}$, and $\{\sqrt{|\lambda_{1a}|}, \sqrt{|\lambda_{2a}|}, \dots\}$ represent a singular value decomposition of the operator $T_{\mu\mu a}^{-1/2} T_{\mu\tau}^*$ where

$$(T_{\mu\mu a}^{-1/2} T_{\mu\tau}^* h)(s) = \sum_{k=1}^{K^*} \sqrt{|\lambda_{ka}|} \phi_{ka}^*(s) \langle \psi_{ka}^*, h \rangle$$

for any $h \in L_2(\mathcal{X})$.

3.2. Comparison to Existing Approaches for Functional Regression. We briefly discuss how this approach compares to existing methods in the literature on functional regression with a functional response.

While the basis functions $\phi_{1k}, \phi_{2k}^*, \dots$ in our analysis are derived from optimality considerations, the procedure we arrive at has a close resemblance to canonical correlation analysis which has previously been proposed for functional regression problems by He, Müller, Wang, and Yang (2010). Our results differ in that for one the basis $\phi_{1k}^*, \dots, \phi_{Kk}^*$ is formally shown to

be optimal for the linear prediction problem considered here. Moreover, the canonical variates need not be ordered according to the eigenvalues λ_k which we show to be the relevant ordering for the IMSE-optimal choice among the eigenfunctions $\phi_1^*, \phi_2^*, \dots$.

To address the potential non-existence of an unregularized solution to (3.4), He, Müller, and Wang (2003) and He, Müller, Wang, and Yang (2010) impose high-level conditions on the cross-correlation operator to ensure existence (see Proposition 4.2 in He, Müller, and Wang (2003)). Since our focus is on prediction, we focus instead on the achievable IMSE, allowing for the possibility that unregularized canonical variates need not be well-defined. This approach parallels the analysis of Cupidon, Eubank, Gilliam, and Ruymgaart (2008) who consider estimation of the largest canonical correlation between two L_2 processes and show that this scalar parameter can be approximated arbitrarily closely via regularized canonical correlation analysis.

Yang, Müller, and Stadtmüller (2011) propose regression based on a singular value decomposition of the operator $T_{\mu\tau}$ rather than $T_{\mu\mu}^{-1/2}T_{\mu\tau}$,

$$(T_{\mu\tau}h)(s) := \sum_{k=1}^K \sqrt{\nu_k} \langle \zeta_k^*, h \rangle \xi_k(s)$$

A finite- K expansion based on spectral analysis of $T_{\mu\tau}$ has no known optimality properties but elegantly sidesteps the problem of inverting $T_{\mu\mu}$ and therefore works under weaker conditions and is numerically stable in the absence of regularization.

Another important approach proposed by Benatia, Carrasco, and Florens (2017) who directly minimize the mean-square error of prediction in a functional linear regression model, subject to a nuclear norm penalization of the projection operator B . The particular appeal of that approach is that it offers a “one-stop” approach towards regularization with a single tuning parameter, and directly optimizes the in-sample predictive performance subject to that penalty. Their approach assumes that B is a Hilbert-Schmidt (kernel) operator which is not guaranteed under our assumptions. Their approach is also designed towards delivering a consistent estimator for B in a setting where G is large.

Our focus is instead on heavily regularized but interpretable solutions $B_{a,K}$ for moderate values of G , where the singular value representation delivers a sparse representation of the operator in terms of a functions of x . The estimated scores can then be used to assess whether the target site is comparable to the experimental sample in terms of the most predictive features identified by the method. The extrapolated CATE can be interpreted as a best linear predictor given the estimated basis functions, and regularization bias results in a potentially suboptimal (with respect to the IMSE), but ultimately valid construction of features from $\mu_g(x; 0)$.

3.3. Estimation. The representation in Corollary 3.1 motivates an estimator of the form

$$\hat{\tau}_{g^*}(x) := \hat{\tau}(x) + \sum_{k=1}^K \hat{t}_{g^*k} \hat{\psi}_{ka}(x)$$

where $\hat{\tau}(x) := \hat{\mu}(x; 1) - \hat{\mu}(x; 0)$, $\hat{t}_{g^*k} = \langle \hat{\mu}_{g^*}, \hat{\phi}_{ka} \rangle$ for a nonparametric estimator $\hat{\mu}_g$ of $\mu_g(x; 0)$, and the basis functions $\hat{\phi}_{1a}, \dots, \hat{\phi}_{Ka}$ are obtained by solving an empirical analog of the generalized eigenvalue problem (3.5).

Here we develop our approach for the case of densely sampled clusters, $n \rightarrow \infty$, for a discussion of the setting with sparse samples, see Appendix A. We estimate $\mu(x; d) := \mathbb{E}[\mu_{g^*}(x; d)]$ and $H(x_1, x_2; d_1, d_2) := \text{Cov}(\mu_{g^*}(x_1; d_1), \mu_{g^*}(x_2; d_2))$ using nonparametric estimators $\hat{\mu}(x; d)$ and $\hat{H}(x_1, x_2; d_1, d_2)$. While our theory is not restricted to one particular choice of nonparametric estimators, following Yao, Müller, and Wang (2005a) we give results for local linear estimators: For each experimental cluster, let

$$\hat{\mu}_g(x; d) := \arg_{b_0, b_1} \min \sum_{i=1}^{n_g} w_{gi}(x; d) (Y_{gi} - b_0 - b_1(x - X_{gi}))^2 \quad (3.9)$$

with nonparametric weights

$$w_{gi}(x; d) := \mathbb{1}\{D_{gi} = d\} K\left(\frac{X_{gi} - x}{h}\right).$$

Here, $K(u)$ is a kernel function with standard properties (see Assumption A.1 in the Appendix for formal conditions on $K(\cdot)$), and the bandwidth $h > 0$ is chosen according to sample size G, n , the dimension of X_{gi} and assumed smoothness of the estimands. We also let

$$\hat{M}_g(x_1, x_2; d_1, d_2) := \arg_{b_0^{(g)}, b_{11}^{(g)}, b_{12}^{(g)}} \min \sum_{j \neq i} H_{gij}(x_1, x_2, \mathbf{b}) w_{gi}(x_1; d) w_{gj}(x_2; d) \quad (3.10)$$

where

$$H_{gij}(x_1, x_2, \mathbf{b}) := \left(Y_{gi} Y_{gj} - b_0^{(g)} - b_{11}^{(g)}(X_{gi} - x_1) - b_{12}^{(g)}(X_{gj} - x_2) \right)^2.$$

We then construct

$$\begin{aligned} \hat{\mu}(x; d) &:= \frac{1}{G-1} \sum_{g=1}^G R_g \hat{\mu}_g(x; d) \\ \hat{H}(x_1, x_2; d_1, d_2) &:= \frac{1}{G-1} \sum_{g=1}^G R_g \hat{M}_g(x_1, x_2; d_1, d_2) - \hat{\mu}(x_1; d_1) \hat{\mu}(x_2; d_2) \end{aligned}$$

In principle, the bandwidth could be chosen differently for estimation of $\hat{\mu}(x; d)$ and $\hat{H}(x_1, x_2; d_1, d_2)$, however in our theory in Appendix A, the optimal rate turns out to be the same for either estimator in the densely sampled case. Apart from kernel-based approaches, other possible methods include series estimators, random forests, or neural networks. The

choice of nonparametric estimator will generally depend on the support of the covariates and other practical considerations.

This estimator is an average of separate local linear estimators for each of the $G - 1$ experimental clusters, in a departure from the approach in Yao, Müller, and Wang (2005a) who propose a local linear estimator based on the pooled data from all $G - 1$ clusters. There are two reasons for a different approach in the densely sampled case: for one we do not assume that attributes (“positions”) are sampled from the same distribution in all clusters, but sites may differ in the distribution of X_{gi} . We furthermore assume “dense” samples from a small number of clusters, whereas they consider scenarios in which n is small, but G grows large. In our setup, cluster-specific moments can be estimated consistently, whereas between-cluster variation is the dominant source of estimation noise due to small G . That source of estimation error would be amplified in a nonparametric regression step, so our approach seeks to avoid that potential problem.

To describe the estimator for the basis functions $\hat{\phi}_1, \dots, \hat{\phi}_K$ let

$$\hat{H}_{\mu\mu}(x_1, x_2) := \hat{H}(x_1, x_2; 0, 0) \quad \text{and} \quad \hat{H}_{\mu\tau}(x_1, x_2) := \hat{H}(x_1, x_2; 1, 0) - \hat{H}(x_1, x_2; 0, 0).$$

In analogy to the definition for the operators $T_{\mu\mu}$ and $T_{\mu\tau}$, we can construct the estimators

$$\begin{aligned} (\hat{T}_{\mu\mu}h)(x) &= \int \hat{H}_{\mu\mu}(x, s)h(x)f_0(s)ds \\ (\hat{T}_{\mu\tau}h)(x) &= \int \hat{H}_{\mu\tau}(x, s)h(x)f_0(s)ds \\ (\hat{T}_{\mu\tau}^*h)(x) &= \int \hat{H}_{\mu\tau}(s, x)h(x)f_0(s)ds \end{aligned} \tag{3.11}$$

for any square integrable function h , and let $\hat{T}_{\mu\mu a} := \hat{T}_{\mu\mu} + a\text{Id}$.

In order to estimate the eigenfunctions $\phi_{1a}^*, \phi_{2a}^*, \dots$, we solve the generalized eigenvalue problem (3.5) after replacing the operators $T_{\mu\tau}, T_{\mu\mu}$ with their estimates as defined above. Specifically, we can find the functions $\hat{\xi}_{1a}, \dots, \hat{\xi}_{Ka}$ solving the eigenvalue problem

$$\hat{T}_{\mu\mu a}^{-1/2} \hat{T}_{\mu\tau} \hat{T}_{\mu\tau}^* \hat{T}_{\mu\mu a}^{-1/2} \hat{\xi}_{ka} = \hat{\lambda}_k \hat{\xi}_{ka} \tag{3.12}$$

and that are associated with the K largest eigenvalues in $\hat{\lambda}_1 \geq \hat{\lambda}_2 \geq \dots$. We then solve for

$$\hat{\phi}_{ka} := \hat{T}_{\mu\mu a}^{-1/2} \hat{\xi}_{ka}. \tag{3.13}$$

Since $\hat{T}_{\mu\mu}$ is a nonnegative (nonnegative definite) operator and $a > 0$, the operator on the left-hand side of (3.12) is Hermitian and compact, and the inverse problem (3.13) is well-posed. To implement the procedure we use linear sieve approximations to the eigenfunctions, which converts (3.12) into a finite-dimensional eigenvalue problem.⁴

We then construct $\hat{\psi}_{ka}$ by applying the estimator of $T_{\mu\tau}^*$ to the estimated eigenfunction $\hat{\phi}_{ka}$,

$$\hat{\psi}_{ka}(x) := \left(\hat{T}_{\mu\tau}^* \hat{\phi}_{ka} \right) (x) \equiv \int \hat{H}_{\mu\tau}(s, x) \hat{\phi}_{ka}(s) f_0(s) ds$$

for $k = 1, \dots, K$. Using these estimates, we then obtain

$$\hat{t}_{g^*k} := \langle \hat{\mu}_{g^*}, \hat{\phi}_{ka} \rangle$$

Substituting this into the formula from Corollary 3.1, our estimate of the conditional ATE $\tau_{g^*}(x)$ is

$$\hat{\tau}_{g^*}(x) = \hat{\tau}(x) + \sum_{k=1}^K \hat{t}_{g^*k} \hat{\psi}_{ka}(x)$$

Appendix A gives convergence rates for these estimators both for densely and sparsely sampled sites. Specifically, assuming equal numbers of cross-sectional observations for each site, $n_g \equiv n$, Theorem A.1 gives the rate

$$r_{Gn} = \frac{1}{G} + h^2 + \left(\frac{\log n}{Gnh^d} \right)^{1/2}$$

for the preliminary nonparametric estimators of mean and covariance functions if sites are **densely sampled** ($n_G \rightarrow \infty$ as $G \rightarrow \infty$) and treatment is randomized among units in each site. If treatment is instead randomized at the site level, the approach to estimating the covariance function $H(x_1, x_2; d_1, d_2)$ has to be modified as discussed in the appendix, resulting in a rate

$$r_{Gn} = \frac{1}{\sqrt{G}} + h^2 + \left(\frac{\log n}{Gnh^d} \right)^{1/2}$$

for the densely sampled case. For **sparsely sampled** sites (n_G bounded), $H(x_1, x_2; d_1, d_2)$ can still be estimated consistently as $G \rightarrow \infty$ by pooling observation pairs across sites. Convergence for eigenfunctions and the IMSE of prediction depends on the asymptotic rate of estimation of the covariance function $H(x_1, x_2; d_1, d_2)$,

$$r_{Gn} = h^2 + \left(\frac{\log G}{Gh^{2d}} \right)^{1/2}$$

whereas the rate for estimating the conditional mean function $\mu(x_1; d_1)$ is faster for reasonable bandwidth choices.

⁴See e.g. Ramsay and Silverman (2005), chapter 8.4.2.

Given these preliminary rates, Theorem A.2 gives a rate

$$\|\hat{\phi}_k - \phi_{ka}\| = O_p(a^{-3/2}r_{Gn})$$

for estimation of the eigenfunctions, and Corollary A.3 shows that the IMSE of prediction using the estimated basis function is

$$|IMSE_K[\hat{\phi}_1, \dots, \hat{\phi}_K] - IMSE_K^*| = O_P(a + a^{-3/2}r_{Gn})$$

Appendix A also provides comparable rates for nonparametric estimation of mean and covariance functions using B-splines instead of local linear regression.

Since the transfer estimate is always a linear projection on the constructed features $\hat{\phi}_k$, these rates illustrate how fast the quality of the prediction improves as we approximate the optimal basis functions ϕ_k^* more closely. In general, that approximation requires the number of sites G to be not too small, especially if treatment was not randomized within each site. The difference in rates between the densely and sparsely sampled cases also illustrates how a larger number of cross-sectional observations n_g within each site can be leveraged to retrieve the optimal predictors more accurately, although in practice typically the number of sites G is the main limiting factor.

3.4. Site-Specific Covariates. A natural extension of the main framework concerns site-specific covariates W_g which may be observed in addition to the unit-level attributes X_{gi} . In this section we sketch a conceptual extension to our approach under the assumption that these covariates satisfy unconfoundedness conditions analogous to those for X_{gi} . When the number of experimental sites is not very large, controlling nonparametrically for a significant number of site covariates is generally not feasible in practice, so we consider this extension to be primarily of theoretical interest. For the purposes of this section, we also regard the G sites as random draws from a superpopulation in order to be able to define conditional expectations given the covariate W_g in a meaningful way.

To be specific, we consider a version of the original problem, where Assumption 2.1 is changed to

$$D_{gi} \perp\!\!\!\perp (Y_{gi}(0), Y_{gi}(1)) | X_{gi}, W_g, R_g = 1$$

and Assumption 2.2 is strengthened to assume that g^* is drawn independently of $Y_{g^*i}(0), Y_{g^*i}(1), X_{g^*i}$, and W_{g^*} . Assuming that the g th cluster represents a random draw from a superpopulation, we can define the conditional expectation

$$\mu(x, w; d) := \mathbb{E}[Y_{g^*i}(d) | X_{g^*i} = x, W_{g^*} = w]$$

and covariance function

$$H(x_1, x_2, w; d_1, d_2) := \mathbb{E} \left[(Y_{g^*1}(d_1) - \mu(x_1, w; d_1))(Y_{g^*2}(d_2) - \mu(x_2, w; d_2)) \middle| X_{g^*1} = x_1, X_{g^*2} = x_2, W_{g^*} = w \right]$$

where expectations are with respect to the joint distribution of potential values, attributes, and W_g in that superpopulation.

We can then apply the previous method conditional on $W_{g^*} = w_{g^*}$, where we replace the unconditional mean function $\mu(x; d)$ with an estimate of estimate $\mu(x; w_{g^*}; d)$, and form the analogs of the covariance operators $T_{\mu\mu}$ and $T_{\mu\tau}$ from estimates of the conditional covariance function $H_{d_1d_2}(x_1, x_2; w_{g^*})$. The conditionally optimal basis functions $\phi_1^*, \dots, \phi_K^*$ are then obtained from an eigenanalysis of the conditional covariance operators given W_{g^*} . Such an approach would effectively amount to a regression adjustment for the mean and covariance functions for $\mu_{g^*}(x; d)$ with respect to W_{g^*} .

For modest values of G , the scope for fully nonparametric adjustments to site-specific covariates is fairly limited for practical purposes, in contrast to “micro” (unit-specific) covariates where our approach can leverage the size of the cross-sectional sample for each site to construct approximately optimal adjustments to estimates for the CATE. Dehejia, Pop-Eleches, and Samii (2021) used machine learning methods to adjust (unconditional) ATE estimates for site-specific covariates, however a fully nonparametric site-specific adjustment to the estimated CATE poses greater challenges given realistic sample sizes.

4. EMPIRICAL APPLICATION

We illustrate our approach with an empirical application to the estimation of the effect of conditional cash transfers on children’s school attendance. In this literature, a conditional cash transfer is a recurring grant paid to an eligible household that is explicitly linked to a child attending school or other household decisions the policy maker wants to encourage, with transfer amounts of the order of 5-20 percent of average household consumption in the target population. In 1998-99 the government of Mexico conducted a large-scale randomized trial during the roll-out of the *PROGRESA/OPORTUNIDADES* program (Schultz (2004) and Todd and Wolpin (2006)), and similar programs have subsequently been implemented in over 50 other countries (see Banerjee, Hanna, Kreindler, and Olken (2017) for a recent summary).

4.1. Data. We combine samples from *PROGRESA* with four additional randomized studies that were conducted in Indonesia (*Program Keluarga Harapan (PKH)*, see Alatas (2011) and Cahyadi, Hanna, Olken, Prima, Satriawan, and Syamsulhakim (2020)), Morocco (*Tayssir*, see Benhassine, Devoto, Duflo, Dupas, and Pouliquen (2015)), Kenya (*Kenya CT-OVC*, Team (2012)), and Ecuador (*Bono de Desarrollo Humano (BDH)*, Edmonds and Schady

(2012)).⁵ Each of these field trials was a multi-site study conducted by the national government, where participants were recruited from a previously selected sample of clusters (schools, villages, or other comparable unit). In each study, clusters were drawn from a subset of the major administrative regions in each of these countries.

It should be noted that there were substantial differences in the exact design of the incentive between these five studies. In particular, Progresa and PKH explicitly make part of the transfer dependent on school attendance, whereas Tayssir experimented with a nudge rather than a strictly conditional transfer. For the remaining two studies in Kenya and Ecuador, cash transfers were unconditional. We deliberately pool the sites to replicate a realistic scenario for which a policy has been adapted to local circumstances, due to practical constraints and the policymaker’s preferences.

Our main focus is on leveraging cross-site variation within each multi-site trial to extract predictive information on site-specific heterogeneity in the CATE. The five study populations in Mexico, Indonesia, Morocco, Ecuador, and Kenya are likely systematically different in terms of many factors that cannot be modeled explicitly, such as the local educational system, the chosen target population within the geographic reach of the study, the specific manner in which the transfer scheme was implemented, etc. Nevertheless, sites also vary substantially within each study, e.g. according to travel distance to urban centers or secondary school, or whether the language of instruction is widely spoken in the community. Hence, some communities in the heterogeneous pool of clusters in, say, Mexico, may still be sufficiently similar to a target location in Morocco or Indonesia in terms of the predictive attributes, as determined by our method. We will assess to what extent between-study variation can be predicted from between site variation on a more disaggregated level.

We retain all observations of households that met the eligibility criteria for the program, and for whom we can reconstruct measures of school attendance and per capita household expenditure at baseline and follow-up, along with children’s age and gender, and the household head’s level of education. For school attendance we use self-reports from baseline and follow up household surveys rather than data from school records or random checks which were only collected for some of the studies used in our analysis. After dropping households with incomplete data and locations with fewer than 15 school-aged children, we obtain a sample of 640 clusters (sites) with average cluster sizes ranging from 18 (PKH, Indonesia) to 47 (PROGRESA, Mexico) and 51 (BDH, Ecuador). PROGRESA and TAYSSIR (Morocco) contribute the largest number of clusters (297 and 238, respectively) compared to 50 for PKH (Indonesia), 31 for BDH (Ecuador), and 24 for CT-OVC (Kenya). For the purposes of

⁵These studies were selected according to ease of access to the underlying microdata, where we excluded one additional study from Colombia (*Subsidios Condicionados a la Asistencia Escolar*, Barrera-Osorio, Bertrand, Linden, and Perez-Calle (2011)) due to our inability to reconstruct baseline attendance data from the replication package.

this analysis we assign equal weight to each cluster. Of those clusters, 434 were treated, the remaining clusters were in the control group.

4.2. Implementation. We compare our approach across three different prediction tasks - as a benchmark, we report some results for the in-sample fit, with $\mu(\cdot)$ and $H(\cdot)$ and resulting basis functions ϕ_k, ψ_k estimated from the full data set. We then consider cross-site prediction where for a given target site g^* , the basis functions are estimated from the remaining $G - 1$ sites, and the transfer estimate is obtained by estimating the principal scores $m_{g^*1}, \dots, m_{g^*K}$ from the baseline for the target site. Finally, we perform cross-study extrapolation, with the predictive model estimated from data excluding all other sites from the study that included the target site, for example predicting the outcome at a Progresa site using only data from sites in the remaining four studies.

Given the small to moderate cluster sizes, we choose an estimation approach suited to sparsely sampled functional data, see also Appendix A. The main difference to the densely sampled case is that the cluster-specific covariate distribution $f_g(x)$ for the weights in (3.9) and (3.10) cannot be estimated nonparametrically. We make the simplifying assumptions that gender and age are independent of location and household per capita expenditure, and per capita expenditure follows a log-normal distribution within each cluster, which we then estimate parametrically.

The setting also differs from the idealized setup discussed in the theoretical sections of the paper in that there is baseline data available for each experimental cluster. Furthermore, in each of these studies, treatment was randomized at the cluster level. We therefore construct predictors from the observed baseline data for $\mu_{gt}(x; 0) := \mathbb{E}[Y_{git}(0)|X_{git} = x]$ at $t = 0$, which are then used to predict conditional expectations $\mu_{gt}(x; 1) := \mathbb{E}[Y_{git}(d)|X_{git} = x]$ for $d \in \{0, 1\}$ and $t = 1$. The covariance operators between $\mu_{g0}(x; 0)$ and $\mu_{g1}(x; 1)$ or $\mu_{g1}(x; 0)$ are then estimated using the treatment and control clusters in the experimental population. We first consider the problem of predicting post-treatment outcomes from baseline outcomes in the treated clusters, where we can validate predictions directly against the observed data at the site level. We then implement the algorithm for predicting conditional average treatment effects, which are not directly observed at the cluster level for any of the experimental sites.

Given the limited number of distinct sites, and also in order to apply consistent variable definitions across studies we restrict the unit-specific covariates X_{gi} to four variables, the child’s gender, the child’s age in years, enrollment status at baseline, and log per-capita household expenditure. We also restrict the estimators for $\mu(\cdot)$ and $H(\cdot)$ to be additively separable in covariates, where we flexibly dummy out gender and age in years, and use B-splines of degree 2 to model variation with respect to log expenditure. Tuning parameters are chosen using cross-validation across clusters, where we separately target the integrated mean-square error of estimating the mean and covariance functions to determine the bandwidths

Prediction using IMSE-Optimal Basis Functions

	baseline mean	K=1	K=2	K=3	K=4	K=5	K=6
in-sample fit	0.1379	0.4398	0.5039	0.5038	0.5167	0.5191	0.4835
cross-site prediction	0.0136	0.3600	0.4484	0.4514	0.4524	0.4603	0.4252
cross-study prediction	-0.0400	0.2164	0.3198	0.2987	0.3282	0.3028	0.3267

Prediction using Functional PC

	baseline mean	K=1	K=2	K=3	K=4	K=5	K=6
in-sample fit	0.1379	0.1377	0.3871	0.3776	0.4051	0.4221	0.4224
cross-site prediction	0.0136	0.0896	0.3743	0.3544	0.3706	0.3878	0.3852
cross-study prediction	-0.0400	0.1519	0.2414	0.2988	0.2868	0.3134	0.3356

TABLE 1. Prediction of Post-Intervention Outcomes $\mu_{g1}(x; 1) - \mu(x; 1)$ using the leading K IMSE-optimal basis functions (top panel) and functional PC (bottom panel) as predictors. Entries correspond to correlation coefficients between actual mean at the site level and the baseline average (first column) and the prediction based on the leading K basis functions (remaining columns).

for local linear regression, and the mean-square error for cross-cluster prediction for the regularization parameter a in (3.5).

4.3. Results. We first report results for prediction of the **model shift in post-intervention outcomes** $\Delta\mu_g(x; 1) := \mu_g(x; 1) - \mu(x; 1)$ using the estimated IMSE-optimal predictors from (3.5), which were estimated using only the 434 treated sites. We assess their performance as predictors at the level of the individual site as well as after aggregating sites within each study. The number of knots for B-spline approximations was determined using (leave-one-site-out) cross-validation, targeting the mean function $\mu(x; d)$ and covariance function $H(x_1, x_2; d_1, d_2)$, respectively. The ridge parameter a was chosen based on estimated cross-site predictive performance, and cross-validation also suggests that for this application the optimal number of basis functions is $K = 2$.

Table 4.3 reports the correlation coefficient between the predicted model shift for the average effect at site g , $\widehat{\Delta\mu_{g1K}} := \frac{1}{n_g} \sum_{i=1}^{n_g} \sum_{k=1}^K \hat{t}_{gk} \hat{\psi}_k(x_{gi})$ with its post-hoc empirical counterpart, $\widehat{\Delta\mu_{g1}} := \frac{1}{n_g} \sum_{i=1}^{n_g} (Y_{gi1} - \hat{\mu}_1(X_{gi}))$. A natural alternative strategy would be to predict post-intervention outcomes using separate regression estimates stratified by average pre-intervention outcomes. In the first column we therefore report correlation coefficients with

Cross-Site Prediction							
Study	actual	K=1	K=2	K=3	K=4	K=5	K=6
MEX	-0.0077	-0.0006	-0.0033	-0.0015	-0.0018	-0.0018	-0.0033
MOR	0.0220	-0.0016	0.0259	0.0231	0.0228	0.0210	0.0266
IDN	0.0037	-0.0003	0.0053	0.0094	0.0086	0.0059	0.0133
KEN	0.0300	0.0353	0.0356	0.0432	0.0591	0.0580	0.0694
ECU	-0.0495	-0.0172	-0.0170	-0.0230	-0.0198	-0.0217	-0.0252

Cross-Study Prediction							
MEX	-0.0077	-0.0064	-0.0014	0.0007	0.0009	0.0004	0.0012
MOR	0.0220	-0.0008	0.0108	0.0213	0.0161	0.0238	0.0290
IDN	0.0037	-0.0004	-0.0006	0.0022	0.0014	-0.0002	0.0016
KEN	0.0300	0.0230	0.0200	0.0283	0.0441	0.0405	0.0412
ECU	-0.0495	-0.0165	-0.0150	-0.0201	-0.0186	-0.0128	-0.0144

TABLE 2. Predictions of post-intervention outcomes $\mu_{g1}(x; 1) - \mu(x; 1)$ using the leading K IMSE optimal basis functions as predictors. Rows correspond to averages across sites for each of the five studies (Progresa, Tayssir, PKH, CT-OVC, BDH), “actual” corresponds to the empirical mean of $\mu_{g1}(x; 1) - \mu(x; 1)$.

the corresponding predictors as a benchmark, where sites were binned into three groups of equal size (terciles) according to average enrollment at baseline.

According to our results, optimal basis functions result in substantially more precise predictions relative to binned estimates and standard FPC, where gains are largest for the first two basis functions, and then plateau for 3 or more components. For example for cross-site prediction, we find a correlation coefficient of around 0.36 (corresponding to an R-square of 0.13) after using only the leading baseline function ($K = 1$), which still gradually improves as additional terms are included. For K larger than 5 or 6, terms are fairly noisily estimated and therefore do not lead to substantial additional improvements. As expected, the strength of correlation for cross-study extrapolation is lower than for cross-site prediction, but still substantial. Stratified estimation by pre-intervention *levels* of outcomes does not appear to extract much predictive information at all, suggesting that the gains observed for our estimator exploit information on how outcomes vary together with covariates at each site.

In Table 4.3, we compare cross-site averages of predictions, where we let \mathcal{G}_s denote the subset of $\{1, \dots, G\}$ corresponding to sites that were part of study $s = 1, \dots, 5$. For each study s we then compare $\frac{1}{|\mathcal{G}_s|} \sum_{g \in \mathcal{G}_s} (\hat{\mu}_{g1K} - \hat{\mu}_1)$ to their “realized” empirical counterparts,

Cross-Site Prediction							
Study	actual	K=1	K=2	K=3	K=4	K=5	K=6
MEX	-0.0077	0.0089	-0.0049	-0.0051	-0.0040	-0.0036	-0.0034
MOR	0.0220	-0.0042	0.0258	0.0285	0.0271	0.0271	0.0281
IDN	0.0037	0.0043	0.0090	0.0221	0.0166	0.0255	0.0213
KEN	0.0300	0.0074	0.0550	0.0943	0.0921	0.0912	0.0961
ECU	-0.0495	0.0047	-0.0138	-0.0182	-0.0213	-0.0251	-0.0371

Cross-Study Prediction							
MEX	-0.0077	0.0005	-0.0032	-0.0066	-0.0013	-0.0021	-0.0018
MOR	0.0220	-0.0011	-0.0043	0.0286	0.0373	0.0364	0.0364
IDN	0.0037	0.0035	0.0077	0.0174	0.0105	0.0168	0.0125
KEN	0.0300	0.0041	0.0340	0.0604	0.0543	0.0505	0.0507
ECU	-0.0495	0.0053	-0.0118	-0.0152	-0.0192	-0.0366	-0.0370

TABLE 3. Predictions of post-intervention outcomes $\mu_{g1}(x; 1) - \mu(x; 1)$ using the leading K functional PC as predictors. Rows correspond to averages across sites for each of the five studies (Progresa, Tayssir, PKH, CT-OVC, BDH), “actual” corresponds to the empirical mean of $\mu_{g1}(x; 1) - \mu(x; 1)$.

$\frac{1}{|\mathcal{G}_s|} \sum_{g \in \mathcal{G}_s} (\hat{\mu}_{g1} - \hat{\mu}_1)$. We find that the predicted average outcomes reflect some of the systematic differences, although especially for BDH and CT-OVC, the numbers and sizes of clusters are smaller, so results are likely noisier than for the first three studies. It should also be noted that the baseline outcome Y_{gi0} is already included as a control for post-intervention outcomes in the specification of μ_1 . Without controlling for state-dependence at the individual level (not reported here), the correlation between pre- and post-intervention outcomes at the site-level is substantially stronger, but the relative comparison between using baseline averages as the “naive” predictor and prediction using K estimated basis functions is qualitatively similar.

We next repeat the same analysis using the respective functional PC for $\hat{\mu}_{g0}(x)$ and $\hat{\mu}_{g1}(x)$, see Table 4.3. Since the general patterns of school attendance as a function of child and household attributes were unlikely to have shifted fundamentally between baseline and follow-up, and the effect of the intervention was sizeable but incremental, we should expect the functional PC for the baseline to be fairly closely aligned with those at follow-up, and therefore perform very well as predictors for post-intervention outcomes. This is confirmed by the quantitative results, where performance is very similar to the IMSE optimal predictors, likely within or close to the margin of error, although we do not formally quantify estimation error for these results.

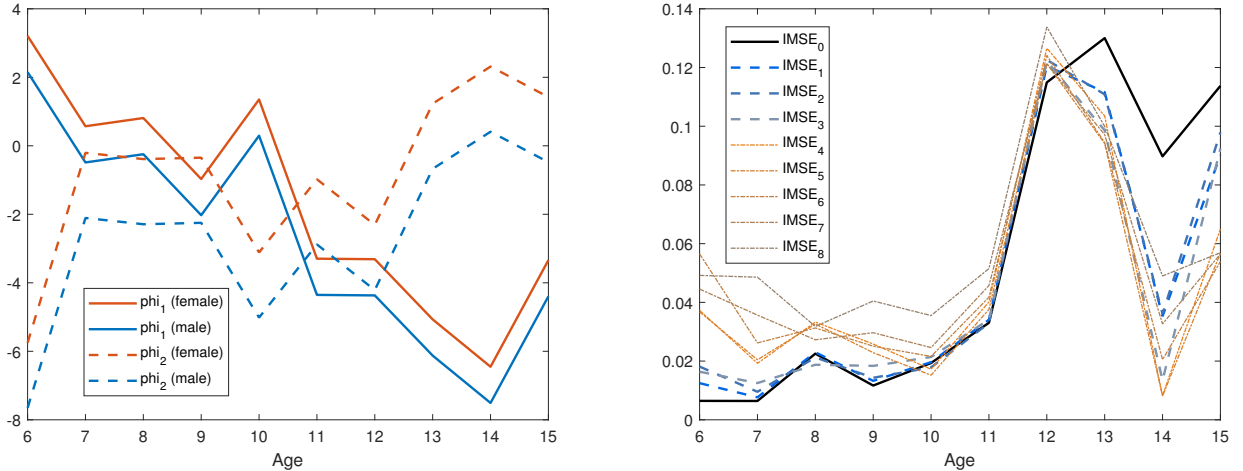


FIGURE 1. Optimal basis functions for predicting $\mu_{g1}(x)$ (left), and conditional MSE of prediction given age using 0 to 8 basis functions (right).

In Figure 4.3, we report estimates of the leading two leading optimal basis functions for predicting conditional post-intervention outcomes. These basis functions do not appear to vary much with income, so we plot ϕ_1, ϕ_2 only as functions of gender and age alone. Since post-intervention outcomes are also observed at all treated sites, we also plot the conditional mean square error for predicting the post-intervention response for those sites, where $IMSE_0$ corresponds to the case in which we use the unadjusted cross-site average as a predictor, and $IMSE_k$ for the prediction using the first k basis functions ϕ_1, \dots, ϕ_k as predictors. While the predictors appear to be responsive to differences in enrollments at young and old ages, most of the improvement in the forecast is for enrollment at ages 12 and above, where (within and across site) variation is generally highest. Most of the improvement in the conditional forecast results from including the first two factors, whereas additional predictors lead to a significant deterioration of the forecast at lower ages. This is in line with the number $K = 2$ of factors selected by cross-validation.

Finally, Figure 4.3 plots the estimated scores corresponding to the leading two basis functions, $\hat{m}_{g1}, \hat{m}_{g2}$ together with variance ellipses corresponding to a 80 percent confidence set for jointly normal variates. We can see that while there is substantial overlap in the support, their distributions vary substantially across the five studies, with especially some sites in the BDH and CT-OVC differing quite substantially from those in the other three studies.

We next repeat the analysis for prediction of **model shifts in site-specific treatment effects** $\tau_g(x) - \tau(x)$, both using IMSE-optimal basis functions and functional PC as predictor (Tables 4.3). These results were obtained combining the data from the 434 treated and 206 control sites, and since the covariance operator of $\mu_g(x; 0)$ with the baseline is estimated

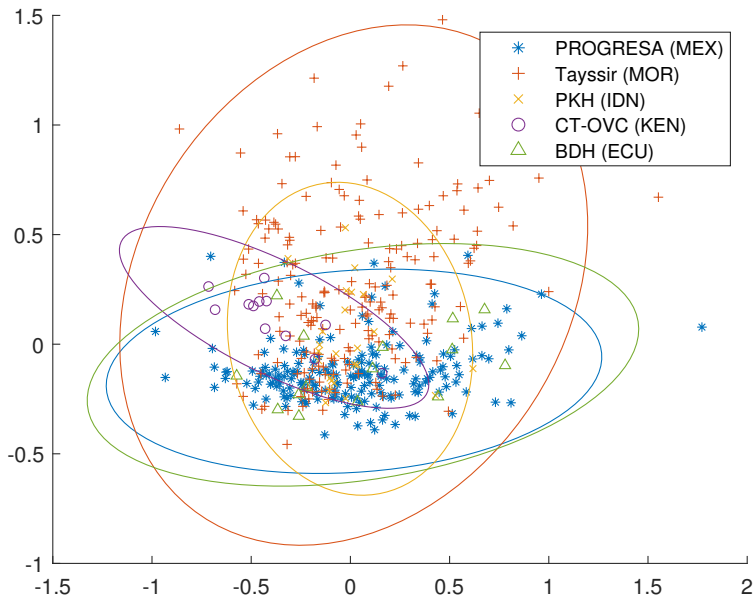


FIGURE 2. Estimated scores for leading $K = 2$ IMSE-optimal predictors of $\mu_{g1}(x)$.

Cross-Site Prediction							
Study	actual	K=1	K=2	K=3	K=4	K=5	K=6
MEX	0.0011	-0.0006	-0.0019	-0.0011	-0.0028	-0.0029	-0.0031
MOR	0.0029	-0.0002	-0.0021	0.0161	0.0198	0.0213	0.0178
IDN	-0.0173	-0.0022	-0.0135	-0.0455	-0.0570	-0.0564	-0.0577
KEN	-0.0506	-0.0394	-0.0301	-0.0253	-0.0245	-0.0197	-0.0198
ECU	-0.0264	-0.0005	-0.0053	-0.0057	-0.0076	-0.0083	-0.0107

Cross-Study Prediction							
Study	actual	K=1	K=2	K=3	K=4	K=5	K=6
MEX	0.0005	-0.0088	-0.0046	-0.0039	-0.0013	0.0040	0.0036
MOR	0.0021	-0.0015	0.0005	0.0309	0.0306	0.0236	0.0154
IDN	-0.0170	-0.0009	-0.0050	-0.0169	-0.0286	-0.0344	-0.0247
KEN	-0.0522	-0.0540	-0.0470	-0.0376	-0.0273	-0.0199	-0.0191
ECU	-0.0258	0.0023	-0.0062	-0.0081	0.0073	0.0033	0.0055

TABLE 4. Prediction of Conditional ATE $\tau_g(x) - \tau(x)$ averaging across sites for each of the five studies (Progresa, Tayssir, PKH, CT-OVC, BDH), using the leading K IMSE optimal basis functions as predictors. “Actual” corresponds to the empirical mean of $\tau_g(x) - \tau(x)$.

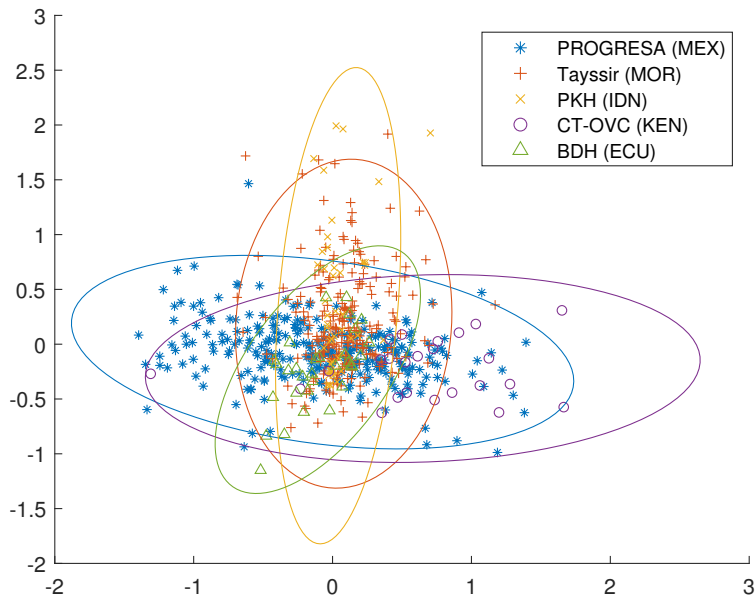


FIGURE 3. Estimated scores for leading $K = 2$ IMSE-optimal predictors of $\tau_g(x)$.

using only data from the substantially smaller control group, we should expect the resulting estimates to be less precise than for predicting post-intervention average outcomes.

In all five RCTs, treatment was randomized at the cluster level, so we can't directly assess the performance of either type of predictor at that level, but we can still aggregate actual and predicted effects at the level of the study. Here, average predictions based on the IMSE optimal basis functions match the sign and approximate magnitudes of post-hoc realized effects for all values of K , whereas at least 3 or 4 functional principal components appear to be necessary to match at least some qualitative aspects of study-level averages. We also report the estimated scores for predicting conditional ATEs plotted in Figure 4.3.

For any of these comparisons, it should also be noted that both types of predictions are based on the unconfounded location assumption (Assumption 2.2), whereas realized conditional effects also reflect systematic differences between studies that can't be predicted by extrapolating intra-study variation among sites. Most importantly, the five studies differ in terms of the exact implementation of the incentive, and also country specific factors. Most importantly, cash transfer for CT-OVC in Kenya and BDH in Ecuador were unconditional, whereas transfers under Progresas, PKH, and Tayssir were conditioned on, or connected to, the child's enrollment in school. While cross-site average treatment effects for those two studies were indeed substantially lower than the cross-study average (first column in Table 4.3), our method appears to replicate most of that difference for the Kenyan sites, whereas it fails to reproduce the deviation from the cross-study average only for Ecuador.

Cross-Site Prediction							
Study	actual	K=1	K=2	K=3	K=4	K=5	K=6
MEX	0.0011	-0.0008	-0.0014	-0.0015	-0.0018	-0.0020	-0.0027
MOR	0.0029	0.0004	0.0153	0.0150	0.0157	0.0160	0.0164
IDN	-0.0173	0.0003	-0.0002	-0.0160	-0.0169	-0.0167	-0.0245
KEN	-0.0506	-0.0321	-0.0308	-0.0202	-0.0152	-0.0151	-0.0132
ECU	-0.0264	0.0018	-0.0025	-0.0018	-0.0095	-0.0182	-0.0185

Cross-Study Prediction							
MEX	0.0005	-0.0005	-0.0010	-0.0027	-0.0022	-0.0027	-0.0026
MOR	0.0021	-0.0003	-0.0073	-0.0288	0.0028	0.0034	0.0031
IDN	-0.0170	-0.0001	0.0018	-0.0022	0.0072	0.0070	0.0075
KEN	-0.0522	-0.0299	-0.0297	-0.0021	0.0031	0.0074	0.0052
ECU	-0.0258	0.0047	-0.0005	0.0047	0.0073	-0.0039	-0.0038

TABLE 5. Prediction of Conditional ATE $\tau_g(x) - \tau(x)$ averaging across sites for each of the five studies (Progesa, Tayssir, PKH, CT-OVC, BDH), using the leading K functional PC as predictors. “Actual” corresponds to the empirical mean of $\tau_g(x) - \tau(x)$.

5. CONCLUSION

We investigate how to exploit observed between-site variation within one or several studies to predict outcomes using baseline data for new “target” sites. The premise of our approach is that agent responses at the micro level follow some universal patterns across study populations. These responses are generally confounded by site-specific factors of an unknown structure, but cross-sectional patterns of attributes and outcome at baseline for each site typically contain useful information regarding those environmental factors in a target site, and may help identify “comparable” sites in the experimental sample. We chose to focus on a nonparametric, linear version of the problem primarily for clarity and ease of implementation, and nonseparable or structural models with sufficiently flexible specifications of site-specific heterogeneity may be another fruitful approach to this problem.

We give a finite-population formulation for the statistical problem of evaluating out of sample forecast performance. We define the target for the transfer estimate as a pseudo-true parameter which reflects the relevant information regarding likely outcomes at the target site that may be learned from previously observed contexts. The corresponding prediction problem is equivalent to functional regression, but given the limited number of sites can only estimate heavily regularized version of the problem. We therefore choose a regularization

approach that targets a small number of “most predictive” features of the distribution of outcomes in the baseline. Those optimal predictors are solutions to a generalized eigenvalue problem in terms of the covariance operators of μ_g and τ_g . The approach can be adapted to sparsely or densely sampled sites, as well as randomization within or between clusters, resulting in different convergence rates.

APPENDIX A. ASYMPTOTIC THEORY

This section gives convergence rates for the estimated eigenfunctions $\hat{\phi}_k, \hat{\psi}_k$ and the resulting integrated mean square error relative to the optimal benchmark $IMSE_K^*$. We consider rates as both G and $n_g \equiv n$ grow to infinity, possibly at different rates. We first state results for the case of densely sampled clusters, $n \rightarrow \infty$ based on local linear estimators for the mean and covariance functions. We then discuss estimation using B-splines, and rates for the sparsely sampled case as well as site-based randomization.

A.1. Nonparametric Estimation of Covariance Functions. We first derive convergence rates for the local linear estimator of the covariance function $H(x_1, x_2; d_1, d_2)$. Following Hansen (2008), we assume the following regarding the kernel function

Assumption A.1. (Kernel Function) *The multivariate kernel function $K : \mathbb{R}^d \rightarrow \mathbb{R}$ satisfies (a) $|K(u)| \leq \bar{K} < \infty$ and $\int |K(u)| du \leq \mu < \infty$. Furthermore, (b) $K(u)$ is differentiable and there exist $\Lambda_1, L < \infty$ and $\nu > 1$ such that $\|\nabla_u K(u)\| \leq \Lambda_1 \min\{1, \|u\|^{-\nu}\}$ for $\|u\| > L$. (c) The first two moments of the kernel satisfy the conditions $\int K(u) du = 1$, $\int uK(u) du = 0$, and $\int uu'K(u) du = \Omega$, a finite, positive definite matrix.*

Parts (a) and (c) are fairly standard in the literature, the bound in part (b) is important for the uniformity arguments. These assumptions are satisfied by commonly used kernel functions such as the Gaussian or Epanechnikov kernel. Hansen (2008) and Graham, Niu, and Powell (2021) consider an alternative set of conditions for kernel functions with bounded support that need not be differentiable, which could be used to replace part (b).

We consider uniform convergence over a compact subset of the support of X , without loss of generality $[0, 1]^d$. We can now state our main result regarding the rate of consistency for the local linear estimator for the conditional mean functions and their covariance kernel:

Theorem A.1. *Suppose that Assumptions 2.1-2.4 and A.1 hold. Furthermore, the bandwidth h satisfies $\left(\frac{n}{\log n}\right)^{1/3} h^d \rightarrow \infty$ and $\left(\frac{\log n}{Gnh^d}\right)^{1/2} \rightarrow 0$. Then the local linear estimators for $\mu(x; \mathbf{d})$ and the covariance operator $H_{d_1 d_2}(x_1, x_2)$ are consistent at the rate*

$$\begin{aligned} \sup_{d, x_1} |\hat{\mu}(x_1, d) - \mu(x_1, d)| &= O_p(r_{Gn}) \\ \sup_{d_1, d_2, x_1, x_2} \left| \hat{H}(x_1, x_2; d_1, d_2) - H(x_1, x_2; d_1, d_2) \right| &= O_p(r_{Gn}) \end{aligned}$$

where $r_{Gn} = \frac{1}{G} + h^2 + \left(\frac{\log n}{Gnh^d}\right)^{1/2}$, and the suprema are for $x_1, x_2 \in [0, 1]^d$. The rate optimal bandwidth minimizing the second term of either error is of the order $h^* = O\left(\left(\frac{\log n}{Gn}\right)^{\frac{1}{4+d}}\right)$, resulting in a rate $\frac{1}{G} + \left(\frac{\log n}{Gn}\right)^{\frac{2}{4+d}}$.

The proof uses uniform consistency results by Hansen (2008) and Graham, Niu, and Powell (2021) for nonparametric regression using cross-sectional and dyadic data and is provided in the appendix. The convergence rate consists of two separate contributions: the first component represents the error from estimating moments from the $G - 1$ experimental clusters, which excludes the single target cluster. The rate for this component is of the order $O_p(G^{-1})$ rather than its square root, owing to the fact that the estimands are the mean and covariance function for the sample of G sites, $G - 1$ out of which are used for estimation. If instead the population of interest consisted of a greater number additional target clusters growing at least at the order of G or an infinite meta-population, the rate on that leading term would instead be $O(G^{-1/2})$.

The second component represents the sampling error in nonparametric estimation of conditional mean functions in each cluster, where the optimal bandwidth sequence balances the respective rates for the smoothing bias and sampling error. It is also instructive to compare the rate to that in Theorem 1 of Yao, Müller, and Wang (2005a) who consider the case of sparse (finite- n) rather than dense samples from each site. For one the effective dimension for nonparametric estimation of the covariance kernel is only d in our problem rather than $2d$, reflecting the fact that the contribution for each cluster is a U-statistic averaging over $\binom{n}{2}$ terms, so that allowing n to grow results in a more favorable rate. A similar phenomenon was pointed out for nonparametric regression with dyadic data in Graham, Niu, and Powell (2021).

A.2. Estimation of Basis Functions ϕ_k, ψ_k . We next consider convergence rates for the estimated eigenfunctions given a preliminary estimator for mean and covariance function for the conditional average treatment effect function $\mu_g(x)$. We distinguish between settings where the optimal predictors ϕ_k^* are well-defined in the absence of regularization according to (3.4) and the general case in which we consider estimation of ϕ_{ka}^* for the regularized version of the problem (3.5), and ψ_{ka}^* given by Corollary 3.1.

We first state result in terms of a generic nonparametric estimator and its convergence rate, both under the inner product norm $\|\cdot\|$ as well as the sup norm. Asymptotic rates based on the local linear estimator are given further below.

Theorem A.2. *Suppose the estimator $\hat{H}(x_1, x_2; d_1, d_2)$ is consistent with rate*

$$\sup_{x_1, x_2, d_1, d_2} \left| \hat{H}(x_1, x_2; d_1, d_2) - H(x_1, x_2; d_1, d_2) \right| = O_p(r_{Gn}).$$

Then the estimators for the generalized eigenvalue problem (3.5) with regularization parameter $a > 0$ are consistent at respective rates $|\hat{\lambda}_k - \lambda_{ka}| = O_p(a^{-3/2}r_{Gn})$, $\|\hat{\psi}_k - \psi_{ka}\| = O_p(a^{-3/2}r_{Gn})$, $\|\hat{\phi}_k - \phi_{ka}\| = O_p(a^{-3/2}r_{Gn})$ for each $k = 1, \dots, K$. Furthermore, $\sup_x |\hat{\psi}_k(x) - \psi_{ka}(x)| = O_p(a^{-3/2}r_{Gn})$ and $\sup_x |\hat{\phi}_k(x) - \phi_{ka}(x)| = O_p(a^{-3/2}r_{Gn})$ for each $k = 1, \dots, K$.

The proof has a similar overall structure as that for results for functional principal components in Gobet, Hoffmann, and Reiß (2004) and Yao, Müller, and Wang (2005a) (Proposition 4.2 and Theorem 2, respectively), but requires some major adjustments. For the problem considered here, estimation of the operator itself requires regularization, and furthermore the rank of all covariance operators is less than or equal to G , treating the population of sites as fixed. We also allow the dimension of x to be greater than one and some of the relevant eigenvalues need not be unique. While each of these adjustments is incremental and leaves the general structure of the argument unchanged, we provide a self-contained proof in Appendix C below.

For the local linear estimator we can immediately obtain the following from Theorems A.1 and A.2:

Corollary A.1. *For each $k = 1, \dots, K$, let $\hat{\psi}_k, \hat{\phi}_k$ and $\hat{\nu}_k, \hat{\lambda}_k$ the estimators for eigenfunctions and eigenvalues using local linear estimators for $\mu(x)$ and $H_{d_1 d_2}(x_1, x_2)$ with a bandwidth sequence h satisfying*

$\left(\frac{n}{\log n}\right)^{1/3} h^d \rightarrow \infty$ and $\left(\frac{\log n}{nh^d}\right)^{1/2} \rightarrow 0$. Under the assumptions for Theorem A.1, the conclusions of Theorem A.2 hold for these estimators with the rate

$$r_{Gn} = \frac{1}{G} + h^2 + \left(\frac{\log n}{Gnh^d}\right)^{1/2}$$

Similarly, we can give the asymptotic rate for estimating the best linear predictor for the conditional average treatment effect as defined in (3.2), where the rates of individual components follow immediately from Theorem A.2.

Corollary A.2. *Suppose the estimators $\hat{\mu}(x; d)$ and $\hat{H}_{d_1 d_2}(x_1, x_2)$ are consistent with rates $\sup_{x_1, d_1} |\hat{\mu}(x_1; d_1) - \mu(x_1; d_1)| = O_p(r_{Gn})$ and $\sup_{x_1, x_2, d_1, d_2} |\hat{H}(x_1, x_2; d_1, d_2) - H(x_1, x_2; d_1, d_2)| = O_p(r_{Gn})$. Then for any fixed value of K , the estimator $\hat{\tau}_g^K(x)$ based on (3.2) is consistent at the rate*

$$\sup_{x \in \mathcal{X}} |\hat{\tau}_g(x) - \tau_g^K(x)| = O_p\left(a^{-3/2} r_{Gn}\right)$$

At present we do not derive the asymptotic distribution for functionals of $\hat{\tau}_g(x)$. Asymptotic normality of certain functionals of estimated eigenfunctions were derived in a different site by Christensen (2014). Whether his strategy of proof can be adapted to derive distributional results for our setup is left for future research.

We finally consider the case in which condition (3.7) holds and the solution to the unregularized problem (3.4) is well defined. It can be seen from the proof of Theorem A.2 that regularization is generally still necessary for estimation of the optimal functions $\phi_1^*, \dots, \phi_K^*$, but we can give a rate with which the IMSE given the estimated functions converges to the lower bound in Lemma 3.3. Specifically, for any K square-integrable functions ϕ_1, \dots, ϕ_K , we define

$$IMSE_K[\phi_1, \dots, \phi_K] := \int \min_{B \in \hat{\mathcal{H}}_K \times L_2(\mathcal{X})} \mathbb{E} [(\tau_g(x) - BP_K \mu_g(x))^2] f_0(x) dx$$

where $P_K : L_2(\mathcal{X}) \rightarrow \mathcal{H}_K$ denotes the operator associated with orthogonal projection onto the closed linear subspace $\mathcal{H}_K := \text{span}(\phi_1, \dots, \phi_K)$. Combining the rate results in Proposition 3.1 and Theorem A.2, we can then give the following

Corollary A.3. *Suppose that the Assumptions of Theorems A.1 and A.2 hold along with Condition (3.7). For the local linear estimator with bandwidth $h^* = O\left(\left(\frac{\log n}{Gn}\right)^{\frac{1}{4+d}}\right)$ and regularization parameter $a > 0$,*

$$|IMSE_K[\hat{\phi}_1, \dots, \hat{\phi}_K] - IMSE_K^*| = O_P\left(a + a^{-3/2} r_{Gn}\right)$$

where $r_{Gn} := \frac{1}{G} + \left(\frac{\log n}{Gn}\right)^{\frac{2}{4+d}}$.

The rate for the IMSE in a and r_{Gn} suggests that this upper bound is minimized at a rate $a = r_{nG}^{2/5}$ for the regularization parameter. For methods of functional data analysis, it is common to determine regularization parameters by cross-validation (see e.g. He, Müller, Wang, and Yang (2010)), however we do not formally establish consistency of such a method.

A.3. Sparsely Sampled Clusters. If the number of observed units in each cluster n_g is bounded or grows at a slow rate relative to G , we have to adapt the strategy for estimating the mean and covariance functions of $\mu_g(x; d)$ along the lines proposed by Yao, Müller, and Wang (2005a) for the problem of functional principal components.

A challenge relative to the densely sampled case is that the site-specific distribution of attributes $f_g(x)$ can no longer be estimated consistently. Instead, we assume that the cluster-specific distribution of attributes X_{gi} is either known or can be estimated parametrically with sufficient precision from the n_g observations in each cluster, so that individual observations can be reweighted accordingly to match the target distribution $f_0(x)$ in each cluster.⁶

Specifically, let

$$\hat{\mu}(x; d) := \arg_{b_0} \min_{b_0, b_1} \sum_{g=1}^G \sum_{i=1}^{n_g} w_{gi}(x; d, h_\mu) (Y_{gi} - b_0 - b_1(x - X_{gi}))^2$$

for $\mu(x; d)$. As before, $K(u)$ is a kernel function satisfying Assumption A.1, and the bandwidth $h > 0$ is chosen according to sample size G, n_g , the dimension of X_{gi} , and assumed smoothness of the estimands. The weights $w_{gi}(x; d, h) := \mathbb{1}\{D_{gi} = d\} \frac{f_0(x)}{f_g(x)} K\left(\frac{X_{gi} - x}{h}\right)$ are assumed to be known. We also let

$$\hat{H}(x_1, x_2; d_1, d_2) := \arg_{b_0^{(g)}} \min_{b_0^{(g)}, b_{11}^{(g)}, b_{12}^{(g)}} \sum_{g=1}^G \sum_{j \neq i} H_{gij}(x_1, x_2, \mathbf{b}) w_{gi}(x_1; d, h_H) w_{gj}(x_2; d, h_H)$$

for an appropriately chosen bandwidth h_H , where $H_{gij}(x_1, x_2, \mathbf{b}) := \left(Y_{gi}Y_{gj} - b_0^{(g)} - b_{11}^{(g)}(X_{gi} - x_1) - b_{12}^{(g)}(X_{gj} - x_2)\right)^2$

Then using arguments parallel to the proof of Theorem A.1, the convergence rates of the local linear estimators for $\mu(x; \mathbf{d})$ and the covariance operator $H_{d_1 d_2}(x_1, x_2)$ are given by

$$\begin{aligned} \sup_{d, x_1} |\hat{\mu}(x_1, d) - \mu(x_1, d)| &= O_p(r_{G\mu}) \\ \sup_{d_1, d_2, x_1, x_2} \left| \hat{H}(x_1, x_2; d_1, d_2) - H(x_1, x_2; d_1, d_2) \right| &= O_p(r_{GH}) \end{aligned}$$

where the sup is taken over $x_1, x_2 \in [0, 1]^d$ and $r_{G\mu} = h_\mu^2 + \left(\frac{\log G}{G h_\mu^d}\right)^{1/2}$ and $r_{GH} = h_H^2 + \left(\frac{\log G}{G h_H^{2d}}\right)^{1/2}$. A similar result was proven under slightly different conditions in Theorem 1 by Yao, Müller, and Wang (2005a).

Comparing these rates to those for the densely sampled case in Theorem A.1, the contributions of order $\frac{1}{G}$ are now unambiguously dominated by the remaining errors. Furthermore, in the rate for the covariance kernel, the bandwidth h_H now appears at the power h_H^{2d} (compared to h_H^d in the dense case). This is a consequence of the fact that the number of unit pairs in each cluster no longer increases to infinity under the sparsely sampled case. As a result, the optimal bandwidths for estimating $\mu(x; d)$ and $H(x_1, x_2; d_1, d_2)$ are generally at different rates and should therefore also be chosen separately in this case. As in the densely sampled case, we can then use Theorem A.2 to determine rates for eigenfunctions and eigenvalues. Unbiased estimators for the scores m_{gk}, t_{gk} are also available, however consistent estimation requires n_g growing large for the sites of interest.

A.4. Cluster-Based Randomization. We can also adapt the approach to the scenario in which treatment assignment is randomized at the cluster level, but a baseline survey of pre-intervention outcomes is available. Specifically, we let $D_{gi} \equiv D_g$ be the assigned treatment for all units in cluster g , and $Y_{git}(d)$ denote the potential value for the policy variable $D_{git} = d$ unit i at site g in period $t = 0, 1$. We then consider the

⁶For the combined studies of conditional cash transfers in the empirical application, this is unproblematic for some of the demographic variables, including the child's age and gender. On the other hand, the means and variances of log per capita household expenditure vary between sites, but separate histograms for each study suggest that the log-normal distribution provides a plausible parametric approximation to the marginal distribution.

problem of predicting post-intervention conditional average treatment effects

$$\tau_{g1}(x) := \mathbb{E}[Y_{gi1}(1) - Y_{gi1}(0) | X_{gi} = x]$$

based on $\mu_{g0}(x) := \mathbb{E}[Y_{gi0}(0) | X_{gi} = x]$, where the covariates X_{gi} are also assumed to be measured at baseline.

With cluster-level randomization, we only observe potential values $Y_{gi1}(1)$ for all units in a cluster g assigned to treatment, $D_g = 1$, or only $Y_{gi1}(0)$ for all units in a control cluster with $D_g = 0$. However under ignorable assignment,

$$D_g \perp\!\!\!\perp Y_{gi0}(0), Y_{gi1}(0), Y_{gi1}(1) | X_{gi}$$

and independent assignment across clusters, we can estimate the covariance function $H_{\mu\tau}(x_1, x_2) := \text{Cov}(\mu_{g0}(x_1), \tau_g(x_2))$ consistently as $G \rightarrow \infty$ via

$$\hat{H}_{\mu\tau}(x_1, x_2) := \hat{H}(x_1, x_2; 0, 1) - \hat{H}(x_1, x_2; 0, 0).$$

where $\hat{H}(x_1, x_2; 0, 1)$ and $\hat{H}(x_1, x_2; 0, 0)$ are nonparametric estimators for $\text{Cov}(\mu_{g0}(x_1), \mu_{g1}(x_2; 1))$ and $\text{Cov}(\mu_{g0}(x_1), \mu_{g1}(x_2; 0))$, respectively, obtained separately from the treatment and control clusters.

With minor modifications of the proofs of Theorem A.1 and Theorem 1 in Yao, Müller, and Wang (2005a) we can then obtain the convergence rates $r_{Gn} = \frac{1}{\sqrt{G}} + \delta_{Gn}^{-1} \left(h^2 + \left(\frac{\log n}{Gnh^d} \right)^{1/2} \right)$ for the densely sampled case where $n_g \equiv n \rightarrow \infty$ for each cluster. For the sparsely sampled case where n_g remains fixed, we obtain $r_{G\mu} = h_\mu^2 + \left(\frac{\log G}{Gh_\mu^d} \right)^{1/2}$ and $r_{GH} = h_H^2 + \left(\frac{\log G}{Gh_H^d} \right)^{1/2}$, so that the rates coincide with the case of within cluster-randomization. The eigenfunctions in (3.5) can then be obtained from Theorem A.2 as before.

A.5. Estimation using B-Splines. This section contains additional results for nonparametric estimation of the mean and covariance functions using B-splines as a convenient alternative to kernel estimation. As before, we consider estimation at covariate values on a compact subset \mathcal{X}^* of \mathbb{R}^d , without loss of generality, $\mathcal{X}^* \equiv [0, 1]^d$. We first define the B-spline basis functions, following the exposition in Chen and Christensen (2015).

We first partition the support of the d' th dimension of the continuously distributed components of X_{gi} with M_d knots $0 \equiv t_{0d'} < \dots < t_{M_d d'} \equiv 1$ for each $d' = 1, \dots, d$. For the B-spline of order $r > 1$ we also set $t_{-(r-1)d'} = t_{-(r-2)d'} = \dots \equiv t_{0d'}$, and for notational simplicity we only consider the case $M_{d'} \equiv M$ and $t_{jd'} \equiv t_j$ for all d' and assume that the mesh ratios for successive spline bases, $\max_{0 \leq j \leq M} \{t_{j+1} - t_j\} / \min_{0 \leq j \leq M} \{t_{j+1} - t_j\}$ are uniformly bounded for all $M = 1, 2, \dots$.

The univariate basis functions are then defined according to

$$\begin{aligned} N_{j,1}(x) &:= \mathbb{1}\{t_j \leq x < t_{j+1}\} \\ N_{j,r'}(x) &:= \frac{x - t_j}{t_{j+r'-1} - t_j} N_{j,r'-1}(x) + \frac{t_{j+1} - x}{t_{j+r'} - t_{j+1}} N_{j+1,r'-1}(x) \end{aligned}$$

recursively for $r' = 1, \dots, r$ and all j and we set $\frac{1}{0} \equiv 0$. The resulting function $N_{j,r}(x)$ are piecewise polynomial of order r and continuously differentiable up to order $r - 1$. After rescaling we denote the basis functions for a particular choice of r and M with

$$b_j^M(x) := \sqrt{M + r} N_{j,r}(x)$$

and denote

$$\mathbf{b}^M(x; d_1) := (b_{-(r-1)}(x) \mathbb{1}\{d_1 = 0\}, \dots, b_M(x) \mathbb{1}\{d_1 = 0\}, b_{-(r-1)}(x) \mathbb{1}\{d_1 = 1\}, \dots, b_M(x) \mathbb{1}\{d_1 = 1\}).$$

where the argument $d_1 \in \{0, 1\}$ corresponds to the treatment indicator.

Noting that we chose the same univariate basis for each dimension, we then define the multivariate spline bases

$$\mathbf{b}^{M,1}(\mathbf{x}_1; d_1) := \bigotimes_{d'=1}^d \mathbf{b}^M(x_{1d'}; d_1)$$

and

$$\mathbf{b}^{M,2}(x_1, x_2; d_1, d_2) := \mathbf{b}^M(x_1; d_1) \otimes \mathbf{b}^M(x_2; d_2)$$

by forming the tensor product of the univariate spline bases, so the resulting dimension of $\mathbf{b}^{M,1}$ is $(M+r)^d$. As for any linear sieve, it is also straightforward to impose additive separability among dimensions of X_{g_i} by omitting all interaction terms among the corresponding univariate basis functions from this tensor product.

Given the sample $X_{g_1}, \dots, X_{g_{n_g}}$ for the g th site, we construct the matrices

$$\mathbf{B}_{g1} := (\mathbf{b}_1^M(X_{g1}; D_{g1}), \dots, \mathbf{b}_1^M(X_{g_{n_g}}; D_{g_{n_g}}))$$

and

$$\mathbf{B}_{g2} := (\mathbf{b}_2^{M,2}(X_{g1}, X_{g2}; D_{g1}, D_{g2}), \dots, \mathbf{b}_2^{M,2}(X_{g_{n_g-1}}, X_{g_{n_g}}; D_{g_{n_g-1}}, D_{g_{n_g}})).$$

We can then define the site-specific estimates

$$\begin{aligned} \hat{\mu}_g(x_1; d_1) &:= \mathbf{b}_w^{M,1}(x_1; d_1) (\mathbf{B}'_{g1} \mathbf{B}_{g1})^{-1} \mathbf{B}'_{g1} \mathbf{Y}_g \\ &=: \frac{1}{n_g} \sum_{i=1}^{n_g} m_{gi}(x_1; d_1) \\ \hat{H}_g(x_1, x_2; d_1, d_2) &:= \mathbf{b}_w^{M,2}(x_1, x_2; d_1, d_2) (\mathbf{B}'_{g2} \mathbf{B}_{g2})^{-1} \mathbf{B}'_{g2} ((\mathbf{Y}_g - \mu_g) \otimes (\mathbf{Y}_g - \mu_g)) \\ &=: \binom{n_g}{2}^{-1} \sum_{1 \leq i < j \leq n_g} H_{n_g ij}(x_1, x_2; d_1, d_2) \end{aligned}$$

The resulting B-spline estimators for the mean and covariance functions are then given by

$$\hat{\mu}(x_1; d_1) \equiv \frac{1}{G} \sum_{g=1}^G \hat{\mu}_g(x_1; d_1)$$

and

$$\hat{H}(x_1, x_2; d_1, d_2) \equiv \frac{1}{G} \sum_{g=1}^G \hat{H}_g(x_1, x_2; d_1, d_2).$$

We can give the following convergence rates for B-spline estimators using this construction:

Proposition A.1. *Suppose that Assumptions 2.1-2.4 hold, and that the number M of knots satisfies $M \rightarrow \infty$ and $\frac{M^d \log n}{n} \rightarrow 0$. Then the B-spline estimators for $\mu(x; \mathbf{d})$ and the covariance operator $H_{d_1, d_2}(x_1, x_2)$ are consistent at the rate*

$$\begin{aligned} \sup_{d, x_1} |\hat{\mu}(x_1, d) - \mu(x_1, d)| &= O_p(r_{Gn}) \\ \sup_{d_1, d_2, x_1, x_2} \left| \hat{H}(x_1, x_2; d_1, d_2) - H(x_1, x_2; d_1, d_2) \right| &= O_p(r_{Gn}) \end{aligned}$$

where $r_{Gn} = \frac{1}{G} + (M/c_n)^{-2} + \left(\frac{M^d \log n}{Gn}\right)^{1/2}$, and the suprema are for $x_1, x_2 \in [0, 1]^d$. The rate optimal number of knots minimizing the second term of either error is of the order $M^* = O\left(\left(\frac{Gn}{\log n}\right)^{\frac{1}{4+d}}\right)$, resulting in a rate $\frac{1}{G} + \left(\frac{\log n}{Gn}\right)^{\frac{2}{4+d}}$.

This result takes the role of Theorem A.1, and convergence rates for estimation of eigenfunctions and the transfer estimator follow by plugging that rate into Theorem A.2 and Corollaries A.2 and A.3. The proof follows closely that of Theorem 2.1 in Chen and Christensen (2015), with only minor modifications to allow for expanding support and two-way averages in estimation of the covariance function. We therefore only provide a brief outline of the formal argument below.

APPENDIX B. PROOFS FOR SECTION 3

Before proving the main result, we give a characterization of the integrated mean square error of projection into closed linear subspaces of $L_2(\mathcal{X})$. Specifically, we consider the mean square error of projection of τ_{g^*} with respect to a general linear transformation μ_{g^*} .

We consider the problem where the domain of the operator B is restricted to \mathcal{H} , a closed linear subspace \mathcal{H} of \mathcal{N}^\perp , which was defined as the orthogonal complement of the null space of $T_{\mu\mu}$, $\mathcal{N} := \ker(T_{\mu\mu})$. It is known that for any linear operator $T : L_2(\mathcal{X}) \rightarrow L_2(\mathcal{X})$, $\text{im}(T)$ and $\ker(T)$ are linear subspaces of $L_2(\mathcal{X})$, and that $\ker(T)$ is closed if the linear operator T is bounded. Since \mathcal{H} is the orthogonal complement of the null space $\ker(T_{\mu\mu})$, it is a closed linear subspace of $L_2(\mathcal{X})$, so this allows for the choice $\mathcal{H} \equiv \mathcal{N}^\perp$. We also let the operator $P : L_2(\mathcal{X}) \rightarrow \mathcal{H}$ to denote the orthogonal projection on \mathcal{H} . Since \mathcal{H} is closed by assumption, that projection is well-defined by the Classical Projection Theorem (Theorem 2 on p.51 in Luenberger (1969)).

We can then characterize the integrated mean square error of projection as follows:

Theorem B.1. (*Integrated MSE of Projection*) *There exists a best linear predictor for τ_{g^*} of the form (2.5) based on μ_{g^*} that is of the form*

$$\tau_{g^*}^*(x) := \int \mu_{g^*}(s)\beta(s, x)f_0(s)ds$$

*If furthermore the operator $PT_{\mu\mu}A^*P : \mathcal{H} \rightarrow \mathcal{H}$ possesses an inverse, the minimized mean square error of prediction satisfies*

$$\int \mathbb{E} [(\tau_{g^*}(x) - \tau_{g^*}^*(x))^2] f_0(x)dx = \mathbb{E}\|\tau_{g^*}\|^2 - \text{tr} (T_{\mu\tau}^*P(PT_{\mu\mu}P)^{-1}PT_{\mu\tau}) \quad (\text{B.1})$$

For the definition of the inverse in (B.1), note that the operator and therefore its inverse are understood to be restricted to the subspace \mathcal{H} .

PROOF: We first consider the case $P = \text{Id}$. The set \mathcal{M} of linear predictors of the form (2.5) can be identified with the Hilbert space $L_2(\mathcal{X} \times \mathcal{X})$ endowed with the scalar product $\langle T_1, T_2 \rangle = \text{tr}(T_1^*T_2) = \int \int g(x_2, x_1)h(x_1, x_2)f_0(x_1)f_0(x_2)dx_1dx_2$ and the trace norm induced by that scalar product.

To obtain a representation of the minimized projection error, we derive a projection analog for the regression model developed in He, Müller, and Wang (2000). We first show that \mathcal{M} is a closed linear subspace of $L_2(\mathcal{X})$: Consider a random element $\phi_{g^*} \in L_2(\mathcal{X})$ and define $H_{\phi_{g^*}, \mu_{g^*}}(x_1, x_2) := \mathbb{E}[\phi_{g^*}(x_1)\mu_{g^*}(x_2; 0)]$ and let $T_{\phi_{g^*}}$ denote the corresponding Hilbert-Schmidt integral operator. We then have that ϕ_{g^*} is orthogonal to $B\mu_{g^*}$ if

$$\begin{aligned} 0 &= \mathbb{E}\langle \phi_{g^*}, B\mu_{g^*} \rangle \\ &= \mathbb{E} \left[\int \phi_{g^*}(x_1)\mu_{g^*}(x_2)\beta(x_1, x_2)f_0(x_1)f_0(x_2)dx_1dx_2 \right] \\ &= \int \mathbb{E} [\phi_{g^*}(x_1)\mu_{g^*}(x_2)] \beta(x_1, x_2)f_0(x_1)f_0(x_2)dx_1dx_2 \\ &= \int H_{\phi_{g^*}, \mu_{g^*}}(x_1, x_2)\beta(x_1, x_2)f_0(x_1)f_0(s)dx_1dx_2 = \text{tr} (T_{\phi_{g^*}}B) \end{aligned}$$

Since B may in particular include the identity, ϕ_{g^*} is orthogonal to \mathcal{M} for any $B \in L_2(\mathcal{X} \times \mathcal{X})$ if and only if $H_{\phi_{g^*}, \mu_{g^*}}(x_1, x_2) \equiv 0$. Since \mathcal{M} is the orthogonal complement of the set of all such vectors $\phi_{g^*} \in L_2(\mathcal{X})$, it is in particular a closed linear subspace of $L_2(\mathcal{X})$.

By the classical projection theorem (Theorem 2 in Luenberger (1969), p.51), it then follows that there exists a unique minimizer $\tau_0^* \in \mathcal{M}$. Furthermore, that minimizer also satisfies the orthogonality condition $\langle m, \tau_{g^*} - \tau_0^* \rangle$ for any $m \in \mathcal{M}$. It follows that

$$\begin{aligned} \min_{B \in L_2(\mathcal{X} \times \mathcal{X})} \mathbb{E} \|\tau_{g^*} - B\mu_{g^*}\|^2 &= \mathbb{E} \|\tau_{g^*}\|^2 - 2\mathbb{E} \langle \tau_{g^*}, \tau_0^* \rangle + \mathbb{E} \|\tau_0^*\|^2 \\ &= \mathbb{E} \|\tau_{g^*}\|^2 - 2(\mathbb{E} \|\tau_{g^*}^*\|^2 + \mathbb{E} \langle \tau_{g^*} - \tau_{g^*}^*, \tau_{g^*}^* \rangle) + \mathbb{E} \|\tau_{g^*}^*\|^2 \\ &= \mathbb{E} \|\tau_{g^*}\|^2 - \mathbb{E} \|\tau_{g^*}^*\|^2 \end{aligned} \quad (\text{B.2})$$

We next characterize the optimal solution $\tau_{g^*}^*$ in terms of the operators $T_{\mu\mu}$ and $T_{\mu\tau}$. Suppose that B_0 with kernel $\beta_0^*(x_1, x_2)$ is such that $\tau_{g^*}^* = B_0\mu_{g^*}$. Then, we have for any $h \in L_2(\mathcal{X})$ that

$$\begin{aligned} (T_{\mu\tau}h)(x_1) &= \int \mathbb{E}[\mu_{g^*}(x_1)\tau_{g^*}(x_2)]h(x_2)f_0(x_2)dx_2 \\ &= \int \mathbb{E}[\mu_{g^*}(x_1)[(B_0\mu_{g^*})(x_2) + \{\tau_{g^*}(x_2) - (B_0\mu)(x_2)\}]]h(x_2)f_0(x_2)dx_2 \\ &= \int \mathbb{E}[\mu_{g^*}(x_1)\mu_{g^*}(x_2)]\beta_0^*(x_2, x_3)f_0(x_2)dx_2h(x_3)f_0(x_3)dx_3 \\ &\quad + \int \mathbb{E}[\mu_{g^*}(x_1)\{\tau_{g^*}(x_3) - (B_0\mu)(x_3)\}]h(x_3)f_0(x_3)dx_3 \\ &= (T_{\mu\mu}B_0h)(x_1) + 0 \end{aligned} \quad (\text{B.3})$$

where the last equality follows from orthogonality of the projection error, noting that $B\mu_{g^*} := \text{Id}\mu_{g^*}$ is in \mathcal{M} .

Now suppose that the minimum is attained at both $B_0\mu_{g^*} \in \mathcal{M}$ and $B_1\mu_{g^*} \in \mathcal{M}$. Then by orthogonality of the projection error,

$$\begin{aligned} \mathbb{E} \|\tau_{g^*} - B_1\mu_{g^*}\|^2 &= \mathbb{E} \|\tau_{g^*} - B_0\mu_{g^*} + (B_0 - B_1)\mu_{g^*}\|^2 \\ &= \mathbb{E} \|\tau_{g^*} - B_0\mu_{g^*}\|^2 + 2\mathbb{E} \langle \tau_{g^*} - B_0\mu_{g^*}, (B_0 - B_1)\mu_{g^*} \rangle + \mathbb{E} \|(B_0 - B_1)\mu_{g^*}\|^2 \\ &= \mathbb{E} \|\tau_{g^*} - B_0\mu_{g^*}\|^2 + \mathbb{E} \|(B_0 - B_1)\mu_{g^*}\|^2 \end{aligned}$$

Hence the minimum can be attained at both B_1 and B_0 iff

$$\begin{aligned} 0 &= \mathbb{E} \|(B_0 - B_1)\mu_{g^*}\|^2 \\ &= \int (\beta_0(x_1, x_2) - \beta_1(x_1, x_2))\mathbb{E}[\mu_{g^*}(x_1)\mu_{g^*}(x_3)](\beta_0(x_3, x_2) - \beta_1(x_3, x_2))f_0(x_1)f_0(x_3)f_0(x_2)dx_1dx_2dx_3 \\ &= \text{tr}((B_0 - B_1)T_{\mu\mu}(B_0^* - B_1^*)) \end{aligned}$$

or equivalently iff $(B_0 - B_1) \in \ker(T_{\mu\mu})$. In particular, the orthogonal projection B_0^* of any solution $B \in L_2(\mathcal{X} \times \mathcal{X})$ onto the closed subspace $\mathcal{N}^\perp \times L_2(\mathcal{X})$ exists and is a solution to the same minimization problem. So without loss of generality we can restrict our attention to the minimization problem

$$\min_{B \in \mathcal{N}^\perp \times L_2(\mathcal{X})} \mathbb{E} \|\tau_{g^*} - B\mu_{g^*}\| \quad (\text{B.4})$$

Noticing that restricted to its range \mathcal{N}^\perp , the operator $T_{\mu\mu}$ possesses an inverse, we can solve the normal equations (B.3) to obtain

$$B_0^*h = T_{\mu\tau}^*T_{\mu\mu}^{-1}h$$

for any $h \in \mathcal{N}^\perp$. Substituting this expression into (B.2), we therefore obtain

$$\min_{B \in L_2(\mathcal{X} \times \mathcal{X})} \mathbb{E} \|\tau_{g^*} - B\mu_{g^*}\|^2 = \mathbb{E} \|\tau_{g^*}\|^2 - \text{tr}(T_{\mu\tau}^* T_{\mu\mu}^{-1} T_{\mu\tau})$$

establishing the claim for $P_1 = \text{Id}$. For the general case, notice that \mathcal{H} was a closed linear subspace of \mathcal{N}^\perp and A was assumed to be invertible on \mathcal{H} , so that the argument continues to apply when restricted to the subspace of linear predictors based on $P\mu_{g^*}$ \square

B.1. Proof of Lemma 3.1. We use the formula from (B.1) with $\tilde{\mathcal{H}}_K := \text{span}(\tilde{\phi}_1, \dots, \tilde{\phi}_K)$ as the linear subspace of $L_1(\mathcal{X})$ spanned by the K orthonormal functions $\tilde{\phi}_1(x), \dots, \tilde{\phi}_K(x)$.

We first consider the operator $\tilde{S}_K := \tilde{P}_K T_{\mu\mu} \tilde{P}_K$. Since $\tilde{\mathcal{H}}_K$ is finite-dimensional, we can identify \tilde{S}_K with a $K \times K$ matrix of coefficients with respect to the basis $\tilde{\phi}_1, \dots, \tilde{\phi}_K$ of $\tilde{\mathcal{H}}_K$,

$$\tilde{S}_K := \left(\langle \tilde{\phi}_k, T_{\mu\mu} \tilde{\phi}_l \rangle \right)_{k,l}$$

Noting that $T_{\mu\mu}$ is injective on \mathcal{N}^\perp we will impose the normalization

$$\langle \tilde{\phi}_k, T_{\mu\mu} \tilde{\phi}_l \rangle = \delta_{k,l} \tag{B.5}$$

so that $\tilde{S}_K = I_K$, the K -dimensional identity matrix.

Furthermore, evaluating the trace using an arbitrarily chosen orthonormal system for $L_2(\mathcal{X})$, we can also verify that

$$\begin{aligned} \text{tr}(T_{\mu\tau}^* \tilde{P}_K \tilde{P}_K T_{\mu\tau}) &= \int \sum_{k=1}^K \left(\int H_{\mu\tau}(x_1, x_2) H_{\mu\tau}(x_3, x_1) \tilde{\phi}_k(x_2) \tilde{\phi}_k(x_3) f_0(x_2) f_0(x_3) dx_2 dx_3 \right) f_0(x_1) dx_1 \\ &= \sum_{k=1}^K \langle \tilde{\phi}_k, T_{\mu\tau} T_{\mu\tau}^* \tilde{\phi}_k \rangle \end{aligned}$$

Hence, using the formula from Theorem B.1,

$$\int \mathbb{E} [(\tau_{g^*}(x) - \tau_{g^*}^*(x))^2] f_0(x) dx = \sum_{k=1}^K \langle \tilde{\phi}_k, T_{\mu\tau} T_{\mu\tau}^* \tilde{\phi}_k \rangle$$

for any collection of functions $\tilde{\phi}_1, \dots, \tilde{\phi}_K$ satisfying the constraint (B.5).

Hence, the mean-square error optimal basis functions are determined by the quadratic program

$$\inf_{\phi_1, \dots, \phi_K} \sum_{k=1}^K \langle \phi_k, T_{\mu\tau} T_{\mu\tau}^* \phi_k \rangle \quad \text{s.t.} \quad \langle \phi_k, T_{\mu\mu} \phi_l \rangle = \delta_{kl} \tag{B.6}$$

which establishes the claim \square

B.2. Proof of Theorem 3.1. From the definition of $IMSE_K^*$, there exist $\tilde{\phi}_{1\varepsilon}, \dots, \tilde{\phi}_{K\varepsilon} \in L_2(\mathcal{X})$, such that $\langle \tilde{\phi}_{k\varepsilon}, T_{\mu\mu} \tilde{\phi}_{l\varepsilon} \rangle = \delta_{kl}$ and

$$IMSE_K \left[\tilde{\phi}_{1\varepsilon}, \dots, \tilde{\phi}_{K\varepsilon} \right] \leq IMSE_K^* + \frac{\varepsilon}{2}$$

Since $\tilde{\phi}_{1\varepsilon}, \dots, \tilde{\phi}_{K\varepsilon} \in L_2(\mathcal{X})$, we can find $L_\varepsilon < \infty$ such that $\|\tilde{\phi}_{k\varepsilon}\| \leq L_\varepsilon$.

These K functions do not necessarily satisfy the regularized orthogonality constraint, rather we find ‘‘close’’ alternative functions $\bar{\phi}_{1\varepsilon}, \dots, \bar{\phi}_{K\varepsilon}$ such that $\langle \bar{\phi}_{k\varepsilon}, T_{\mu\mu a} \bar{\phi}_{l\varepsilon} \rangle = \delta_{kl}$. Since the operator $T_{\mu\mu a}$ is Hermitian and positive, we can define a scalar product $\langle u, v \rangle_a := \langle u, T_{\mu\mu a} v \rangle$. We first obtain K functions $\check{\phi}_{1\varepsilon}, \dots, \check{\phi}_{K\varepsilon}$ that satisfy the orthogonality constraints $\langle \check{\phi}_{k\varepsilon}, \check{\phi}_{l\varepsilon} \rangle = 0$ for all $k \neq l$. To that end, we use the Gram-Schmidt

procedure with respect to the scalar product $\langle \cdot, \cdot \rangle_a$, where $\check{\phi}_{1\varepsilon} := \tilde{\phi}_{1\varepsilon}$, and

$$\check{\phi}_{k\varepsilon} := \tilde{\phi}_{k\varepsilon} - \sum_{l=1}^{k-1} \frac{\langle \tilde{\phi}_{k\varepsilon}, \check{\phi}_{l\varepsilon} \rangle_a}{\langle \check{\phi}_{l\varepsilon}, \check{\phi}_{l\varepsilon} \rangle_a} \check{\phi}_{l\varepsilon}$$

Defining $c_{kk} = 1$ and $c_{lk} := -\frac{\langle \tilde{\phi}_{k\varepsilon}, \check{\phi}_{l\varepsilon} \rangle_a}{\langle \check{\phi}_{l\varepsilon}, \check{\phi}_{l\varepsilon} \rangle_a}$ for $k \neq l$, we can confirm by induction that

$$\check{\phi}_{k\varepsilon} = \tilde{\phi}_{k\varepsilon} - \sum_{l=1}^{k-1} d_{lk} \tilde{\phi}_{l\varepsilon}$$

where $d_{lk} = \sum_{\mathcal{J}(l,k)} \prod_{s=2}^{|k-l|} c_{j_s j_{s-1}}$, and $\mathcal{J}(l,k)$ is the set of all (j_1, \dots, j_s) such that $s \leq |k-l|$ and $j_1 < j_2 < \dots < j_s$. For notational convenience, we also define $d_{kk} = 1$.

We now recursively bound c_{kl} and d_{kl} for $k \neq l$. Due to the constraint on $\tilde{\phi}_{1\varepsilon}, \dots, \tilde{\phi}_{K\varepsilon}$ it follows for any $k \neq l$,

$$\langle \tilde{\phi}_{k\varepsilon}, \tilde{\phi}_{l\varepsilon} \rangle_a = \langle \check{\phi}_{k\varepsilon}, T_{\mu\mu} \tilde{\phi}_{l\varepsilon} \rangle + a \langle \check{\phi}_{k\varepsilon}, \tilde{\phi}_{l\varepsilon} \rangle = a \langle \check{\phi}_{k\varepsilon}, \tilde{\phi}_{l\varepsilon} \rangle$$

Hence we can calculate the scalar products

$$\begin{aligned} \langle \tilde{\phi}_{k\varepsilon}, \tilde{\phi}_{l\varepsilon} \rangle_a &= a \sum_{j=1}^l d_{lj} \langle \tilde{\phi}_{k\varepsilon}, \tilde{\phi}_{j\varepsilon} \rangle \\ \langle \tilde{\phi}_{k\varepsilon}, \tilde{\phi}_{k\varepsilon} \rangle_a &= 1 + \sum_{l=1}^{k-1} d_{kl}^2 + a \sum_{j=1}^{k-1} \sum_{l=1}^{k-1} d_{kj} d_{kl} \langle \tilde{\phi}_{j\varepsilon}, \tilde{\phi}_{l\varepsilon} \rangle \end{aligned}$$

for any $k \neq l$. In particular, denoting $\bar{d}_k := \max\{|d_{kl}| : k > l\}$, we can bound

$$\begin{aligned} \left| \langle \tilde{\phi}_{k\varepsilon}, \tilde{\phi}_{l\varepsilon} \rangle_a \right| &\leq a(1 + (k-1)\bar{d}_k)L_\varepsilon^2 \\ \left| \langle \tilde{\phi}_{k\varepsilon}, \tilde{\phi}_{k\varepsilon} \rangle_a - 1 - \sum_{l=1}^{k-1} d_{kl}^2 \right| &\leq aL_\varepsilon^2(1 + (k-1)^2\bar{d}_k^2) \end{aligned}$$

Hence for a satisfying $2a^2 \leq (L_\varepsilon^2 K^2)^{-1}$, we can bound $\bar{d}_2 := |c_{21}| \leq 2aL_\varepsilon^2$. It then follows by induction over k that $|c_{kl}| \leq 4aL_\varepsilon^2$ and

$$\bar{d}_k \leq 8aL_\varepsilon^2$$

for each $k = 1, \dots, K$.

To obtain functions $\bar{\phi}_{1\varepsilon}, \dots, \bar{\phi}_{K\varepsilon}$ with the desired property, we furthermore need to impose the scale normalization $\langle \bar{\phi}_{k\varepsilon}, \bar{\phi}_{k\varepsilon} \rangle_a = 1$. Since $\check{\phi}_{k\varepsilon} = \sum_{j=1}^k d_{kj} \tilde{\phi}_{j\varepsilon}$,

$$\langle \check{\phi}_{k\varepsilon}, \check{\phi}_{k\varepsilon} \rangle_a = \left\langle \sum_{j=1}^k \tilde{\phi}_{j\varepsilon}, T_{\mu\mu} \langle \check{\phi}_{k\varepsilon}, \check{\phi}_{k\varepsilon} \rangle \tilde{\phi}_{j\varepsilon} \right\rangle + a \langle \check{\phi}_{k\varepsilon}, \check{\phi}_{k\varepsilon} \rangle$$

Since $d_{kk} = 1$, we can then bound

$$\left| \langle \check{\phi}_{k\varepsilon}, \check{\phi}_{k\varepsilon} \rangle_a - 1 \right| \leq K\bar{d}_k^2 + aL_\varepsilon^2 \leq (K+8)aL_\varepsilon^2$$

We can therefore form

$$\bar{\phi}_k := (\langle \check{\phi}_{k\varepsilon}, \check{\phi}_{k\varepsilon} \rangle_a)^{-1/2} \check{\phi}_{k\varepsilon}$$

By construction, $\bar{\phi}_{1\varepsilon}, \dots, \bar{\phi}_{K\varepsilon}$ satisfy the constraints $\langle \bar{\phi}_{k\varepsilon}, \bar{\phi}_{l\varepsilon} \rangle_a = \delta_{kl}$ and, using standard bounding arguments

$$\|\bar{\phi}_{k\varepsilon} - \tilde{\phi}_{k\varepsilon}\| \leq 10KaL_\varepsilon^3$$

for any sufficiently small value of $a > 0$.

It remains to be shown by a continuity argument that the IMSE achieved by $\bar{\phi}_{1\varepsilon}, \dots, \bar{\phi}_{K\varepsilon}$ is greater than $IMSE_K^* + \varepsilon$ for a sufficiently close to zero. Using the formula from (B.1), we can write the IMSE for a given set of basis functions as

$$IMSE_K[\phi_1, \dots, \phi_K] = \text{tr}(C_K^{-1}A_K)$$

where C_K and A_K can be identified with $K \times K$ matrices $A_K = (A_{kl})$ and $C_K = (C_{kl})$, and

$$C_{kl} := \langle \phi_k, T_{\mu\mu}\phi_l \rangle$$

and

$$A_{kl} := \langle \phi_k, T_{\mu\tau}T_{\mu\tau}^*\phi_l \rangle$$

By assumption, for the basis functions $\tilde{\phi}_{1\varepsilon}, \dots, \tilde{\phi}_{K\varepsilon}$ we have $C_{kl} = \delta_{kl}$ so that the corresponding matrix is the K -dimensional identity matrix. Furthermore, the operators $T_{\mu\mu}$ and $T_{\mu\tau}T_{\mu\tau}^*$ are compact with largest eigenvalue equal to $\nu_1 < \infty$ and $\lambda_1 < \infty$, respectively. Since $\|\tilde{\phi}_{k\varepsilon} - \bar{\phi}_{k\varepsilon}\| \leq aB_9K\varepsilon^3$, there exists a constant $\kappa_\varepsilon < \infty$ such that

$$|IMSE_K[\bar{\phi}_{1\varepsilon}, \dots, \bar{\phi}_{K\varepsilon}] - IMSE_K[\tilde{\phi}_{1\varepsilon}, \dots, \tilde{\phi}_{K\varepsilon}]| \leq \kappa_\varepsilon a \quad (\text{B.7})$$

for a sufficiently small, which establishes the desired conclusion \square

We also note that the convergence rate for $|IMSE_K(a) - IMSE_K^*|$ as a function of a generally depends on the eigenvalues of $T_{\mu\mu}$ and $T_{\mu\tau}$, where L_ε in the preceding proof may diverge as $\varepsilon \rightarrow 0$. We leave this question for future research.

Proof of Proposition 3.1. Since $T_{\mu\mu}$ is injective on $\ker(T_{\mu\mu})^\perp$, any function ϕ_k^* solving the generalized eigenvalue problem (3.4) at eigenvalue λ_k can be equivalently characterized by $\phi_k^* := T_{\mu\mu}^{-1/2}\chi_k^*$, where χ_k^* is an eigenfunction

$$T_{\mu\mu}^{-1/2}T_{\mu\tau}T_{\mu\tau}^*T_{\mu\mu}^{-1/2}\chi_k^* = \lambda_k\chi_k^*$$

at the same eigenvalue λ_k . In what follows we also write $S := T_{\mu\mu}^{-1/2}T_{\mu\tau}T_{\mu\tau}^*T_{\mu\mu}^{-1/2}$. Without loss of generality we also assume that eigenvalues are ordered according to $\lambda_1 \geq \lambda_2 \geq \dots$, and $\lambda_K > 0$.

We next argue that under the condition (3.7), S is compact: it follows immediately from the Karhunen-Loève expansion (3.6) that we can write

$$\begin{aligned} (T_{\mu\mu}h)(x) &= \sum_{k=1}^{\infty} \mathbb{E}[\alpha_{g^*k}^2] \langle \xi_k, h \rangle \xi_k(x) \\ (T_{\mu\tau}h)(x) &= \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \mathbb{E}[\alpha_{g^*k}\beta_{g^*l}] \langle \zeta_l, h \rangle \xi_k(x), \end{aligned}$$

with the analogous expression for the adjoint $T_{\mu\tau}^*$.

Since ξ_1, ξ_2, \dots is a basis of $\ker(T_{\mu\mu})^\perp$, we can therefore evaluate the trace of S in terms of that basis to obtain

$$\text{tr}(S) = \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \frac{\mathbb{E}[\alpha_{g^*k}\beta_{g^*l}]^2}{\mathbb{E}[\alpha_{g^*k}^2]}$$

which is finite by (3.7). In particular, the sequence of compact operators S_K defined as the analog of S after truncating the respective Karhunen-Loève expansions for μ_{g^*} and τ_{g^*} after the K leading principal components converges to S under the trace norm, so that S is also compact. Since S is self-adjoint and nonnegative and therefore has a discrete spectrum of nonnegative eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq 0$ with associated eigenfunctions $\chi_1^*, \chi_2^*, \dots \in L_2(\mathcal{X})$.

It remains to be shown that the norm of $\phi_k^* := T_{\mu\mu}^{-1/2}\chi_k^*$ is also bounded. Since χ_k^* is an eigenfunction of S at eigenvalue $\lambda_k > 0$, we can write

$$\phi_k^* := \lambda_k^{-1}T_{\mu\mu}^{-1/2}S\chi_k^*.$$

Hence, the norm of ϕ_k^* is given by

$$\|\phi_k^*\|^2 = \lambda_k^{-2}\langle T_{\mu\mu}^{-1/2}S\chi_k^*, T_{\mu\mu}^{-1/2}S\chi_k^* \rangle = \lambda_k^{-2}\langle \chi_k^*, ST_{\mu\mu}^{-1}S\chi_k^* \rangle$$

noting that S and $T_{\mu\mu}$ are self-adjoint. Moreover, expressing $T_{\mu\mu}$ and $T_{\mu\tau}$ in terms of the Karhunen-Loève representations (3.6), we can use the Cauchy-Schwarz inequality to bound

$$\text{tr}(ST_{\mu\mu}^{-1}S) \leq \left(\sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \frac{\mathbb{E}[\alpha_{g^*k}\beta_{g^*l}]^2}{\mathbb{E}[\alpha_{g^*k}^2]^{3/2}} \right)^2$$

which is finite under (3.7). Noting that $S^r T_{\mu\mu}^{-1} S^r$ is self-adjoint, this establishes that the operator is also trace-class and therefore compact with operator norm bounded by $\text{tr}(ST_{\mu\mu}^{-1}S)$.

In particular, since $\lambda_1 \geq \dots \lambda_K > 0$ by assumption, we can bound

$$\max_{k=1, \dots, K} \|\phi_k^*\|^2 \leq |\lambda_K|^{-2} \text{tr}(ST_{\mu\mu}^{-1}S) \max_k \|\chi_k^*\|^2$$

where $\|\chi_k^*\|$ is finite for each k since $\chi_k^* \in L_2(\mathcal{X})$.

We can then apply the argument from the proof of Theorem 3.1 where we choose $\tilde{\phi}_{k\varepsilon}(x) \equiv \phi_k^*(x)$, the solutions to (3.4) corresponding to the k th largest eigenvalue for $k = 1, \dots, K$. Since those functions are chosen independently of ε , the bound B_ε is fixed at some finite value B_0 , so that the claim follows immediately from (B.7), noting that $\kappa_\varepsilon \equiv \kappa_0$ is constant. \square

B.3. Proof of Corollary 3.1. By construction, the optimal basis for the regularized problem 3.5 satisfies the constraint $\langle \phi_k^*, (T_{\mu\mu} + a\text{Id})\phi_l^* \rangle = \delta_{kl}$. Hence, we can rewrite the $K \times K$ matrix $P_K^* T_{\mu\mu} P_K^* = I_K - aP_K^*$, and use the Neumann series to obtain its inverse, $(P_K^* T_{\mu\mu} P_K^*)^{-1} = I_K + \frac{a}{1-a} P_K^*$. From the proof of Theorem B.1, the projection of τ_{g^*} onto the optimal basis is therefore given by

$$\tau_{g^*K}^*(x) := \sum_{k=1}^K \langle \mu_{g^*}, \phi_k^* \rangle \frac{1+a}{1-a} (T_{\mu\tau}^* \phi_k^*)(x)$$

which establishes the formula given in the Corollary \square

APPENDIX C. PROOFS FOR SECTION A

C.1. Proof of Theorem A.1. We use the main result in Graham, Niu, and Powell (2021) which adapts Theorems 2 and 10 in Hansen (2008) to nonparametric regression for dyadic data, rather than conventional sample averages. We first apply their results separately for each clusters $g = 1, \dots, G$, where we strengthen the rate conditions to ensure uniformity across clusters. We then aggregate the cluster-specific estimates to obtain the first and second conditional moments across clusters.

C.1.1. Convergence Rate for Kernel Averages. The local linear estimator can be expressed in terms of weighted averages of products of X_{gi}, d_{gi}, Y_{gi} . For a general notation, let $W_{sgi} = (a_{0s} + a_{1s}X_{gi})(b_{0s} + b_{1s}Y_{gi})$ be a function of X_{gi}, Y_{gi} that is affine in Y_{gi} given fixed coefficients $a_{0s}, b_{0s}, a_{1s}, b_{1s}$. We consider uniform

convergence of conventional and dyadic kernel averages

$$\begin{aligned}\hat{\Psi}_g(x_1; d_1) &:= \frac{1}{nh^d} \sum_{i=1}^n W_{1gi} K\left(\frac{x_1 - x_{gi}}{h}\right) \mathbb{1}\{d_{gi} = d_1\} \\ \hat{\Omega}_g(x_1, x_2; d_1, d_2) &:= \binom{n}{2}^{-1} h^{-2d} \frac{1}{2} \sum_{i \neq j} W_{1gi} W_{2gj} K\left(\frac{x_1 - x_{gi}}{h}\right) K\left(\frac{x_2 - x_{gj}}{h}\right) \mathbb{1}\{d_{gi} = d_1, d_{gj} = d_2\}\end{aligned}$$

for each $g = 1, \dots, G$ such that $R_g = 1$.

Lemma C.1. *Suppose that the bandwidth g satisfies $\left(\frac{n}{\log n}\right)^{1/3} h^d \rightarrow \infty$ and $\left(\frac{\log n}{nh^d}\right)^{1/2}$. Under Assumptions 2.4 and A.1, the kernel averages $\hat{\Psi}_g$ and $\hat{\Omega}_g$ converge uniformly to their respective expectations at the rate*

$$\begin{aligned}\max_{g=1, \dots, G} R_g \sup_{x_1 \in [0, 1]^d} \left| \hat{\Psi}_g(x_1; d_1) - \mathbb{E}[\hat{\Psi}_g(x_1; d_1)] \right| &= O_P\left(\left(\frac{\log n}{nh^d}\right)^{1/2}\right) \\ \max_{g=1, \dots, G} R_g \sup_{x_1, x_2 \in [0, 1]^d} \left| \hat{\Omega}_g(x_1, x_2; d_1, d_2) - \mathbb{E}[\hat{\Omega}_g(x_1, x_2; d_1, d_2)] \right| &= O_P\left(\left(\frac{\log n}{nh^d}\right)^{1/2}\right)\end{aligned}\tag{C.1}$$

for any $d_1, d_2 \in \{0, 1\}$.

PROOF: We prove this result using Theorem 3.2 in Graham, Niu, and Powell (2021). Note first that, since W_{gi} are conditionally i.i.d., Assumption 2.4 implies Assumptions 3.1 and 3.3 (a) in Graham, Niu, and Powell (2021) for $Z_{gij} := W_{gi} W_{gj}$. Also, Assumption A.1 subsumes Assumptions 3.2 and 3.3 (b) in Graham, Niu, and Powell (2021). Moreover, for $s \geq 3$, lengthy but elementary rate calculations confirm that any bandwidth sequence with $\left(\frac{n}{\log n}\right)^{1/3} h^d \rightarrow \infty$ satisfies the additional bandwidth conditions required for their theorem.

Their argument can then be adapted to achieve uniform convergence of $\hat{\Psi}_{gs}(x_1; d_1)$ and $\hat{\Omega}_{gs}(x_1, x_2; d_1, d_2)$ with respect to x_1, x_2 and g . To that end, the grid $\mathcal{X}_n^* \{w_{n1}, \dots, w_{nL_n}\}$ is chosen in a way such that the set $[0, 1]^d$ is covered by the collection of balls of radius $a_n h$. We then replace the approximating grid introduced on p.19 of Graham, Niu, and Powell (2021) with $\mathcal{X}_n^* \times \{1, \dots, G\}$, resulting in $L_n := G \left(h^{-1} \left(\frac{\log n}{nh^d}\right)^{1/2}\right)^d$ partition elements. We can therefore conclude that

$$\max_{g=1, \dots, G} R_g \sup_{x_1, x_2 \in [0, 1]^d} \left| \hat{\Omega}_{gs}(x_1, x_2; d_1, d_2) - \mathbb{E}[\hat{\Omega}_{g1}(x_1, x_2; d_1, d_2)] \right| = O_P\left(\frac{\log n}{nh^d}\right)^{1/2}\tag{C.2}$$

for $s = 1, 2$. The claim regarding $\hat{\Psi}(x_1; d_1)$ is proven in an analogous manner using Theorem 2 in Hansen (2008), whose conditions are subsumed under those for Theorem 3.2 in Graham, Niu, and Powell (2021) \square

C.1.2. *Proof of Theorem A.1.* We now complete the proof of Theorem A.1. We consider the general case of estimating the conditional expectation

$$\Psi_g(x; d) \equiv \Psi_g(x_1, x_2; d_1, d_2) := \mathbb{E}[W_{1gi}, W_{2gj} | X_{gi} = x, X_{gj} = x_2, D_{gi} = d_1, D_{gj} = d_2]$$

and $\Lambda(x_1, x_2; d_1, d_2) := \frac{1}{G} \sum_{g=1}^G \Lambda_g(x_1, x_2; d_1, d_2)$. for general W_{1gi}, W_{2gj} . The corresponding cluster-specific local linear estimator

$$\hat{\Psi}_g(x_1, x_2; d_1, d_2) := \arg_{b_0^{(g)}} \min_{b_0^{(g)}, b_{11}^{(g)}, b_{12}^{(g)}} \sum_{i=1}^{n_g} \sum_{j \neq i} \Psi_{gij}(x_1, x_2; \mathbf{b}) w_{gi}(x_1; d_1) w_{gj}(x_2; d_2)$$

where we denote $\Psi_{gij}(x_1, x_2; \mathbf{b}) := \left(W_{1gi}W_{2gj} - b_0^{(g)} - b_{11}^{(g)}(X_{gi} - x_1) - b_{12}^{(g)}(X_{gj} - x_2) \right)$, and as before, $w_{gi}(x_1; d_1) := K\left(\frac{X_{gi} - x_1}{h}\right) \mathbb{1}\{d_{gi} = d_1\}$.

As in the proof of Theorem 10 in Hansen (2008), we can write each local linear estimator as

$$\hat{\Lambda}_g(x; d) = \frac{\hat{m}_g + \hat{S}'_g \hat{M}_g^{-1} \hat{N}_g}{\hat{f}_g - \hat{S}'_g \hat{M}_g^{-1} \hat{S}_g}$$

where for greater legibility, we write $(x, d) := (x_1, x_2; d_1, d_2)$ and suppress dependence on d_1, d_2 wherever possible, and terms on the right-hand side are defined as follows:

$$\begin{aligned} \hat{m}_g &= \hat{m}_g(x; d) := \binom{n}{2}^{-1} h^{-2d} \frac{1}{2} \sum_{i \neq j} W_{gi} W_{gj} w_{gi}(x_1; d_1) w_{gj}(x_2; d_2) \\ \hat{f}_g &= \hat{f}_g(x; d) := \binom{n}{2}^{-1} h^{-2d} \frac{1}{2} \sum_{i \neq j} w_{gi}(x_1; d_1) w_{gj}(x_2; d_2) \\ \hat{S}_g &= \hat{S}_g(x; d) := \binom{n}{2}^{-1} h^{-2d} \frac{1}{2} \sum_{i \neq j} \left(\frac{x - X_{gij}}{h} \right) w_{gi}(x_1; d_1) w_{gj}(x_2; d_2) \\ \hat{M}_g &= \hat{M}_g(x; d) := \binom{n}{2}^{-1} h^{-2d} \frac{1}{2} \sum_{i \neq j} \left(\frac{x - X_{gij}}{h} \right) \left(\frac{x - X_{gij}}{h} \right)' w_{gi}(x_1; d_1) w_{gj}(x_2; d_2) \\ \hat{N}_g &= \hat{N}_g(x; d) := \binom{n}{2}^{-1} h^{-2d} \frac{1}{2} \sum_{i \neq j} \left(\frac{x - X_{gij}}{h} \right) W_{gij} w_{gi}(x_1; d_1) w_{gj}(x_2; d_2) \end{aligned}$$

Applying Lemma C.1 component by component, each of these terms converges uniformly to its expectation. Specifically, denoting $b_n := \left(\frac{\log n}{nh^d}\right)^{1/2}$, and $\Sigma := \int uu'K(u)du$, standard calculations for conditional moment estimation using local linear regression (see also the proofs of Theorems 8 and 10 in Hansen (2008)) then yield

$$\begin{aligned} \hat{m}_g(x; d) &= m_g(x; d) + O(h^2) + O_p(b_n) \\ \hat{f}_g(x; d) &= f_g(x; d) + O(h^2) + O_p(b_n) \\ \hat{S}_g(x; d) &= h\Sigma \nabla_x f_g(x; d) + O(h^2) + O_p(b_n) \\ \hat{M}_g(x; d) &= \Sigma f_g(x; d) + O(h^2) + O_p(b_n) \\ \hat{N}_g(x; d) &= h\Sigma \nabla_x m_g(x; d) + O(h^2) + O_p(b_n) \end{aligned}$$

uniformly in $(x; d)$, where $m_g(x; d) := \Psi_g(x; d) f_g(x; d)$.

We can now confirm that $b_n^{1/3} h \equiv \left(\frac{n}{\log n}\right)^{1/3} h^d \rightarrow \infty$ implies that

$$\frac{h}{b_n} = \left(\frac{n}{\log n}\right) h^{d+1} = \left[\left(\frac{n}{\log n}\right)^{1/3} h^d \right]^3 h^{1-2d} \rightarrow \infty$$

for any $d \geq 1$. Hence, collecting terms,

$$\begin{aligned} \left| \hat{S}_g(x; d)' \hat{M}_g(x; d)^{-1} \hat{N}_g(x; d) - h^2 \frac{\nabla_x f_g(x; d)' \Sigma \nabla_x m_g(x; d)}{f_g(x; d)} \right| &= O_p\left(\left\{ \frac{h^2}{f_g(x; d)} + h \right\} b_n\right) \\ &\leq O_p\left(h^2 \delta_{G_n}^{-1} b_n + h b_n\right) = h O_p(b_n) \end{aligned}$$

where convergence is uniform in $(x; d)$.

Hence, from standard rate calculations

$$\begin{aligned}
\hat{\Psi}_g(x; d) &= \frac{\hat{m}_g + \hat{S}'_g \hat{M}_g^{-1} \hat{N}_g}{\hat{f}_g - \hat{S}'_g \hat{M}_g^{-1} \hat{S}_g} \\
&= \frac{\Psi_g(x; d) f_g(x; d) + O(h^2) + O_P(b_n + hb_n)}{f_g(x; d) + O(h^2) + O_P(b_n + hb_n)} \\
&= \Psi_g(x; d) + O_P(b_n) + O(h^2)
\end{aligned}$$

Since units $i = 1, \dots, n$ are sampled independently in each location, the $O_P(\cdot)$ terms are independent across locations $g = 1, \dots, G$ with expectation of order $o(h^2)$.

Hence, aggregating over $g = 1, \dots, G$,

$$\hat{\Psi}(x_1, x_2; d_1, d_2) = \frac{1}{G-1} \sum_{g=1}^G R_g \hat{\Psi}_g(x_1, x_2; d_1, d_2)$$

Hence, by the triangle inequality

$$\begin{aligned}
\left| \hat{\Psi}(x_1, x_2; d_1, d_2) - \Psi(x_1, x_2; d_1, d_2) \right| &\leq \left| \frac{1}{G-1} \sum_{g=1}^G R_g \hat{\Psi}_g(x_1, x_2; d_1, d_2) - \Psi_g(x_1, x_2; d_1, d_2) \right| \\
&\quad + \left| \frac{1}{G-1} \sum_{g=1}^G R_g |\Psi_g(x_1, x_2; d_1, d_2) - \Psi(x_1, x_2; d_1, d_2)| \right| \\
&= O_P\left(\frac{b_n + h^2}{G^{1/2}}\right) + O_P\left(\frac{1}{G}\right)
\end{aligned}$$

since R_g is equal to zero for a single unit g^* selected at random and one otherwise, where we use unconfoundness of location, Assumption 2.2 and bounded conditional moments in Assumption 2.4. By our previous arguments, convergence is also uniform with respect to the arguments $x_1, x_2; d_1, d_2$.

We can immediately verify that $\hat{\mu}(x; d)$ and $\mu(x; d)$ correspond to $\hat{\Psi}(x; d)$ and $\Psi(x; d)$, respectively, for the case $W_{1gi} = Y_{gi}$ and $W_{2gj} = 1$, so that

$$\sup_{x \in [0,1]^d} |\hat{\mu}(x; d) - \mu(x; d)| = O_P\left(\frac{b_n + h^2}{G^{1/2} \delta G n^{-1}}\right) + O_P\left(\frac{1}{G}\right)$$

For the covariance kernel $H(x_1, x_2; d_1, d_2)$, we can set $W_{1gi} = Y_{gi}$ and $W_{2gj} = Y_{gj}$ so that the cluster-specific local linear estimator

$$\begin{aligned}
\hat{\Psi}_g(x_1, x_2; d_1, d_2) &:= \arg_{b_0^{(g)}} \min_{b_0^{(g)}, b_{11}^{(g)}, b_{12}^{(g)}} \sum_{i=1}^{n_g} \sum_{j \neq i} \left\{ \mathbb{1}\{D_{gi} = d_1, D_{gj} = d_2\} \left(Y_{gi} Y_{gj} - b_0^{(g)} - b_{11}^{(g)} (X_{gi} - x_1) - b_{12}^{(g)} (X_{gj} - x_2) \right) \right\} \\
&\quad \times w_{gi}(x_1; d_1) w_{gj}(x_2; d_2)
\end{aligned}$$

is uniformly consistent for any $g = 1, \dots, G$ with $R_g = 1$ so that for

$$\hat{H}(x_1, x_2; d_1, d_2) = \frac{1}{G-1} \sum_{g=1}^G R_g \hat{\Psi}_{d_1 d_2, g}(x_1, x_2; d_1, d_2) - \bar{\mu}(x_1; d_1) \bar{\mu}(x_2; d_2)$$

we can conclude

$$\sup_{x_1, x_2 \in [0,1]^d} |\hat{H}(x_1, x_2; d_1, d_2) - H(x_1, x_2; d_1, d_2)| = O_P\left(\frac{b_n + h^2}{G^{1/2} \delta G n^{-1}}\right) + O_P\left(\frac{1}{G}\right)$$

establishing the convergence rates for a general choice of the bandwidth sequence subject to the rate conditions in the theorem.

Since by standard arguments the bias is of the order h^2 , the rate of the root mean square error is minimized at bandwidth sequences such that $h^2 = \left(\frac{\log n}{Gnh^d}\right)^{1/2}$ so that such a sequence must go to zero at a rate $h^* = O\left(\frac{\log n}{Gn}\right)^{\frac{1}{4+d}}$. \square

C.2. Proof of Proposition A.1. We give the argument for estimation of $H(x_1, x_2; d_1, d_2)$, the proof for the mean function $\mu(x_1; d_1)$ follows as a special case. We let H_g^* denote the projection of H_g onto the spline basis under the empirical measure. Parallel to the case of kernel estimation in Graham, Niu, and Powell (2019), the estimation error in $\hat{H}_g(x_1, x_2; d_1, d_2)$ can be decomposed into

$$\begin{aligned}\hat{H}_g(x_1, x_2; d_1, d_2) &= H_g^*(x_1, x_2; d_1, d_2) + \frac{2}{n_g} \sum_i H_{gn_g i}^{(1)} + \binom{n_g}{2}^{-1} \sum_{i < j} H_{gn_g ij}^{(2)} \\ &=: H_g^*(x_1, x_2; d_1, d_2) + T_{gn_g}(1) + T_{gn_g}^{(2)}\end{aligned}$$

where

$$\begin{aligned}H_{gn_g i}^{(1)} &= \mathbb{E}[H_{n_g ij} | Y_{gi}, X_{gi}, \mathbf{X}_g] - \mathbb{E}[H_{n_g ij}, \mathbf{X}_g] \\ H_{gn_g ij}^{(2)} &= \mathbb{E}[H_{n_g ij} | Y_{gi}, Y_{gj}, X_{gi}, X_{gj}, \mathbf{X}_g] - H_{gn_g i}^{(1)} - H_{gn_g j}^{(1)} + \mathbb{E}[H_{n_g ij}, \mathbf{X}_g]\end{aligned}$$

and $H_{n_g ij} \equiv H_{n_g ij}(x_1, x_2; d_1, d_2)$.

The variance bound can then be derived following the arguments in the proof of the i.i.d. case for Lemma 2.3 in Chen and Christensen (2015): By assumption, the term $T_{gn_g}(1)$ directly satisfies the conditions of their lemma. For $T_{gn_g}(2)$, we set $h := 1/M$ and note that by assumption $\frac{\log n}{nh^d} \rightarrow 0$, so that an analogous bound for the second term follows from arguments completely analogous to the proof of claim (ii) in Lemma 3.4 of Graham, Niu, and Powell (2021). The triangle inequality then yields

$$\text{Var} \left(\sup_{x_1, x_2, d_1, d_2} \left| \hat{H}_g(x_1, x_2; d_1, d_2) - H_g^*(x_1, x_2; d_1, d_2) \right| \right) \lesssim \frac{(M+r)^d \log n}{n},$$

noting that from known facts about tensor products of polynomial spline bases (see p.450 in Chen and Christensen (2015)), $\lambda_{Kn} \lesssim O(1)$.

Given these bounds, aggregation of the site specific estimates is completely analogous to the case of kernel-based estimation in the proof of Theorem A.1 and yields

$$\sup_{x_1, x_2, d_1, d_2} \left| H_g^*(x_1, x_2; d_1, d_2) - H_g(x_1, x_2; d_1, d_2) \right| \lesssim \left(\frac{(M+r)^d \log n}{n} \right)^{1/2} + M^{-2} + G^{-1}$$

which establishes the claim \square

C.3. Proof of Theorem A.2. For the following formal arguments we let $\|\cdot\|_F$ denote the trace operator norm $\|T\|_F := \text{tr}(T^*T)$. We start by proving the following Lemma:

Lemma C.2. *Suppose that S is a compact, self-adjoint operator with eigenvalues $\lambda_1 \geq \lambda_2, \dots$, counted by their multiplicity, and corresponding eigenfunctions ϕ_1, ϕ_2, \dots . Then for any sequence \hat{S} of compact, self-adjoint operators with eigenvalues $\hat{\lambda}_1 \geq \hat{\lambda}_2, \dots$ such that $\|\hat{S} - S\|_F = O_P(r_{Gn})$ we can choose the eigenfunctions $\hat{\phi}_1, \hat{\phi}_2, \dots$ such that*

$$\begin{aligned}|\hat{\lambda}_k - \lambda_k| &= O_P(r_{Gn}) \\ \|\hat{\phi}_k - \phi_k\| &= O_P(r_n)\end{aligned} \tag{C.3}$$

for each $k = 1, 2, \dots$ such that $\lambda_k > 0$.

PROOF: We follow closely the proofs for Proposition 4.2 in Gobet, Hoffmann, and Reiß (2004) and Theorem 2 in Yao, Müller, and Wang (2005a). Since S is compact, existence of eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots$ and eigenfunctions ϕ_1, ϕ_2, \dots follows from Mercer's Theorem (see Happ and Greven (2018) for a multivariate generalization where \mathcal{X} may be of dimension greater than one).

We define the resolvent maps of the operators S and \hat{S} ,

$$R(z) := (S - z\text{Id})^{-1}, \quad \text{and } \hat{R}(z) := (\hat{S} - z\text{Id})^{-1}$$

Defining the resolvent sets $\varrho(S)$ and $\varrho(\hat{S})$ via $\varrho(T) := \{z \in \mathbb{C} : T - z\text{Id} \text{ is invertible}\}$, we have for $z \in \varrho(S) \cap \varrho(\hat{S})$,

$$\begin{aligned} \hat{R}(z) &= (S - z\text{Id} + (\hat{S} - S))^{-1} \\ &= (R(z)^{-1} + (\hat{S} - S)R(z)R(z)^{-1})^{-1} \\ &= R(z) (\text{Id} + (\hat{S} - S)R(z))^{-1} \\ &= R(z) + R(z) \sum_{s=1}^{\infty} ((S - \hat{S})R(z))^s \end{aligned}$$

where the last equality uses a Neumann representation of the inverse. Therefore, if $\|\hat{S} - S\|_F \|R(z)\|_F < 1$, we can use the triangle inequality for the (trace) operator norm to bound

$$\|\hat{R}(z) - R(z)\|_F \leq \sum_{s=1}^{\infty} \left\| R(z) \left((S - \hat{S})R(z) \right)^s \right\| \leq \frac{\|\hat{S} - S\|_F \|R(z)\|_F^2}{1 - \|\hat{S} - S\|_F \|R(z)\|_F} \quad (\text{C.4})$$

Now, consider the k th eigenvalue λ_k . Since the operator S is self-adjoint and compact, its spectrum is real-valued and separated. In particular any nonzero eigenvalue λ_k has only finite multiplicity $m_k < \infty$, and there exists $\varrho_k > 0$ such that the ϱ_k -ball around λ_k in the complex plane \mathbb{C} does not contain any other eigenvalue different from λ_k .

We then let $\Gamma_k : [0, 2\pi] \rightarrow \mathbb{C}$ be the positively oriented Jordan curve

$$\Gamma_k(t) := \lambda_k + \varrho_k/2 e^{it}$$

around λ_k with radius $\varrho_k/2$. By the Cauchy integral formula and the Hilbert's resolvent equations (equations (2.4) and (2.5) in Chatelin (1983)) it can be verified that the operator

$$P_k := -\frac{1}{2i\pi} \int_{\Gamma_k} R(z) dz$$

is the orthogonal projector onto the eigenspace of S at the eigenvalue λ_k (Theorem 2.27 in Chatelin (1983)). We can similarly define

$$\hat{P}_k := -\frac{1}{2i\pi} \int_{\Gamma_k} \hat{R}(z) dz$$

Since the nonzero eigenvalues of \hat{S} are also separated and of finite multiplicities, we can assume without loss of generality that the curve Γ_k encloses a finite number of eigenvalues of \hat{S} , and that no eigenvalues of \hat{S} lie on the curve (otherwise we can replace the radius $\varrho_k/2$ with any other number in the interval $(0, \varrho_k)$). By Cauchy's integral formula, \hat{P}_k is the sum of the orthogonal projectors onto the eigenspaces of \hat{S} associated with the eigenvalues of \hat{S} enclosed by Γ_k . In particular, \hat{P}_k is an orthogonal projector into a linear subspace of finite dimension.

Next we define

$$M_k := \sup \{ \|R(z)\| : z \in \Gamma_k \} < \infty$$

and assume that $\varepsilon := \|\hat{S} - S\|_F \leq \frac{1}{2M_k}$, so that in particular the bound (C.4) holds, and we can use (C.4) to bound

$$\begin{aligned} \|\hat{P}_k - P_k\|_F &\leq \frac{1}{2\pi} \int_{\Gamma_k} \|\hat{R}(z) - R(z)\|_F dz \\ &\leq \frac{\varrho_k}{2} \frac{\|\hat{S} - S\|_F M_k^2}{1 - \|\hat{S} - S\|_F M_k} \\ &\leq \varrho_k M_k^2 \varepsilon =: B_k \end{aligned}$$

Since $\|\hat{P}_k - P_k\|_F \leq B_k < \|P_k\|_F$ for n sufficiently large, $\hat{P}_k \neq 0$. In particular, the intersection of the $\varrho_k/2$ ball around λ_k with the spectrum of \hat{S} is nonempty. Now, let ϕ_k be an eigenvector of S associated with the eigenvalue λ_k , and let $\hat{\phi}_k$ be a vector of unit length in the eigenspace of \hat{S} corresponding to an eigenvalue $\hat{\lambda}_k$ with $|\hat{\lambda}_k - \lambda_k| \leq \varrho_k/2$. Without loss of generality, we choose $\hat{\phi}_k$ such that $\langle \hat{\phi}_k, \phi_k \rangle > 0$ and that ϕ_k is orthogonal to all other eigenvectors of \hat{S} at eigenvalue $\hat{\lambda}_k$. In particular, $\hat{P}_k \phi_k = \langle \phi_k, \hat{\phi}_k \rangle \hat{\phi}_k$, so that

$$\begin{aligned} \|\hat{P}_k - P_k\|^2 &\geq \|(\hat{P}_k - P_k)\phi_k\|^2 = \|\hat{P}_k \phi_k - \phi_k\|^2 \\ &= 1 - 2\langle \phi_k, \hat{P}_k \phi_k \rangle + \|\hat{P}_k \phi_k\|^2 \\ &= 1 - (\langle \hat{\phi}_k, \phi_k \rangle)^2 \end{aligned}$$

Furthermore,

$$\begin{aligned} \|\hat{\phi}_k - \phi_k\|^2 &\leq 2 - 2\langle \hat{\phi}_k, \phi_k \rangle \leq 2(1 - \langle \hat{\phi}_k, \phi_k \rangle)(1 + \langle \hat{\phi}_k, \phi_k \rangle) \\ &= 2 \left(1 - (\langle \hat{\phi}_k, \phi_k \rangle)^2 \right) \\ &\leq 2\|\hat{P}_k - P_k\|^2 \leq 2B_k \end{aligned}$$

Reversing the roles of S and \hat{S} , we can similarly find an eigenvector of S at eigenvalue λ_k for any vector $\hat{\phi}_k$ in the eigenspace of \hat{S} at an eigenvalue $\hat{\lambda}_k$ with $|\hat{\lambda}_k - \lambda_k| \leq \varrho_k/2$, such that $\|\phi_k - \hat{\phi}_k\|$ satisfies the same bound. The convergence rate for the eigenvalues then follows from Slutsky's Lemma applied to the formula characterizing the k th eigenvalue, $\lambda_k = \langle \phi_k, S\phi_k \rangle$ \square

We now complete the proof of Theorem A.2: Since $\hat{\phi}_k$ are defined by the generalized eigenvalue problem

$$\hat{T}_{\mu\tau} \hat{T}_{\mu\tau}^* \hat{\phi}_k = \hat{\lambda}_k \hat{T}_{\mu\mu\alpha} \hat{\phi}_k$$

and $\hat{T}_{\mu\mu\alpha}$ is injective, we can equivalently rewrite

$$\hat{\phi}_k := \hat{T}_{\mu\mu\alpha}^{-1/2} \hat{\chi}_k$$

where $\hat{\chi}_k$ solves the eigenvalue problem

$$\hat{S} \hat{\chi}_k = \hat{\lambda}_k \hat{\chi}_k$$

and $\hat{S} := \hat{T}_{\mu\mu\alpha}^{-1/2} \hat{T}_{\mu\tau} \hat{T}_{\mu\tau}^* \hat{T}_{\mu\mu\alpha}^{-1/2}$. We therefore first derive the convergence rate for $\hat{\chi}_k$ with respect to χ_k , the eigenfunction associated with the k th largest eigenvalue λ_k of $S := T_{\mu\mu\alpha}^{-1/2} T_{\mu\tau} T_{\mu\tau}^* T_{\mu\mu\alpha}^{-1/2}$.

Since by assumption of the theorem, the covariance functions $H_{\mu\mu}$ and $H_{\mu\tau}$ are estimated uniformly consistently at the rate r_{Gn} , it follows immediately that the corresponding Hilbert-Schmidt operators converge at the same rate under the trace (operator) norm, $\|\hat{T}_{\mu\mu} - T_{\mu\mu}\|_F = O_p(r_{Gn})$ and $\|\hat{T}_{\mu\tau} - T_{\mu\tau}\|_F = O_p(r_{Gn})$, follows immediately.

We furthermore confirm that the operator $S_0 := T_{\mu\mu}^{-1/2}T_{\mu\tau}T_{\mu\tau}^*T_{\mu\mu}^{-1/2}$ is compact. From the proof of Lemma B.1, $\min_B \|\tau_g - B\mu_g\|^2 = \text{tr}(T_{\mu\tau}^*T_{\mu\mu}^{-1}T_{\mu\tau})$ where the operator $T_{\mu\mu}$ is understood to be restricted to $\ker(T_{\mu\mu})^\perp$. Therefore,

$$\begin{aligned} \text{tr}(T_{\mu\mu}^{-1/2}T_{\mu\tau}T_{\mu\tau}^*T_{\mu\mu}^{-1/2}) &= \text{tr}(T_{\mu\tau}^*T_{\mu\mu}^{-1}T_{\mu\tau}) \\ &= \min_B \|\tau_g - B\mu_g\|^2 \leq \|\tau_g\|^2 < \infty \end{aligned}$$

Since S_0 is self-adjoint, it follows that it is also trace class and therefore compact. Since $T_{\mu\mu a}^{-1/2}T_{\mu\mu}^{1/2}$ and its transpose are compact for any $a \geq 0$, it also follows that $S \equiv S_a$ is compact for any $a \geq 0$ as well. \hat{S} can be shown to be compact by the same argument applied to sample analogs.

Next, define $A_a := (T_{\mu\mu} + a\text{Id})^{1/2} \equiv (T_{\mu\mu}^{1/2} + a^{1/2}\text{Id})$ and $\hat{A}_a := (\hat{T}_{\mu\mu}^{1/2} + a^{1/2}\text{Id})$. We can then check that

$$\hat{A}_a^{-1} - A_a^{-1} = \hat{A}_a^{-1}(\hat{A}_a - A_a)A_a^{-1} = \hat{A}_a^{-1}(\hat{T}_{\mu\mu}^{1/2} - T_{\mu\mu}^{1/2})A_a^{-1/2}$$

The difference between \hat{S} and S can be written as

$$\hat{S} - S = \hat{T}_{\mu\mu a}^{-1/2}\hat{T}_{\mu\tau}\hat{T}_{\mu\tau}^*\hat{T}_{\mu\mu a}^{-1/2} - T_{\mu\mu a}^{-1/2}T_{\mu\tau}T_{\mu\tau}^*T_{\mu\mu a}^{-1/2} = R_1 + R_2 + R_3$$

where

$$\begin{aligned} R_1 &= \hat{T}_{\mu\mu a}^{-1/2}\hat{T}_{\mu\tau}\hat{T}_{\mu\tau}^*(\hat{T}_{\mu\mu a}^{-1/2} - T_{\mu\mu a}^{-1/2}) \\ &= \hat{T}_{\mu\mu a}^{-1/2}\hat{T}_{\mu\tau}\hat{T}_{\mu\tau}^*\hat{T}_{\mu\mu a}^{-1/2}(\hat{T}_{\mu\mu a}^{1/2} - T_{\mu\mu a}^{1/2})T_{\mu\mu a}^{-1/2} \\ &= \hat{S}(\hat{T}_{\mu\mu a}^{1/2} - T_{\mu\mu a}^{1/2})\hat{T}_{\mu\mu a}^{-1/2} \\ R_2 &= T_{\mu\mu a}^{-1/2}(\hat{T}_{\mu\tau}\hat{T}_{\mu\tau}^* - T_{\mu\tau}T_{\mu\tau}^*)\hat{T}_{\mu\mu a}^{-1/2} \\ R_3 &= (\hat{T}_{\mu\mu a}^{-1/2} - T_{\mu\mu a}^{-1/2})T_{\mu\tau}T_{\mu\tau}^*T_{\mu\mu a}^{-1/2} \\ &= \hat{T}_{\mu\mu a}^{-1/2}(\hat{T}_{\mu\mu a}^{1/2} - T_{\mu\mu a}^{1/2})S \end{aligned}$$

Since $\hat{T}_{\mu\mu}$ and $T_{\mu\mu}$ are nonnegative, the eigenvalues of $\hat{T}_{\mu\mu a}^{1/2}$ and $T_{\mu\mu a}^{1/2}$ are bounded from below by $a^{-1/2}$. It therefore follows that $\|R_1\| = O(a^{-1/2}r_{Gn})$, $\|R_2\| = O(a^{-1}r_{Gn})$, and $\|R_3\| = O(a^{-1/2}r_{Gn})$ under the trace norm. Hence together with the triangle inequality, Lemma C.2 implies that $\hat{\chi}_k^* - \chi_k$ converges at a rate $O_P(a^{-1}r_{Gn})$. The conclusion of the Theorem then follows from the observation that the largest eigenvalue of $\hat{T}_{\mu\mu a}^{-1/2}$ is bounded by $a^{-1/2}$ \square

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