Conditional Distributional Treatment Effect with Kernel Conditional Mean Embeddings and U-Statistic Regression

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Abstract

We propose to analyse the conditional distributional treatment effect (CoDiTE), which, in contrast to the more common conditional average treatment effect (CATE), is designed to encode a treatment’s distributional aspects beyond the mean. We first introduce a formal definition of the CoDiTE associated with a distance function between probability measures. Then we discuss the CoDiTE associated with the maximum mean discrepancy via kernel conditional mean embeddings, which, coupled with a hypothesis test, tells us whether there is any conditional distributional effect of the treatment. Finally, we investigate what kind of conditional distributional effect the treatment has, both in an exploratory manner via the conditional witness function, and in a quantitative manner via U-statistic regression, generalising the CATE to higher-order moments. Experiments on synthetic, semi-synthetic and real datasets demonstrate the merits of our approach.

1. Introduction

Analysing the effect of a treatment (medical drug, economic programme, etc.) has long been a problem of great importance, and has attracted researchers from diverse domains, including econometrics (Imbens & Wooldridge, 2009), political sciences (Künzel et al., 2019), healthcare (Foster et al., 2011) and social sciences (Imbens & Rubin, 2015). The field has naturally received much attention of statisticians over the years (Rosenbaum, 2002; Rubin, 2005; Imbens & Rubin, 2015), and in the past few years, the machine learning community has started applying its own armoury to this problem – see Section 1.2 for a succinct review.

1 Traditional methods for treatment effect evaluation focus on the analysis of the average treatment effect (ATE), such as an increase or decrease in average income, inequality or poverty, aggregated over the population. However, the ATE is not informative about the individual responses to the intervention and how the treatment impact varies across individuals (known as treatment effect heterogeneity). The study of conditional average treatment effect (CATE) has been proposed to analyse such heterogeneity in the mean treatment effect. Although sufficient in many cases, the CATE is still an average. As such, it fails to capture information about distributional aspects of the treatment beyond the mean. A significant amount of interest exists for developing methods that can analyse distributional treatment effects conditioned on the covariates (Chang et al., 2015; Bitler et al., 2017; Shen, 2019; Chernozhukov et al., 2020; Hohberg et al., 2020; Briseño Sanchez et al., 2020).

Our contributions are as follows. Firstly, we formally define the conditional distributional treatment effect (CoDiTE) associated with a chosen distance function between distributions. Then we use kernel conditional mean embeddings (Song et al., 2013; Park & Muandet, 2020a) to analyse the CoDiTE associated with the maximum mean discrepancy (Gretton et al., 2012). Coupled with a statistical hypothesis test, this can determine whether there exists any effect of the treatment, conditioned on a set of covariates. Finally, we use conditional witness functions and U-statistic regression to investigate what kind of effect the treatment has.

1.1. Problem Set-Up: Potential Outcomes Framework

Throughout this paper, we take $(\Omega, \mathcal{F}, P)$ as the underlying probability space, $\mathcal{X}$ as the input space and $\mathcal{Y} \subseteq \mathbb{R}$ as the output space. Let $Z : \Omega \to \{0, 1\}$, $X : \Omega \to \mathcal{X}$ and $Y_0, Y_1, Y : \Omega \to \mathcal{Y}$ be random variables representing, respectively, the treatment assignment, covariates, the potential outcomes under control and treatment, and the observed outcome, i.e. $Y = Y_0(1 - Z) + Y_1Z$. For example, $Z$ may indicate whether a subject is administered a medical treatment ($Z = 1$) or not ($Z = 0$). The potential outcomes $Y_1, Y_0$ respectively correspond to subject’s responses had they received treatment or not. The covariates $X$ corre-
Figure 1. Toy illustration of higher-order heterogeneity that cannot be captured by CATE. (a) Data. $X \sim \text{Uniform}[0,1]$, $Y_0 = 3 + 5X + X < 0.3 \cdot N + 71X > 0.3(1 + (X - 0.3))N$ and $Y_1 = 4X + X < 0.3 \cdot N + 71X > 0.3(1 + (X - 0.3))N$, where $N \sim \mathcal{N}(0,1)$; in particular, the CATE is increasing with $X$. (b) Hypothesis test (Section 4.2) Each of the hypotheses $P_{Y_0|X} \equiv P_{Y_0|X}, P_{Y_1|X} \equiv P_{Y_1|X}$ and $P_{Y_0|X} \equiv P_{Y_1|X}$ are tested 100 times. The last (false) hypothesis is rejected in most tests, while the first two (true) hypotheses are not rejected in most tests, meaning that both type I and type II errors are low. (c) Conditional witness function (Section 5.1). The conditional witness function is close to zero for all $Y$ at $X \geq 0.5$, demonstrating that $P_{Y_0|X}$ and $P_{Y_1|X}$ are similar in this region of $X$. For $X < 0.4$, the witness function is positive in regions where the density of $Y_1$ is higher than that of $Y_0$, and negative in regions where the density of $Y_0$ is higher than that of $Y_1$. (d) U-statistic regression (Section 5.2). True conditional standard deviation (in black) is estimated (in red and blue for control and treatment groups respectively) as a function of $X$ via U-statistic regression (since variance is a U-statistic) and the square-root operation. We see that the standard deviation increases linearly for $X \geq 0.3$.

CoDiTE with CMEs and U-Statistic Regression

respond to subject’s characteristics such as age, gender, race that could influence both the potential outcomes and the choice of treatment. We denote the distributions of random variables by subscripting $P$, e.g. $P_X$ for the distribution of $X$. Throughout, we impose the mild condition that conditional distribution $P(· | X)$ admits a regular version ( Çınlar, 2011, p.150, Definition 2.4, Proposition 2.5).

Each unit $i = 1, ..., n$ is associated with an independent copy $(X_i, Z_i, Y_{0i}, Y_{1i})$ of $(X, Z, Y_0, Y_1)$. However, for each $i = 1, ..., n$, we observe either $Y_{0i}$ or $Y_{1i}$; this missing value problem is known as the fundamental problem of causal inference ( Holland, 1986), preventing us from directly computing the difference in the outcomes under treatment and control for each unit. As a result, we only have access to samples $\{(x_i, z_i, y_{i1})\}_{i=1}^{n}$ of $(X, Z, Y)$. We write $n_0 = \sum_{i=1}^{n} 1_{z_i=0}$ and $n_1 = \sum_{i=1}^{n} 1_{z_i=1}$ for the control and treatment sample sizes, and denote the control and treatment samples by $\{(x_0^i, y_{i1})\}_{i=1}^{n_0}$ and $\{(x_1^i, y_{i1})\}_{i=1}^{n_1}$.

We assume strong ignorability (Rosenbaum & Rubin, 1983):

unconfoundedness $\quad Z \perp (Y_0, Y_1) \mid X$; and

overlap $\quad 0 < e(X) = P(Z = 1 \mid X) = E[Z \mid X] < 1$.

Causal treatment effects are then identifiable from observational data, since $P_{Y_0|X} = P_{Y_0|X,Z=0} = P_{Y_1|X,Z=0}$, and similarly for $P_{Y_1|X}$. The quantity $e(X)$ is the propensity score. In a randomised experiment, $e(X)$ is known and controlled (Imbens & Rubin, 2015, p.40, Definition 3.10).

The usual objects of interest in the treatment effect literature are the average treatment effect (ATE), $E[Y_1 - Y_0]$, and the conditional average treatment effect (CATE), $T(x) = E[Y_1 - Y_0 \mid X = x]$. In this paper, we propose to extend the analysis to compare other aspects of the conditional distributions, $P_{Y_0|X}$ and $P_{Y_1|X}$. One compelling reason to do this is that estimating CATE is inherently a problem of comparing two means, and as such, is only meaningful if the corresponding variances are given. Consider the toy example in Figure 1. The CATE is constructed to be increasing with $X$, but taking into account the variance, the treatment effect is clearly more pronounced for small values of $X$. For example, the probability of $Y_1$ being greater than $Y_0$ is much higher for smaller values of $X$.

Beyond the mean and variance, researchers may also be interested in other higher-moment treatment effect heterogeneity, such as Gini’s mean difference or skewness, or indeed how the entire conditional densities of the control and treatment groups differ given the covariates, in an exploratory fashion. Panels (b), (c) and (d) in Figure 1 demonstrate each of the steps we propose in this paper applied to this toy dataset: hypothesis testing of equality of conditional distributions, the conditional witness function and U-statistic regression (variance, in this instance), respectively.

1.2. Related Work & Summary of Contributions

In the past few years the machine learning community has focused much effort on models for estimating the CATE function. Some approaches include Gaussian processes (Alaa & van der Schaar, 2017; 2018), Bayesian regression trees (Hill, 2011; Hahn et al., 2020), random forests (Wager & Athey, 2018), neural networks (Johansson et al., 2016; Shalit et al., 2017; Louizos et al., 2017; Atan et al., 2018; Shi et al., 2019), GANs (Yoon et al., 2018), boosting and adaptive regression splines (Powers et al., 2018) and kernel mean embeddings (Singh et al., 2020).

Distributional extensions of the ATE have been considered by many authors. Abadie (2002) tested the hypotheses of
equality and stochastic dominance of the marginal outcome distributions \( P_{Y_0} \) and \( P_{Y_1} \), whereas Kim et al. (2018); Muan- 
det et al. (2018) focus on estimating \( P_{Y_0} \) and \( P_{Y_1} \), or some distance between them. These works do not consider treatment effect heterogeneity. Singh et al. (2020, Appendix C) consider CATE as well as distributional treatment effect, and while it seems that the ideas can straightforwardly be extended to conditional distributional treatment effect, it is not explicitly considered in the paper.

The CoDiTE incorporates both distributional considerations of treatment effects and treatment effect heterogeneity. Interest has been growing, especially in the econometrics literature, for such analyses – indeed, Bitler et al. (2017) provided concrete evidence that in some settings, the CATE does not suffice. Existing works that analyse the CoDiTE can be split into three categories, depending on how distributions are characterised: (i) quantiles, (ii) cumulative distributional functions, and (iii) specific distributional parameters, such as the mean, variance, skewness, etc. In category (i), quantile regression is a powerful tool (Koenker, 2005); however, in order to get a distributional picture via quantiles, one needs to estimate a large number of quantiles, and issues of crossing quantiles arise, whereby estimated quantiles are non-monotone. In category (ii), Chernozhukov et al. (2013; 2020) propose splitting \( Y \) into a grid and regressing for the cumulative distribution function at each point in the grid, but this also brings issues of non-monotonicity of the cumulative distribution function, similar to crossing quantiles. Shen (2019) estimates the cumulative distribution functions \( P(Y_0 < y^*) \) and \( P(Y_1 < y^*) \) for each \( y^* \in Y \) given each value of \( X = x \) by essentially applying the Nadaraya-Watson conditional U-statistic of Stute (1991) to the U-kernel \( h(y) = 1(y \leq y^*) \). In category (iii), generalised additive models for location, scale and shape (GAMLSS) (Stasinopoulos et al., 2017) have been applied for CoDiTE analysis (Hoehberg et al., 2020; Briseño Sanchez et al., 2020), but being a parametric model, despite its flexibility, the researcher has to choose a model beforehand to proceed, and issues of model misspecification are unavoidable.

Interest has also always existed for hypothesis tests in the context of treatment effect analysis, especially in econometrics (Imbens & Wooldridge, 2009, Sections 3.3 and 5.12). Abadie (2002) tested the equality between the marginal distributions of \( Y_0 \) and \( Y_1 \), while Crump et al. (2008) tested for the equality of \( \mathbb{E}[Y_1 | X] \) and \( \mathbb{E}[Y_0 | X] \). Lee & Whang (2009); Lee (2009); Chang et al. (2015); Shen (2019) were interested, among others, in the hypothesis of the equality of \( P_{Y_1 | X} \) and \( P_{Y_0 | X} \), which we consider in Section 4.2.

Summary of Contributions We characterise distributions in two ways – first as elements in a reproducing kernel Hilbert space via kernel conditional mean embeddings, which, to the best of our knowledge, is a novel attempt in the treatment effect literature, and secondly via specific distributional parameters, as in category (iii). The former characterisation gives us a novel way of testing for the equality of conditional distributions, as well as an exploratory tool for density comparison between the groups via conditional witness functions. For the latter characterisation, we provide, to the best of our knowledge, a novel U-statistic regression technique by generalising kernel ridge regression, which, in contrast to GAMLSS, is fully nonparametric. Neither characterisation requires the estimation of a large number of quantities, unlike characterisations via quantiles or cumulative distribution functions.

2. Preliminaries

In this section, we briefly review reproducing kernel Hilbert space embeddings and U-statistics. A more complete introduction can be found in Appendix A.

2.1. Reproducing Kernel Hilbert Space Embeddings

Let \( l : Y \times Y \to \mathbb{R} \) be a (scalar) positive definite kernel on \( Y \) with reproducing kernel Hilbert space (RKHS) \( \mathcal{H} \) (Berlinet & Thomas-Agnan, 2004, p.7, Definition 1). Given a random variable \( Y \) on \( Y \), satisfying \( \mathbb{E}[(\sqrt{l(Y,Y)})] < \infty \), the kernel mean embedding of \( Y \) is defined as \( \mu_Y(·) = \mathbb{E}[l(Y,·)] \) (Smola et al., 2007, Eqn. (2a)). Given two random variables \( Y \) and \( Y' \), the maximum mean discrepancy (MMD) between them is defined as \( \| \mu_Y - \mu_{Y'} \|_\mathcal{H} \) (Gretton et al., 2012, Lemma 4), where \( \mu_Y - \mu_{Y'} \) is the (unnormalised) witness function (Gretton et al., 2012, Section 2.3; Lloyd & Ghahramani, 2015, Eqn. (3.2)). If the embedding is injective from the space of probability measures on \( Y \) to \( \mathcal{H} \), then we say that \( l \) is characteristic (Fukumizu et al., 2008, Section 2.2), in which case the MMD is a proper metric.

Given another random variable \( X \) on \( X \), the conditional mean embedding (CME) of \( Y \) given \( X \) is defined as \( \mu_{Y|X} = \mathbb{E}[l(Y,·) | X] \) (Park & Muandet, 2020a, Definition 3.1)\(^2\).

Denote by \( L^2(\mathcal{X}, P_X; \mathcal{H}) \) the Hilbert space of (equivalence classes of) measurable functions \( F : \mathcal{X} \to \mathcal{H} \) such that \( \| F(·) \|_2^2 \) is \( P_X \)-integrable, with inner product \( \langle F_1, F_2 \rangle_{L^2(\mathcal{X}, P_X; \mathcal{H})} = \int_{\mathcal{X}} \langle F_1(x), F_2(x) \rangle_{\mathcal{H}} dP_X(x) \). Given an operator-valued kernel \( \Gamma : \mathcal{X} \times \mathcal{X} \to \mathcal{L}(\mathcal{H}) \), where \( \mathcal{L}(\mathcal{H}) \) is the Banach space of bounded linear operators \( \mathcal{H} \to \mathcal{H} \), there exists an associated vector-valued RKHS of functions \( \mathcal{X} \to \mathcal{H} \) (Carmeli et al., 2006, Definition 2.1, Definition 2.2, Proposition 2.3).

2.2. U-Statistics

Let \( Y_1, \ldots, Y_r \) be independent copies of \( Y \), and let \( h : Y^r \to \mathbb{R} \) be a symmetric function, i.e. for any permutation \( \pi \)

\[^2\]We use the conditional expectation interpretation of the CME. An interpretation of the CME as an operator from an RKHS on \( \mathcal{X} \) to \( \mathcal{H} \) also exists (Song et al., 2009; 2013; Fukumizu et al., 2013).
of \((1, \ldots, r), h(y_1, \ldots, y_r) = h(y_{\pi(1)}, \ldots, y_{\pi(r)})\), such that
\(h(Y_1, \ldots, Y_r)\) is integrable. Given i.i.d. copies \(Y_i \overset{\text{i.i.d.}}{\sim} Y\), the \(U\)-statistic (Hoeffding, 1948; Serfling, 1980, p. 172) for an unbiased estimation of \(\theta(P_Y) = \mathbb{E}[h(Y_1, \ldots, Y_r)]\) is
\[\hat{\theta}(Y_1, \ldots, Y_n) = \frac{1}{N(n)} \sum h(Y_{i_1}, \ldots, Y_{i_n})\]
where \(N(n)\) is the binomial coefficient and the summation is over the \(\binom{n}{r}\) combinations of \(r\) distinct elements \(\{i_1, \ldots, i_r\}\) from \(\{1, \ldots, n\}\).

This has been extended to the conditional case (Stute, 1991). Given another random variable \(X\) on \(\mathcal{X}\) and independent copies \(X_1, \ldots, X_r\) of it, we can consider the estimation of \(\theta(P_{Y|X}) = \mathbb{E}[h(Y_1, \ldots, Y_r)|X_1, \ldots, X_r]\). Stute (1991); Derumigny (2019) extend the Nadaraya-Watson regressor (Nadaraya, 1964; Watson, 1964) to estimate \(\theta(P_{Y|X})\).

3. Conditional Distributional Treatment Effect

In this section, we generalise the notion of CATE to account for distributional differences between treatment and control groups, rather than just the mean difference.

**Definition 3.1.** Let \(D\) be some distance function between probability measures. We define the conditional distributional treatment effect (CoDiTE) associated with \(D\) as
\[U_D(x) = D(P_{Y|X=x}, P_{Y|X=x}).\]

Here, the choice of \(D\) depends on what characterisation of distributions is used (c.f. Section 1.2). For example, if \(D(P_{Y|X=x}, P_{Y|X=x}) = \mathbb{E}[Y_1|X=x] - \mathbb{E}[Y_0|X=x]\), we recover the CATE, i.e. \(U_D(x) = T(x)\), thereby showing that the CoDiTE is a strict generalisation of the CATE. Different choices of \(D\) will require different estimators.

The usual performance metric of a CATE estimator \(\hat{T}\) is the precision of estimating heterogeneous effects (PEHE) (first proposed in sample form by Hill (2011, Section 4.3); we report the population-level definition, found in, for example, Alaa & Van Der Schaar (2019, Eqn. (5)):
\[\|\hat{T} - T\|_2^2 = \mathbb{E}[|\hat{T}(X) - T(X)|^2].\]

We propose a performance metric of an estimator of the CoDiTE in an exactly analogous manner.

**Definition 3.2.** Given a distance function \(D\), for an estimator \(\hat{U}_D\) of \(U_D\), we define the precision of estimating heterogeneous distributional effects (PEHDE) as
\[\psi_D(\hat{U}_D) = \|\hat{U}_D - U_D\|_2^2 = \mathbb{E}[|\hat{U}_D(X) - U_D(X)|^2].\]

Again, if \(D\) measures the difference in expectations, then the associated PEHDE \(\psi_D\) reduces to the usual PEHE.

Henceforth, we explore different choices of the distance function \(D\), as well as methods of estimating the corresponding CoDiTE \(U_D\), to answer the following questions:

**Q1** Are \(P_{Y|X}\) and \(P_{Y|X}\) different? In other words, is there any distributional effect of the treatment? (Section 4)

**Q2** If so, how does the distribution of the treatment group differ from that of the control group? (Section 5)

4. CoDiTE associated with MMD via CMEs

In this section, we answer Q1, i.e. we investigate whether the treatment has any effect at all. To this end we choose \(D\) to be the MMD with the associated kernel \(l\) being characteristic. Then writing \(\mu_{Y|X}\) and \(\mu_{Y|X}\) for the CMEs of \(Y_0\) and \(Y_1\) given \(X\) respectively (c.f. Section 2.1), we have
\[U_{\text{MMD}}(x) = \text{MMD}(P_{Y|X=x}, P_{Y|X=x}) = \|\mu_{Y|X=x} - \mu_{Y|x=x}\|_H.\]

Since \(l\) is characteristic, \(P_{Y|X=x}\) and \(P_{Y|X=x}\) are equal if and only if \(\text{MMD}(P_{Y|X=x}, P_{Y|X=x}) = 0\). What makes the MMD a particularly convenient choice is that for each \(x \in \mathcal{X}, P_{Y|X=x}\) and \(P_{Y|X=x}\) are represented by individual elements \(\mu_{Y|X=x}\) and \(\mu_{Y|X=x}\) in the RKHS \(H\), which means that we can estimate the associated CoDiTE simply by performing regression with \(\mathcal{X}\) as the input space and \(H\) as the output space, as will be shown in the next section.

4.1. Estimation and Consistency

We now discuss how to obtain empirical estimates of \(U_{\text{MMD}}(x)\). Recall that, by the unconfoundedness assumption, we can estimate \(\mu_{Y|X}\) and \(\mu_{Y|X}\) separately from control and treatment samples respectively. We perform operator-valued kernel regression (Micchelli & Pontil, 2005; Kadri et al., 2016) in separate vector-valued RKHSs \(G_0\) and \(G_1\), endowed with kernels \(\Psi_0(l, \cdot) = k_0(\cdot, \cdot)\text{Id}\) and \(\Psi_1(l, \cdot) = k_1(\cdot, \cdot)\text{Id}\), where \(k_0, k_1 : \mathcal{X} \times \mathcal{X} \to \mathbb{R}\) are scalar-valued kernel and \(\text{Id} : H \to H\) is the identity operator. Following Park & Muandet (2020a, Eqn. (4)), the empirical estimates \(\hat{\mu}_{Y|X}\) and \(\hat{\mu}_{Y|X}\) of \(\mu_{Y|X}\) and \(\mu_{Y|X}\) are constructed, for each \(x \in \mathcal{X}\), as
\[
\hat{\mu}_{Y|X=0} = k_0^T(x)W_0l_0 \in G_0
\]
and
\[
\hat{\mu}_{Y|X=1} = k_1^T(x)W_1l_1 \in G_1,
\]
where
\[W_0 = (K_0 + n_0 \lambda_{n_0} I_{n_0})^{-1}, W_1 = (K_1 + n_1 \lambda_{n_1} I_{n_1})^{-1},\]
\[K_0|1 \leq i, j \leq n_0 = k_0(x^0_i, x^0_j), K_1|1 \leq i, j \leq n_1 = k_1(x^1_i, x^1_j),\]
\[\lambda_{n_0} > 0, \lambda_{n_1} > 0\] are regularisation parameters, \(I_{n_0}\) and \(I_{n_1}\) are identity matrices, \(k_0(x) = \langle k_0(x^0_i, x) \rangle, \ldots, \langle k_0(x^0_{n_0}, x) \rangle\rangle^T\), \(k_1(x) = \langle k_1(x^1_i, x) \rangle, \ldots, \langle k_1(x^1_{n_1}, x) \rangle\rangle^T\), \(l_0 = \langle l(y^0_1), \ldots, l(y^0_{n_0}) \rangle\rangle^T\) and \(l_1 = \langle l(y^1_1), \ldots, l(y^1_{n_1}) \rangle\rangle^T\).

By plugging in the estimates (2) in the expression (1) for \(U_{\text{MMD}}\), we can construct \(\hat{U}_{\text{MMD}}\) as
\[
\hat{U}_{\text{MMD}}(x) = \|\hat{\mu}_{Y|X=0} - \hat{\mu}_{Y|X=1}\|_H.
\]
The next lemma establishes a closed-form expression for \(\hat{U}_{\text{MMD}}\) based on the control and treatment samples.
Algorithm 1 Kernel conditional discrepancy (KCD) test of conditional distributional treatment effect

```
Input: data \{ \{(x_i, z_i, y_i)\}_{i=1}^n \}, significant level \( \alpha \), kernels \( k_0, k_1, l \), regularisation parameters \( \lambda_0, \lambda_1 \), no. of permutations \( m \).
Calculate \( \hat{t} \) using Lemma 4.4 based on the input data.
KLR of \( z_i \) against \( x_i \) to obtain \( \hat{e}(x_i) \).
for \( k = 1 \) to \( m \) do
  For each \( i = 1, \ldots, n \), sample \( \hat{z}_i \sim \text{Bernoulli}(\hat{e}(x_i)) \).
  Calculate \( \hat{t}_k \) from the new dataset \( \{x_i, \hat{z}_i, y_i\}_{i=1}^n \).
end for
Calculate the \( p \)-value as \( p = \frac{1+\sum_{i=1}^m \mathbb{I}\{t_i \geq \hat{t}\}}{1+m} \).
if \( p < \alpha \) then
  Reject \( H_0 \).
end if
```

**Lemma 4.1.** For each \( x \in X \), we have

\[
\hat{U}_{\text{MMD}}^2(x) = k_0^2(x)W_0L_0W_0^T k_0(x) - 2k_0^2(x)W_0LW_1^T k_1(x) + k_1^2(x)W_1L_1W_1^T k_1(x),
\]

where

\[
[L_0]_{1 \leq i, j \leq n_0} = l(y_i^0, y_j^0), \quad [L]_{1 \leq i \leq n_0, 1 \leq j \leq n_1} = l(y_i^0, y_j^1) \quad \text{and} \quad [L_1]_{1 \leq i, j \leq n_1} = l(y_i^1, y_j^1).
\]

The proof of this, and all other results, are deferred to Appendix C. The next theorem shows that, using universal kernels \( \Gamma_0, \Gamma_1 \) (Carmeli et al., 2010, Definition 4.1), \( \hat{U}_{\text{MMD}} \) is universally consistent with respect to the PEHDE.

**Theorem 4.2** (Universal consistency). Suppose that \( k_0, k_1 \) and \( l \) are bounded, that \( \Gamma_0 \) and \( \Gamma_1 \) are universal, and that \( \lambda_{n_0} \) and \( \lambda_{n_1} \) decay at slower rates than \( O(n_0^{-1/2}) \) and \( O(n_1^{-1/2}) \) respectively. Then as \( n_0, n_1 \to \infty \),

\[
\psi_{\text{MMD}}(\hat{U}_{\text{MMD}}) = \mathbb{E}[ (\hat{U}_{\text{MMD}}(X) - U_{\text{MMD}}(X))^2 ] \xrightarrow{\text{P}} 0.
\]

**4.2. Statistical Hypothesis Testing**

We are interested in whether or not the two conditional distributions \( P_{Y|X} \) and \( P_{Y|X^t} \), corresponding to control and treatment, are equal. The hypotheses are then

\begin{align*}
H_0: \quad & P_{Y|X=x} = P_{Y|X=x^t} \ 	ext{for all } x \in X, \\
H_1: \quad & \text{there exists } A \subseteq X \text{ with positive measure such that } P_{Y|X=x} \neq P_{Y|X=x^t} \text{ for all } x \in A.
\end{align*}

The null hypothesis \( H_0 \) means that the treatment has no effect for any of the covariates, whereas the alternative hypothesis \( H_1 \) means that the treatment has an effect on some of the covariates, where the effect is distributional. For notational simplicity, we write \( P_{Y|X} \equiv P_{Y|X^t} \) if \( H_0 \) holds.

We use the following criterion for \( P_{Y|X} \equiv P_{Y|X^t} \), which we call the kernel conditional discrepancy (KCD):

\[
t = \mathbb{E}[\|\hat{\mu}_{Y|X} - \hat{\mu}_{Y|X^t}\|_2^2].
\]

The following lemma tells us that \( t \) can indeed be used as a criterion of \( P_{Y|X} \equiv P_{Y|X^t} \).

**Lemma 4.3.** If \( t \) is a characteristic kernel, \( P_{Y|X} \equiv P_{Y|X^t} \) if and only if \( t = 0 \).

Next, we define a plug-in estimate \( \hat{t} \) of \( t \), which we will use as the test statistic of our hypothesis test:

\[
\hat{t} = \frac{1}{n} \sum_{i=1}^n \|\hat{\mu}_{Y|X=x_i} - \hat{\mu}_{Y|X^t=x_i}\|^2.
\]

Then we have a closed-form expression for \( \hat{t} \) as follows.

**Lemma 4.4.** We have

\[
\hat{t} = \frac{1}{n} \text{Tr}(K_0W_0L_0W_0^T K_0^T) - \frac{2}{n} \text{Tr}(K_0W_0LW_1^T K_1^T) + \frac{1}{n} \text{Tr}(K_1W_1L_1W_1^T K_1^T),
\]

where \( K_0, L_1 \) and \( L \) are as defined in Lemma 4.1 and \( [K_0]_{1 \leq i \leq n_0, 1 \leq j \leq n_0} = k_0(x_i, x_j^0) \) and \( [K_1]_{1 \leq i \leq n_0, 1 \leq j \leq n_1} = k_1(x_i, x_j^1) \).

The consistency of \( \hat{t} \) in the limit of infinite data is shown in the following theorem.

**Theorem 4.5.** Under the same assumptions as in Theorem 4.2, we have \( t \xrightarrow{\text{P}} t \) as \( n_0, n_1 \to \infty \).

Unfortunately, it is extremely difficult to compute the (asymptotic) null distribution of \( t \) analytically, and so we resort to resampling the treatment labels to simulate the null distribution. To ensure that our resampling scheme respects the control and treatment covariate distributions \( P_X|Z=0 \) and \( P_X|Z=1 \), we follow the conditional resampling scheme of Rosenbaum (1984). We first estimate the propensity score \( \hat{e}(x_i) \) for each datapoint \( x_i \) (e.g. using kernel logistic regression (KLR) (Zhu & Hastie, 2005; Marteau-Ferey et al., 2019)), and then resample each data label from this estimated propensity score. By repeating this resampling procedure and computing the test statistic on each resampled dataset, we can simulate from the null distribution of the test statistic. Finally, the test statistic computed from the original dataset is compared to this simulated null distribution, and the null hypothesis is rejected or not rejected accordingly. The exact procedure is summarised in Algorithm 1.

**5. Understanding the CoDiTE**

After determining whether \( P_{Y|X} \) and \( P_{Y|X^t} \) are different via MMD-associated CoDiTE and hypothesis testing, we now turn to Q2, i.e. we investigate how they are different.
5.1. Conditional Witness Functions

For two real-valued random variables, the witness function between them is a useful tool for visualising where their densities differ, without explicitly estimating the densities (Gretton et al., 2012, Figure 1; Lloyd & Ghahramani, 2015, Figure 1). We extend this to the conditional case with the (unnormalised) conditional witness function \( \mu_{Y|X=x} - \mu_{Y|X=x'} \).

Let us fix \( x \in X \). The witness function between \( P_{Y|X=x} \) and \( P_{Y|X=x'} \) is \( \mu_{Y|X=x} - \mu_{Y|X=x'} : Y \to \mathbb{R} \). For \( y \in Y \) in regions where the density of \( P_{Y|X=x} \) is greater than that of \( P_{Y|X=x'} \), we have \( \mu_{Y|X=x}(y) - \mu_{Y|X=x'}(y) > 0 \). For \( y \) in regions where the converse is true, we similarly have \( \mu_{Y|X=x}(y) - \mu_{Y|X=x'}(y) < 0 \). The greater the difference in density, the greater the magnitude of the witness function. For each \( y \in Y \), the associated CoDiTE is

\[
U_{\text{witness},y}(x) = \mu_{Y|X=x}(y) - \mu_{Y|X=x'}(y).
\]

The estimates in (2) can be plugged in to obtain the estimate \( \hat{U}_{\text{witness},y} = \hat{\mu}_{Y|X=x}(y) - \hat{\mu}_{Y|X=x'}(y) \). Since convergence in the RKHS norm implies pointwise convergence (Berlinet & Thomas-Agnan, 2004, p.10, Corollary 1), Theorem 4.2 implies the consistency of \( \hat{U}_{\text{witness},y} \) with respect to the corresponding PEHDE. Clearly, if \( X \) is more than 1-dimensional, heat maps as in Figure 1(c) cannot be plotted; however, fixing a particular \( x \in X \), \( \mu_{Y|X=x} - \mu_{Y|X=x'} \) can be plotted against \( y \), since \( Y \subseteq \mathbb{R} \). Such plots will be informative of where the density of \( P_{Y|X=x} \) is greater than that of \( P_{Y|X=x'} \) and vice versa.

5.2. CoDiTE associated with Specific Distributional Quantities via U-statistic Regression

Next, we consider CoDiTE on specific distributional quantities, such as the mean, variance or skewness, or some function thereof. For example, Briseño Sanchez et al. (2020, Eqn. (2)) were interested, in addition to the CATE, in the treatment effect on the standard deviation \( U_D(x) = \text{std}(Y_1|X = x) - \text{std}(Y_0|X = x) \). Our motivating example in Figure 1 could inspire a “standardised” version of the CATE\(^3\):

\[
U_D(x) = \frac{\mathbb{E}[Y_1|X = x] - \mathbb{E}[Y_0|X = x]}{\sqrt{\text{Var}(Y_1|X = x) + \text{Var}(Y_0|X = x)}}. \tag{3}
\]

Many of these quantities can be represented as the expectation of a U-kernel, i.e. \( \mathbb{E}[h(Y_1, ..., Y_r)] \) (c.f. Section 2.2). For example, \( h(y) = y \) gives the mean, \( h(y_1, y_2) = \frac{1}{2}(y_1 - y_2)^2 \) gives the variance and \( h(y_1, y_2) = |y_1 - y_2| \) gives Gini’s mean difference. We consider their conditional counterparts, i.e. \( \theta(P_{Y_0|X}|P_{X}) = \mathbb{E}[h(Y_{01}, ..., Y_{0r})|X_1, ..., X_r] \) and \( \theta(P_{Y_1|X}|P_{X}) = \mathbb{E}[h(Y_{11}, ..., Y_{1r})|X_1, ..., X_r] \) (c.f. Section 2.2). By Çınlar (2011, p.146, Theorem 1.17), there exist functions \( F_0, F_1 : \mathcal{X}^r \to \mathbb{R} \) such that \( F_0(X_1, ..., X_r) = \theta(P_{Y_0|X}) \) and \( F_1(X_1, ..., X_r) = \theta(P_{Y_1|X}) \).

Estimation of \( F_0 \) and \( F_1 \) can be done via U-statistic regression, by generalising kernel ridge regression as follows. As in Section 4.1, let \( k_0 : \mathcal{X} \times \mathcal{X} \to \mathbb{R} \) be a kernel on \( \mathcal{X} \) with RKHS \( \mathcal{H}_0 \). Then if we define \( k_0^r : \mathcal{X}^r \times \mathcal{X}^r \to \mathbb{R} \) as

\[
k_0^r((x_1, ..., x_r), (x'_1, ..., x'_r)) = k_0(x_1, x'_1)k_0(x_r, x'_r).
\]

Berlinet & Thomas-Agnan (2004, p.31, Theorem 13) tells us that \( k_0^r \) is a reproducing kernel on \( \mathcal{X}^r \) with RKHS \( \mathcal{H}_0^r = \mathcal{H}_0 \otimes \cdots \otimes \mathcal{H}_0 \), the \( r \)-times tensor product of \( \mathcal{H}_0 \), whose elements are functions \( \mathcal{X}^r \to \mathbb{R} \). We estimate \( F_0 \) in \( \mathcal{H}_0^r \). Given any \( F \in \mathcal{H}_0^r \), the natural least-squares risk is

\[
\mathcal{E}(F) = \mathbb{E}[((F(X_1, ..., X_r) - h(Y_{01}, ..., Y_{0r}))^2].
\]

Recalling the control sample \( \{(x_{0i}, y_{0i})\}_{i=1}^{n_0} \), we solve the following regularised least-squares problem:

\[
\hat{F}_0 = \arg \min_{F \in \mathcal{H}_0^r} \left\{ \hat{\mathcal{E}}(F) + \lambda_{n_0} \|F\|_{\mathcal{H}_0^r}^2 \right\} \tag{4}
\]

where the empirical least-squares risk \( \hat{\mathcal{E}}(F) \) is defined as

\[
\hat{\mathcal{E}}(F) = \frac{1}{n_0 \choose r} \sum_{i_1, ..., i_r} (F(x_{0i_1}, ..., x_{0i_r}) - h(y_{0i_1}, ..., y_{0i_r}))^2,
\]

with the summation over the \( n_0 \choose r \) combinations of \( r \) distinct elements \( \{i_1, ..., i_r\} \) from \( \{1, ..., n_0\} \). Note that \( \hat{\mathcal{E}}(F) \) is itself a U-statistic for the estimation of \( \mathcal{E}(F) \). The following is a representer theorem for the problem in (4).

**Theorem 5.1.** The solution \( \hat{F}_0 \) to the problem in (4) is

\[
\hat{F}_0(x_1, ..., x_r) = \sum_{i_1, ..., i_r} k_0(x_{0i_1}, x_{0i_2})...k_0(x_{0i_r}, x_{0i_r})c_{i_1, ..., i_r}^0,
\]

where the coefficients \( c_{i_1, ..., i_r} \in \mathbb{R} \) are the unique solution of the \( n_0 \) linear equations,

\[
\sum_{j_1, ..., j_r=1}^{n_0} \left( k_0(x_{0j_1}, x_{0j_2})...k_0(x_{0j_r}, x_{0j_r}) \right) c_{j_1, ..., j_r}^0 = \lambda_{n_0} \delta_{i_1, j_1}...\delta_{i_r, j_r} c_{j_1, ..., j_r}^0 = h(y_{0i_1}, ..., y_{0i_r}).
\]

Note that if \( r = 1 \) and \( h(y) = y \), we recover the usual kernel ridge regression. The following result shows that this estimation procedure is universally consistent.
Table 1. Root mean square error in estimating the conditional standard deviation, with standard error from 100 simulations, for GAMLSS (implemented via the R package gamlss (Rigby & Stasinopoulos, 2005)) and our U-statistic regression via generalised kernel ridge regression (U-regression KRR; implemented via the Falkon library on Python (Rudi et al., 2017; Meanti et al., 2020)). Lower is better.

| Method         | Setting SN          | Setting LN          | Setting HN          |
|----------------|---------------------|---------------------|---------------------|
|                | Control             | Treatment           | Control             | Treatment           |
| GAMLSS         | 0.17 ± 0.031        | 0.767 ± 0.414       | 3.3 ± 0.55          | 15.44 ± 8.128       |
| U-regression KRR| 0.13 ± 0.059        | 0.16 ± 0.059        | 1.1 ± 0.31          | 2.16 ± 0.61         |

Figure 2. Hypothesis testing and witness functions on the IHDP dataset. (a) Hypothesis test is conducted on 100 simulations for each setting, with the bar chart showing proportion of tests rejected for each setting. In setting “LN”, where the variance overwhelms the CATE, the test does not reject the hypothesis \( P_{Y|X} = P_{Y|X} \), whereas in the other two settings, the hypothesis is rejected. (b) At both \( X = a \) and \( X = b \), the density of the control group is larger than that of the treatment group around \( Y = 0 \), and the reverse is true around \( Y = 4 \), showing the marked effect of the treatment. (c) At both \( X = a \) and \( X = b \), the density of the control and treatment groups are roughly equal for all \( Y \), whereas at \( X = b \), the witness function clearly shows where the density of one group dominates the other. The juxtaposition of witness functions at different points in the covariate space is an exploratory tool to compare the relative strength of the treatment effect.

**Theorem 5.2.** Suppose \( k_0^* \) is a bounded and universal kernel and that \( X_{n_0}^0 \) decays at a slower rate than \( O(n_0^{-1/2}) \). Then as \( n_0 \to \infty \),

\[
\mathbb{E}\left[ \left( \bar{F}_0(X_1, ..., X_r) - F_0(X_1, ..., X_r) \right)^2 \right] \xrightarrow{p} 0.
\]

A consistent estimate \( \hat{F}_1 \) of \( F_1 \) is obtained by exactly the same procedure, using the treatment sample \( \{(x_i^1, y_i^1)\}_{i=1}^n \).

6. Experiments

6.1. Semi-synthetic IHDP Data

We demonstrate the use of our methods on the Infant Health and Development Program (IHDP) dataset (Hill, 2011, Section 4). The covariates are taken from a randomised control trial, from which a non-random portion is removed to imitate an observational study. The reason for its popularity in the CATE literature is that, for each datapoint, the outcome is simulated for both treatment and control, enabling cross-validation and evaluation, which is usually not possible in observational studies due to the missing counterfactuals. Existing works first define the noiseless response surfaces for the control and treatment groups, and generate realisations of the potential outcomes by applying Gaussian noise with constant variance across the whole dataset.

This last assumption of constant variance is somewhat unrealistic, but of little importance in evaluating CATE estimators. In our experiments, we modify the data generating process in three different ways, all of which have the same parallel linear mean response surfaces, with the CATE of 4 (“response surface A” in Hill (2011)). In setting “SN” (“small noise”), the standard deviation of the noise is constant at 1, so that the CATE of 4 translates to a meaningful treatment effect. In setting “LN” (“large noise”), the standard deviation of the noise is constant at 20, meaning that the mean difference in the response surfaces is negligible in comparison. In this case, our test does not reject the hypothesis that the two conditional distributions are the same, and there is no case for further investigation (see middle bar in Figure 2(a)). In setting “HN” (“heterogeneous noise”), the standard deviation is heterogeneous across the dataset, so that the standard deviation is 1 for some data points while others have standard deviation of 20. The exact data generating process is detailed in Appendix B.

In setting “HN”, let us consider points \( a, b \in X \) with \( \text{sd}(Y|X = a) = 20 \) and \( \text{sd}(Y|X = b) = 1 \). Then even though the CATE at \( a \) and \( b \) are equal at 4, we have \( \text{sd}(Y_1 - Y_0|X = a) \gg \text{sd}(Y_1 - Y_0|X = b) \), such that there is a pronounced treatment effect at \( b \), while the variance engulfs the treatment effect at \( a \). The comparative magnitudes of the witness functions conditioned on \( a \) and \( b \) confirm this heterogeneity (see Figure 2(d)). In Table 1, the quality of estimation of the standard deviation via our U-statistic
regression is compared with GAMLSS (Stasinopoulos et al., 2017) estimation for each setting.

An immediate benefit is a better understanding of the treatment. Even a perfect CATE estimator cannot capture such heterogeneity in distributional treatment effect (variance, in this case). As argued in Section 1.1, any method that involves comparing mean values (of which CATE is one) should also take into account the variance for it to be meaningful. This will give a clearer picture of the subpopulations on which there is a marked treatment effect, and those on which it is weaker, than relying on the CATE alone. Such knowledge should in turn influence policy decisions, in terms of which subpopulations should be targeted. We note that recently Jesson et al. (2020) considered CATE uncertainty in IHDP in the context of a different task: making or deferring treatment recommendations while using Bayesian neural networks, focusing on cases where overlap fails or under covariate shift; however, distributional considerations can be important even when overlap is satisfied and no covariate shift takes place.

6.2. Real Outcomes: LaLonde Data

In this section, we apply the proposed methods to LaLonde’s well-known National Supported Work (NSW) dataset (LaLonde, 1986; Dehejia & Wahba, 1999) which has been used widely to evaluate estimators of treatment effects. The outcome of interest $Y$ is the real earnings in 1978, with treatment $Z$ being the job training. We refer the interested readers to Dehejia & Wahba (1999, Sec. 2.1) for a detailed description of the dataset. As income distributions are known to be skewed to the right, it may be interesting to investigate not only the CATE, but the entire distributions.

The test rejects the hypothesis $P_{Y_1|X} = P_{Y_0|X}$ with p-value of 0.013. As a demonstration of the kind of exploratory analysis that can be conducted using the conditional witness functions, we focus our attention on a subset of the data on which the overlap condition is satisfied – Black, unmarried participants up to the age of 25, who were unemployed in both 1974 and 1975. Figure 3 shows the witness function for each individual in this subset, with the colour of the curve delineating whether the corresponding individual has a high school diploma.

We can see clearly that for those without a high school diploma, the treatment effect is not so pronounced, whereas there is a marked treatment effect for those with it. Negative values of the witness function for small income values mean that we are more likely to get small income values from the control group than the treatment group, whereas larger income values are more likely to come from the treatment group, as indicated by the positive values of the witness functions. In particular, the tail of the blue curves to the right implies a skewness of the density of the treated group relative to the control group, and the treatment group continues to have larger density than the control group for high income values ($> 25000$), albeit to a lesser extent. Such comparison of densities in different regions of $Y$ is not possible with the CATE, which is a simple difference of the means between the control and treated groups.

7. Discussion & Conclusion

In this paper, we discussed the analysis of the conditional distributional treatment effect (CoDiTE). We first propose a new kernel-based hypothesis test via kernel conditional mean embeddings to see whether there exists any CoDiTE. Then we proceeded to investigate the nature of the treatment effect via conditional witness functions, revealing where and how much the conditional densities differ, and U-statistic regression, which is informative about the differences in specific conditional distributional quantities.

We foresee that much of the work that has been done by the machine learning community on treatment effect analysis, although cast mostly in the context of CATE, applies for the CoDiTE. Examples include meta learners (Künzel et al., 2019), model validation (Alaa & Van Der Schaar, 2019), subgroup analysis (Su et al., 2009; Lee et al., 2020) and covariate balancing (Gretton et al., 2009; Kallus, 2018). Overo

A major obstacle in any covariate-conditional analysis of treatment effect is this: when the covariate space is high-dimensional, the accuracy and reliability of the estimates deteriorate significantly due to the curse of dimensionality, and we heavily rely on changes to be smooth across the covariate space. This limitation is present not only in methods presented in this paper, but any CATE or CoDiTE analysis. While out of scope for the present paper, it is of interest to investigate how to mitigate this problem.

Last but not least, we argue that the conditional distributional treatment effect can play an important role in making fair and explainable decisions as it provides a more complete picture of the treatment effect. On the one hand, policymakers can use tools that we develop to identify the groups of
individuals for which the outcome distributions differ most through the effect modifiers. On the other hand, the presence of effect modification that is associated with sensitive attributes such as race, ethnicity, and gender creates challenges for decision makers. If they knew that there is effect modification by race, for example, certain groups of individuals may be treated unfairly. In practice, our tools can potentially be used to detect the discrepancy between outcome distributions conditioned on these sensitive attributes, which is also an interesting avenue for future work.

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A. Background Material

In this section, we give a more detailed review of the background on reproducing kernel Hilbert space embeddings and U-statistics. Interested readers can refer to Berlinet & Thomas-Agnan (2004); Muandet et al. (2017) for the former, and Serfling (1980, Chapter 5) for the latter.

A.1. Reproducing Kernel Hilbert Space Embeddings

Let $\mathcal{H}$ be a vector space of real-valued functions on $\mathcal{Y}$, endowed with the structure of a Hilbert space via an inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$. Let $\| \cdot \|_{\mathcal{H}}$ be the associated norm, i.e. $\|f\|_{\mathcal{H}} = (\langle f, f \rangle_{\mathcal{H}})^{1/2}$ for $f \in \mathcal{H}$.

**Definition A.1** (Berlinet & Thomas-Agnan (2004, p.7, Definition 1)). A function $l : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$ is a reproducing kernel of the Hilbert space $\mathcal{H}$ if and only if

(i) for all $y \in \mathcal{Y}$, $l(y, \cdot) \in \mathcal{H}$;

(ii) for all $y \in \mathcal{Y}$ and for all $f \in \mathcal{H}$, $\langle f, l(y, \cdot) \rangle_{\mathcal{H}} = f(y)$ (the reproducing property).

A Hilbert space of functions $\mathcal{Y} \rightarrow \mathbb{R}$ which possesses a reproducing kernel is called the reproducing kernel Hilbert space (RKHS).

For any $y \in \mathcal{Y}$, denote by $e_y : \mathcal{H} \rightarrow \mathbb{R}$ the evaluation functional at $y$, i.e. $e_y(f) = f(y)$ for $f \in \mathcal{H}$. Riesz representation theorem can be used to prove the following lemma.

**Lemma A.2** (Berlinet & Thomas-Agnan (2004, p.9, Theorem 1)). A Hilbert space of functions $\mathcal{Y} \rightarrow \mathbb{R}$ has a reproducing kernel if and only if all evaluation functionals $e_y, y \in \mathcal{Y}$ are continuous on $\mathcal{H}$.

Next, we characterise reproducing kernels.

**Definition A.3** (Berlinet & Thomas-Agnan (2004, p.10, Definition 2)). A function $l : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$ is called a positive definite function if, for all $n \geq 1$, any $a_1, \ldots, a_n \in \mathbb{R}$ and any $y_1, \ldots, y_n \in \mathcal{Y}$,

$$\sum_{i,j=1}^{n} a_i a_j l(y_i, y_j) \geq 0.$$  

A reproducing kernel is a positive definite function, since, by the reproducing property,

$$\sum_{i,j=1}^{n} a_i a_j l(y_i, y_j) = \left\| \sum_{i=1}^{n} a_i l(y_i, \cdot) \right\|_{\mathcal{H}}^2 \geq 0$$

(see Berlinet & Thomas-Agnan (2004, p.13, Lemma 2)). The Moore-Aronszajn Theorem (Aronszajn, 1950) shows that the set of positive definite functions and the set of reproducing kernels on $\mathcal{Y} \times \mathcal{Y}$ are identical.

**Theorem A.4** (Berlinet & Thomas-Agnan (2004, p.19, Theorem 3)). Let $l$ be a positive definite function on $\mathcal{Y} \times \mathcal{Y}$. Then there exists a unique Hilbert space of functions $\mathcal{Y} \rightarrow \mathbb{R}$ with $l$ as its reproducing kernel. The subspace $\mathcal{H}$ of $\mathcal{H}$ spanned by $\{l(y, \cdot) : y \in \mathcal{Y}\}$ is dense in $\mathcal{H}$, and $\mathcal{H}$ is the set of functions $\mathcal{Y} \rightarrow \mathbb{R}$ which are pointwise limits of Cauchy sequences in $\mathcal{H}$ with the inner product

$$\langle f, g \rangle_{\mathcal{H}} = \sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_i \beta_j l(y_i, y_j)$$

where $f = \sum_{i=1}^{n} \alpha_i l(y_i, \cdot)$ and $g = \sum_{j=1}^{m} \beta_j l(y_j, \cdot)$.

Examples of commonly used kernels in Euclidean spaces include the linear kernel $l(y, y') = y \cdot y'$, the monomial kernel $l(y, y') = (y \cdot y')^p$, the polynomial kernel $l(y, y') = (y \cdot y' + 1)^p$, the Gaussian kernel $l(y, y') = e^{-\frac{1}{2} \|y-y'\|^2}$ and the Laplacian kernel $l(y, y') = e^{-\frac{1}{2\sigma^2} \|y-y'\|}$.

Kernel methods in machine learning turns linear methods into non-linear ones using the so-called “kernel trick”, whereby individual datapoints $y \in \mathcal{Y}$ are “embedded” into an RKHS $\mathcal{H}$ with reproducing kernel $l$ via the mapping $y \mapsto l(y, \cdot)$. The
RKHS is high- (and often infinite-)dimensional, and performing a linear method (e.g. linear regression, support vector machine, principal component analysis, etc.) in $\mathcal{H}$ with datapoints $l(y_i, \cdot), i = 1, \ldots, n$, instead of the original space $\mathcal{Y}$ with datapoints $y_i, i = 1, \ldots, n$, results in a nonlinear method in the original space. Please see Schölkopf & Smola (2001) for more details.

Recently, this idea of RKHS embeddings has been extended to embed entire (conditional) distributions, rather than individual datapoints, via the expectation. Suppose $Y$ is a random variable taking values in $\mathcal{Y}$, with distribution $P_Y$. Assuming the integrability condition $\int_{\mathcal{Y}} \sqrt{f(y)} dP_Y(y) < \infty$, we define the kernel mean embedding $\mu_{P_Y} \in \mathcal{H}$ of the measure $P_Y$, or the random variable $Y$, as

$$\mu_{P_Y}(\cdot) = \mathbb{E}[l(Y, \cdot)] = \int_{\mathcal{Y}} l(y, \cdot) dP_Y(y) = \int_{\Omega} l(Y(\omega), \cdot) dP(\omega).$$

Note that the integrand $l(Y, \cdot)$ is an element in a Hilbert space (and therefore a Banach space), so the integral is not the usual Lebesgue integral on $\mathbb{R}$. There are a number of ways in which one can define integration on a Banach space (Schwabik & Ye, 2005). Among those, the Bochner integral (Dinculeanu, 2000, p.15, Definition 35) is the simplest and most intuitive one, and suffices for our purposes. Riesz representation theorem is again used to prove the following mean embedding version of the reproducing property.

**Lemma A.5 (Smola et al. (2007)).** For each $f \in \mathcal{Y}$,

$$\mathbb{E}[f(Y)] = \int_{\mathcal{Y}} f(y) dP_Y(y) = \langle f, \mu_{P_Y} \rangle_{\mathcal{H}}.$$

Using the kernel mean embedding, we can define a distance function, called the maximum mean discrepancy (Gretton et al., 2012), between two random variables $Y$ and $Y'$ on $\mathcal{Y}$, or equivalently, two probability measures $P_Y$ and $P_{Y'}$, as

$$\text{MMD}(Y, Y') = \left\| \mu_{P_Y} - \mu_{P_{Y'}} \right\|_{\mathcal{H}}.$$

The name maximum mean discrepancy comes from the following lemma.

**Lemma A.6 (Gretton et al. (2012, Lemma 4)).** We have

$$\text{MMD}(Y, Y') = \sup_{f \in \mathcal{H}, \|f\|_{\mathcal{H}} \leq 1} \left\{ \mathbb{E}[f(Y)] - \mathbb{E}[f(Y')] \right\}.$$

In this alternative definition of the MMD, the function in the unit ball of $\mathcal{H}$ that maximises $\mathbb{E}[f(Y)] - \mathbb{E}[f(Y')]$ is called the witness function (Gretton et al., 2012, Section 2.3). It can easily be seen that the witness function is in fact

$$\frac{\mu_{P_Y} - \mu_{P_{Y'}}}{\| \mu_{P_Y} - \mu_{P_{Y'}} \|_{\mathcal{H}}}.$$

Lloyd & Gahramani (2015) uses the unnormalised witness function $\mu_{P_Y} - \mu_{P_{Y'}}$ for model criticism.

The MMD is not a proper metric, since $Y$ and $Y'$ may be distinct and still give $\text{MMD}(Y, Y') = 0$, depending on the kernel $l$ that is used. The notion of characteristic kernels is therefore essential, since it tells us whether the associated RKHS is rich enough to enable us to distinguish distinct distributions based on their embeddings.

**Definition A.7 (Fukumizu et al. (2008, Section 2.2)).** Denote by $\mathcal{P}$ the set of all probability measures on $\mathcal{Y}$. A positive definite kernel $l$ is characteristic if the kernel mean embedding map $\mathcal{P} \rightarrow \mathcal{H} : P_Y \mapsto \mu_{P_Y}$ is injective.

For example, of the aforementioned kernels, the Gaussian and Laplacian kernels are characteristic, whereas the linear, monomial and polynomial kernels are not. The MMD associated with a characteristic kernel is then a proper metric between probability measures on $\mathcal{Y}$. See Sriperumbudur et al. (2010; 2011); Simon-Gabriel & Schölkopf (2018) for various characterisations of characteristic kernels.

Now we discuss conditional embedding of distributions into RKHSs. Suppose $X$ is a random variable on a space $\mathcal{X}$.

**Definition A.8 (Park & Muandet (2020a, Definition 3.1)).** The conditional mean embedding of the random variable $Y$, or equivalently, the distribution $P_Y$, is the Bochner conditional expectation (as defined in Dinculeanu (2000, p.45, Definition 38))

$$\mu_{P_{Y|X}} = \mathbb{E}[l(Y, \cdot) \mid X].$$

Notice that this is a straightforward extension of the kernel mean embedding $\mu_{P_Y} = \mathbb{E}[l(Y, \cdot)]$ to the conditional case.
A.2. U-Statistics

Suppose \(Y_1, Y_2, ..., Y_r\) are independent copies of the random variable \(Y\), i.e. they are independent and all have distribution \(P_Y\). Let \(h: Y^r \to \mathbb{R}\) be a symmetric function (called a kernel in the U-statistics literature; confusion must be avoided with the reproducing kernel used throughout this paper), i.e. for any permutation \(\pi\) of \(\{1, ..., r\}\), we have \(h(y_1, ..., y_r) = h(y_{\pi(1)}, ..., y_{\pi(r)})\). Suppose we would like to estimate a function of the form

\[
\theta(P_Y) = \mathbb{E}[h(Y_1, ..., Y_r)] = \int_{Y^r} \int_{Y^r} h(y_1, ..., y_r) \, dP_Y(y_1) ... dP_Y(y_r).
\]

The corresponding U-statistic for an unbiased estimation of \(\theta(P_Y)\) based on a sample \(Y_1, ..., Y_n\) of size \(n \geq r\) is given by

\[
\hat{\theta}(P_Y) = \frac{1}{\binom{n}{r}} \sum h(Y_{i_1}, ..., Y_{i_r}),
\]

where \(\binom{n}{r}\) is the binomial coefficient and the summation is over the \(\binom{n}{r}\) combinations of \(r\) distinct elements \(\{i_1, ..., i_r\}\) from \(\{1, ..., n\}\). Clearly, since the expectation of each summand yields \(\theta(P_Y)\), we have \(\mathbb{E}[\hat{\theta}(P_Y)] = \theta(P_Y)\), so U-statistics are unbiased estimators.

Some examples of \(h\) and the corresponding estimator include the sample mean \(h(y) = y\), the sample variance \(h(y_1, y_2) = \frac{1}{2}(y_1 - y_2)^2\), the sample cumulative distribution up to \(y^*\) \(h(y) = 1(y \leq y^*)\), the \(k\)th sample raw moment \(h(y) = y^k\) and Gini’s mean difference \(h(y_1, y_2) = |y_1 - y_2|\).

To the best of our knowledge, Stute (1991) was the first to consider a conditional counterpart of U-statistics. Let \(X_1, ..., X_r\) be independent copies of the random variable \(X\). We are now interested in the estimation of the following quantity:

\[
\theta(P_{Y|X}) = \mathbb{E}[h(Y_1, ..., Y_r) \mid X_1, ..., X_r].
\]

By Çınlar (2011, p.146, Theorem 1.17), \(\theta(P_{Y|X})\) can be considered as a function \(X^r \to \mathbb{R}\), such that for each \(r\)-tuple \(\{x_1, ..., x_r\}\), we have

\[
\theta\left(P_{Y|X}\right)(x_1, ..., x_r) = \mathbb{E}[h(Y_1, ..., Y_r) \mid X_1 = x_1, ..., X_r = x_r].
\]

The simplest case is when \(r = 1\) and \(h(y) = y\). In this case, the estimand reduces to \(f(X) = \mathbb{E}[Y \mid X]\), which is the usual regression problem for which a plethora of methods exist. Suppose we have a sample \((X_i, Y_i)_{i=1}^n\). One such regression method is the Nadaraya-Watson kernel smoother:

\[
\hat{f}(x) = \frac{\sum_{i=1}^n Y_i K\left(\frac{x - X_i}{a}\right)}{\sum_{i=1}^n K\left(\frac{x - X_i}{a}\right)},
\]

where \(K\) is the so-called “smoothing kernel” and \(a\) is the bandwidth. This was extended by Stute (1991) to \(r \geq 1\) and more general \(h:\)

\[
\hat{\theta}\left(P_{Y|X}\right)(x_1, ..., x_r) = \frac{\sum h(Y_{i_1}, ..., Y_{i_r}) \prod_{j=1}^r K\left(\frac{x_j - X_{i_j}}{a}\right)}{\sum \prod_{j=1}^r K\left(\frac{x_j - X_{i_j}}{a}\right)},
\]

where the sums are over the \(\binom{n}{r}\) combinations of \(r\) distinct elements \(\{i_1, ..., i_r\}\) from \(\{1, ..., n\}\) as before. Derumigny (2019) considers a parametric model of the form

\[
\Lambda\left(\theta\left(P_{Y|X}\right)(x_1, ..., x_r)\right) = \psi(x_1, ..., x_r)^T \beta^*.
\]

where \(\Lambda\) is a strictly increasing and continuously differentiable “link function” such that the range of \(\Lambda \circ \theta\) is exactly \(\mathbb{R}\), \(\beta^* \in \mathbb{R}^a\) is the true parameter and \(\psi(\cdot) = (\psi_1(\cdot), ..., \psi_a(\cdot))^T \in \mathbb{R}^a\) is some basis, such as polynomials, exponentials, indicator functions etc. However, the estimation of \(\beta^*\) still makes use of the Nadaraya-Watson kernel smoothers considered above.

Of course, Nadaraya-Watson kernel smoothers are far from being the only method of regression that can be extended to estimate conditional U-statistics, and in the main body of the paper (Section 5.2), we consider extending kernel ridge regression for this purpose.
B. More Details on IHDP Dataset

In this section, we give more details on the data generating process of the semi-synthetic IHDP (Infant Health and Development Program) dataset that was first used in the treatment effect literature by Hill (2011).

The data consists of 25 covariates: birth weight, head circumference, weeks born preterm, birth order, first born, neonatal health index, sex, twin status, whether or not the mother smoked during pregnancy, whether or not the mother drank alcohol during pregnancy, whether or not the mother took drugs during pregnancy, the mother’s age, marital status, education attainment, whether or not the mother worked during pregnancy, whether she received prenatal care, and 7 dummy variables for the 8 sites in which the family resided at the start of the intervention.

These covariates are originally taken from a randomised experiment, and included information about the ethnicity of the mothers. Hill (2011) removed all children with nonwhite mothers from the treatment group, which is clearly a non-random (biased) portion of the data, thereby imitating an observational study. This leaves 608 children in the control group and 139 in the treatment group. The overlap condition is now only satisfied for the treatment group.

In creating the parallel linear response surfaces, which are used in all three of the settings “SN”, “LN” and “HN”, we let \( \mathbb{E}[Y_0|X] = \beta X + 4 \) and \( \mathbb{E}[Y_1|X] = \beta X + 4 \), where the 25-dimensional coefficient vector \( \beta \) is generated in the same way as in Alaa & Schaar (2018): for the 6 continuous variables (birth weight, head circumference, weeks born preterm, birth order, neonatal health index, mother’s age), the corresponding coefficients is sampled from \( \{0, 0.1, 0.2, 0.3, 0.4\} \) with probabilities \( \{0.5, 0.125, 0.125, 0.125, 0.125\} \) respectively, whereas for the other 19 binary variables, the corresponding coefficients are sampled from \( \{0, 0.1, 0.2, 0.3, 0.4\} \) with probabilities \( \{0, 0.6, 0.1, 0.1, 0.1\} \) respectively.

Finally, we generate realisations of the potential outcomes by adding noise to the mean response surfaces. We let \( Y_0 = \beta X + \epsilon(X) \) and \( Y_1 = \beta X + 4 + \epsilon(X) \), where \( \epsilon(X) \) is \( \epsilon_{SN} \) in setting “SN”, \( \epsilon(X) = \epsilon_{LN} \) in setting “LN” and \( \epsilon(X) = X_6 \epsilon_{SN} + (1-X_6) \epsilon_{LN} \) in setting “HN”, with \( \epsilon_{SN} \sim \mathcal{N}(0, 1^2) \) and \( \epsilon_{LN} \sim \mathcal{N}(0, 20^2) \). The covariate \( X_6 \) corresponds to the sex of the child, and was chosen because there are roughly the same number of each sex in both the control and the treatment groups.

C. Proofs

Lemma 4.1. For each \( x \in \mathcal{X} \), we have

\[
\hat{U}_{MMD}^2(x) = k_0^T(x)W_0L_0W_0^Tk_0(x) - 2k_0^T(x)W_0LW_1^Tk_1(x) + k_1^T(x)W_1L_1W_1^Tk_1(x),
\]

where \( [L_0]_{1 \leq i, j \leq n_0} = l(y_{0i}^0, y_{0j}^0), [L_1]_{1 \leq i \leq n_1, 1 \leq j \leq n_1} = l(y_{1i}^0, y_{1j}^0) \) and \( [L_1]_{1 \leq i \leq n_1} = l(y_{1i}^0, y_{1j}^0) \).

Proof. We use the reproducing property of \( \mathcal{H} \) and (2) to see that, for any \( x \in \mathcal{X} \),

\[
\hat{U}_{MMD}^2(x) = \left\| \hat{\mu}_{Y_1|X=x} - \hat{\mu}_{Y_0|X=x} \right\|_{\mathcal{H}}^2
= \left\| k_0^T(x)W_0L_0W_0^Tk_0(x) - 2k_0^T(x)W_0LW_1^Tk_1(x) + k_1^T(x)W_1L_1W_1^Tk_1(x) \right\|_{\mathcal{H}}^2
= \sum_{i,j=1}^{n_0} k_0(x, x_i^0)W_{0,ij}l(y_{0i}^0, \cdot) + \sum_{i,j=1}^{n_0} k_0(x, x_j^0)W_{0,ji}l(y_{0j}^0, \cdot)
- 2 \sum_{i,j=1}^{n_0} k_0(x, x_i^0)W_{0,ij}l(y_{0j}^0, \cdot) + \sum_{i,j=1}^{n_1} k_1(x, x_i^0)W_{1,ij}l(y_{1j}^0, \cdot)
+ \sum_{i,j=1}^{n_1} k_1(x, x_j^0)W_{1,ji}l(y_{1j}^0, \cdot)
= \sum_{i,j,p,q=1}^{n_0} k_0(x, x_i^0)W_{0,ij}l(y_{0i}^0, y_{0j}^0)W_{0,qp}^Tk_0(x_p^0, x)
- 2 \sum_{i,j,p,q=1}^{n_0} \sum_{i,j=1}^{n_1} k_0(x, x_i^0)W_{0,ij}l(y_{0i}^0, y_{1j}^0)W_{1,qp}^Tk_1(x_i^0, x)
- 2 \sum_{i,j,p,q=1}^{n_0} \sum_{i,j=1}^{n_1} k_0(x, x_i^0)W_{0,ij}l(y_{0i}^0, y_{1j}^0)W_{1,qp}^Tk_1(x_i^0, x)
\]
\[\sum_{i,j,p,q=1}^{n_t} k_i(x, x_i^1)W_{i,j}l(y_j, y_q^1)W_{i,j}^T k_i(x, x)\]
\[= k_0^T(x)W_0L_0W_0^T k_0(x) - 2k_0^T(x)W_0LW_0^T k_1(x) + k_1^T(x)W_1L_1W_1^T k_1(x).\]

\[\psi_{\text{MMD}}(\hat{U}_{\text{MMD}}) = \mathbb{E}\left[(\hat{U}_{\text{MMD}}(X) - U_{\text{MMD}}(X))^2\right] \overset{P}{\to} 0.\]

**Theorem 4.2.** Suppose that \(k_0, k_1, I\) are bounded, that \(\Gamma_0\) and \(\Gamma_1\) are universal, and that \(\lambda_{n_0}\) and \(\lambda_{n_1}\) decay at slower rates than \(O(n_0^{-1/2})\) and \(O(n_1^{-1/2})\) respectively. Then as \(n_0, n_1\to\infty\),
\[\psi_{\text{MMD}}(\hat{U}_{\text{MMD}}) = \mathbb{E}\left[(\hat{U}_{\text{MMD}}(X) - U_{\text{MMD}}(X))^2\right] \overset{P}{\to} 0.\]

**Proof.** The simple inequality \(\|a + b\|^2 \leq 2\|a\|^2 + 2\|b\|^2\) holds in any Hilbert space. Using this, we see that
\[\psi_{\text{MMD}}(\hat{U}_{\text{MMD}}) = \mathbb{E}\left[(\hat{U}_{\text{MMD}}(X) - U_{\text{MMD}}(X))^2\right] \leq 2\mathbb{E}\left[\int_{\mathcal{X}} |\bar{\mu}_{Y_i|X} - \mu_{Y_i|X}\|^2 dP_{X|Y_i}(x)\right] + 2\mathbb{E}\left[\int_{\mathcal{X}} |\bar{\mu}_{Y_0|X} - \mu_{Y_0|X}\|^2 dP_{X|Y_0}(x)\right]\]
\[\overset{P}{\to} 0.\]

Hence, it suffices to know that
\[\mathbb{E}\left[\int_{\mathcal{X}} |\bar{\mu}_{Y_i|X} - \mu_{Y_i|X}\|^2 dP_{X|Y_i}(x)\right] \overset{P}{\to} 0 \quad \text{and} \quad \mathbb{E}\left[\int_{\mathcal{X}} |\bar{\mu}_{Y_0|X} - \mu_{Y_0|X}\|^2 dP_{X|Y_0}(x)\right] \overset{P}{\to} 0.\]

But this follows immediately from Park & Muandet (2020b), so the proof is complete.

**Lemma 4.3.** If \(l\) is a characteristic kernel, \(P_{Y_i|X} \equiv P_{Y_1|X}\) if and only if \(t = 0\).

**Proof.** We can assume without loss of generality that \(P_{Y_0|X}\) and \(P_{Y_1|X}\) are obtained from a regular version of \(P(\cdot|X)\). Then by (Park & Muandet, 2020a, Theorem 2.9), there exist \(C_0, C_1 \in \mathcal{F}\) with \(P(C_0) = P(C_1) = 1\) such that for all \(\omega \in C_0, \mu_{Y_0|X}(\omega) = \int_{\mathcal{Y}} l(y, \cdot) dP_{Y_0|X}(\omega)(y)\) and for all \(\omega' \in C_1, \mu_{Y_1|X}(\omega') = \int_{\mathcal{Y}} l(y, \cdot) dP_{Y_1|X}(\omega')(y)\).

Suppose for contradiction that there exists some measurable \(A \subseteq \mathcal{X}\) with \(P_X(A) > 0\) such that for all \(x \in A, \mu_{Y_0|X=x} \neq \int_{\mathcal{Y}} l(y, \cdot) dP_{Y_0|X=x}(y)\). Then \(P(X^{-1}(A)) = P_X(A) > 0\), and hence \(P(X^{-1}(A) \cap C_0) > 0\). For all \(x \in X^{-1}(A) \cap C_0\), we have \(X(\omega) \in A\), and hence
\[\mu_{Y_0|X}(\omega) \neq \int_{\mathcal{Y}} l(y, \cdot) dP_{Y_0|X=X(\omega)}(y) = \int_{\mathcal{Y}} l(y, \cdot) dP_{Y_0|X=X(\omega)}(y) = \mu_{Y_0|X}(\omega).\]

This is a contradiction, hence there does not exist a measurable \(A \subseteq \mathcal{X}\) with \(P_X(A) > 0\) such that for all \(x \in A, \mu_{Y_0|X=x} \neq \int_{\mathcal{Y}} l(y, \cdot) dP_{Y_0|X=x}(y)\). Therefore, there must exist some measurable \(A_0 \subseteq \mathcal{X}\) with \(P_X(A_0) = 1\) such that for all \(x \in A_0, \mu_{Y_0|X=x} = \int_{\mathcal{Y}} l(y, \cdot) dP_{Y_0|X=x}(y)\). Similarly, there must exist some measurable \(A_1 \subseteq \mathcal{X}\) with \(P_X(A_1) = 1\) such that for all \(x \in A_1, \mu_{Y_1|X=x} = \int_{\mathcal{Y}} l(y, \cdot) dP_{Y_1|X=x}(y)\).

(\implies) Suppose that \(P_{Y_i|X} \equiv P_{Y_1|X}\). This means that there exists a measurable \(A \subseteq \mathcal{X}\) with \(P_X(A) = 1\) such that for all \(x \in A, the measures \(P_{Y_0|X=x}(\cdot)\) and \(P_{Y_1|X=x}(\cdot)\) are the same. Then for all \(x \in A \cap A_0 \cap A_1\),
\[\mu_{Y_0|X=x} = \int_{\mathcal{Y}} l(y, \cdot) dP_{Y_0|X=x}(y) \quad \text{since } x \in A_0\]
\[\int_{\mathcal{Y}} l(y, \cdot) dP_{Y_1|X=x}(y) \quad \text{since } x \in A\]
where \( k \) Since 

Now suppose that \( P_{\cdot \mid X = x} = P_{\cdot \mid X = x} = P_{\cdot \mid X = x} \) for all \( x \in A \cap A_0 \cap A_1 \), we have \( P_{\cdot \mid X = x} = P_{\cdot \mid X = x} = P_{\cdot \mid X = x} \) almost everywhere. Hence,

\[
t = E \left[ \left\| \mu_{Y_1 \mid X = x} - \mu_{Y_0 \mid X = x} \right\|^2_H \right] = 0
\]

( \( \iff \) ) Now suppose that \( t = 0 \), i.e. \( \mu_{Y_0 \mid X = x} = \mu_{Y_1 \mid X = x} \). Say on a measurable set \( A \subseteq X \) with \( P_X(A) = 1 \). Suppose \( x \in A \cap A_0 \cap A_1 \). Then

\[
\int_y l(y, \cdot) dP_{Y_1 \mid X = x} (y) = \mu_{Y_0 \mid X = x} = \mu_{Y_1 \mid X = x} = \int_y l(y, \cdot) dP_{Y_1 \mid X = x} (y)
\]

since \( x \in A_0 \) and \( x \in A \). Then

Since \( k \) is characteristic, this means that \( P_{Y_0 \mid X = x} \) and \( P_{Y_1 \mid X = x} \) are the same measure. As before, we have \( P_X(A \cap A_0 \cap A_1) = 1 \), hence \( P_{Y_0 \mid X} \equiv P_{Y_1 \mid X} \).

Lemma 4.4. We have

\[
\hat{\epsilon} = \frac{1}{n} \text{Tr} \left( \tilde{K}_0 W_0 L_0 W_0^T \tilde{K}_0^T \right) - \frac{2}{n} \text{Tr} \left( \tilde{K}_0 W_0 L W_0^T \tilde{K}_1^T \right) + \frac{1}{n} \text{Tr} \left( \tilde{K}_1 W_1 L_1 W_1^T \tilde{K}_1^T \right)
\]

where \( L_0, L_1 \) and \( L \) are as defined in Lemma 4.1 and \([\tilde{K}_0]_{1 \leq i \leq n, 1 \leq j \leq n_0} = k_0(x_i, x_j)\) and \([\tilde{K}_1]_{1 \leq i \leq n_1, 1 \leq j \leq n_1} = k_1(x_i, x_j)\).

Proof. See that, using the reproducing property in \( \mathcal{H} \) again,

\[
\hat{\epsilon} = \frac{1}{n} \sum_{i=1}^{n} \left\| \tilde{\mu}_{Y_1 \mid X = x_i} - \tilde{\mu}_{Y_0 \mid X = x_i} \right\|^2_H
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \left\{ \left\| \tilde{\mu}_{Y_1 \mid X = x_i} \right\|^2_H - 2 \left\{ \tilde{\mu}_{Y_1 \mid X = x_i}, \tilde{\mu}_{Y_0 \mid X = x_i} \right\}_H + \left\| \tilde{\mu}_{Y_0 \mid X = x_i} \right\|^2_H \}
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \left\{ \left\| k_0^T (x_i) W_0 L_0 \right\|^2_H - 2 \left\{ k_0^T (x_i) W_0 L_0, k_0^T (x_i) W_1 L_1 \right\}_H + \left\| k_0^T (x_i) W_1 L_1 \right\|^2_H \}
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \left\{ \sum_{q=1}^{n_0} \sum_{p=1}^{n_0} k_0(x_p, x_i) W_{0, pq} l(y_q^0, \cdot), \sum_{r,s=1}^{n_1} k_0(x_r, x_i) W_{0, rs} l(y_s^0, \cdot) \right\}_H
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \left\{ \sum_{q=1}^{n_0} \sum_{p=1}^{n_0} k_0(x_p, x_i) W_{0, pq} l(y_q^0, \cdot), \sum_{r,s=1}^{n_1} k_1(x_r, x_i) W_{1, rs} l(y_s^1, \cdot) \right\}_H
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \left\{ \sum_{q=1}^{n_0} \sum_{p=1}^{n_0} k_0(x_p, x_i) W_{0, pq} l(y_q^0, y_s^0) W^T_{0, sr} k_0(x_r, x_i) \right\}_H
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \left\{ \sum_{q=1}^{n_0} \sum_{p=1}^{n_0} k_0(x_p, x_i) W_{0, pq} l(y_q^0, y_s^0) W^T_{1, sr} k_1(x_r, x_i) \right\}_H
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \left\{ \sum_{q=1}^{n_0} \sum_{p=1}^{n_0} k_0(x_p, x_i) W_{0, pq} l(y_q^0, y_s^0) W^T_{0, sr} k_0(x_r, x_i) \right\}_H
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \left\{ \sum_{q=1}^{n_0} \sum_{p=1}^{n_0} k_0(x_p, x_i) W_{0, pq} l(y_q^0, y_s^0) W^T_{1, sr} k_1(x_r, x_i) \right\}_H
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \left\{ \sum_{q=1}^{n_0} \sum_{p=1}^{n_0} k_0(x_p, x_i) W_{0, pq} l(y_q^0, y_s^0) W^T_{0, sr} k_0(x_r, x_i) \right\}_H
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \left\{ \sum_{q=1}^{n_0} \sum_{p=1}^{n_0} k_0(x_p, x_i) W_{0, pq} l(y_q^0, y_s^0) W^T_{1, sr} k_1(x_r, x_i) \right\}_H
\]
\[
\sum_{i=1}^{n} \left( \frac{1}{n} \right) \left\{ \text{Tr} \left( \hat{K}_0 W_0 \hat{L}_0 W_0^T \hat{K}_0^T \right) - 2 \text{Tr} \left( \hat{K}_0 W_0 \hat{W}_1 \hat{K}_1^T \right) + \text{Tr} \left( \hat{K}_1 \hat{W}_1 \hat{L}_1 \hat{W}_1^T \hat{K}_1^T \right) \right\}
\]

**Theorem 4.5.** Under the same assumptions as in Theorem 4.2, we have \( \hat{t} \xrightarrow{p} t \) as \( n_0, n_1 \to \infty \).

**Proof.** We decompose \( |\hat{t} - t| \) as follows using the triangle inequality:

\[
|\hat{t} - t| = \frac{1}{n} \sum_{i=1}^{n} \left| \mu_{\hat{Y}_1|X=x_i} - \mu_{\hat{Y}_0|X=x_i} \right|^2 - \mathbb{E} \left[ \left| \mu_{\hat{Y}_1|X} - \mu_{\hat{Y}_0|X} \right|^2 \right]
\]

Here, the first term converges to 0 in probability by the uniform law of large numbers. For the second term, see that

\[
\mathbb{E} \left[ \left| \mu_{\hat{Y}_1|X} - \mu_{\hat{Y}_0|X} \right|^2 \right] - \mathbb{E} \left[ \left| \mu_{\hat{Y}_1|X} - \mu_{\hat{Y}_0|X} \right|^2 \right] = - \mathbb{E} \left[ \left| \mu_{\hat{Y}_1|X} - \mu_{\hat{Y}_0|X} \right|^2 \right]
\]

which converges to 0 in probability by the uniform law of large numbers.

Here, we have

\[
\mathbb{E} \left[ \left| \mu_{\hat{Y}_1|X} - \mu_{\hat{Y}_0|X} \right|^2 \right] \xrightarrow{p} 0 \quad \text{and} \quad \mathbb{E} \left[ \left| \mu_{\hat{Y}_1|X} - \mu_{\hat{Y}_0|X} \right|^2 \right] \xrightarrow{p} 0
\]

as in the proof of Theorem 4.2, so we are done.

**Theorem 5.1.** The solution \( \hat{F}_0 \) to the problem in (4) is

\[
\hat{F}_0(x_1, \ldots, x_r) = \sum_{i_1, \ldots, i_r = 1}^{n_0} k_0(x_{i_1}, x_1) \cdots k_0(x_{i_r}, x_r) c_{i_1, \ldots, i_r}
\]

where the coefficients \( c_{i_1, \ldots, i_r} \in \mathbb{R} \) are the unique solution of the \( n^r \) linear equations

\[
\sum_{j_1, \ldots, j_r = 1}^{n_0} \left( k_0(x_{i_1}, x_{j_1}) \cdots k_0(x_{i_r}, x_{j_r}) + \binom{n_0}{r} \lambda_{n_0} \delta_{i_1, j_1} \cdots \delta_{i_r, j_r} \right) c_{j_1, \ldots, j_r} = h(y_{i_1}, \ldots, y_{i_r}).
\]

**Proof.** Recall from (4) that

\[
\hat{F}_0 = \text{arg min}_{F \in \mathcal{H}_0} \left\{ \frac{1}{n_0} \sum_{r} \left( F(x_{i_1}, \ldots, x_{i_r}) - h(y_{i_1}, \ldots, y_{i_r}) \right)^2 + \lambda_{n_0} \|F\|^2_{\mathcal{H}_0} \right\},
\]

where the summation is over the \( \binom{n_0}{r} \) combinations of \( r \) distinct elements \( \{i_1, \ldots, i_r\} \) from 1, \ldots, \( n_0 \). Write

\[
\hat{F}_0(x_1, \ldots, x_r) = \sum_{i_1, \ldots, i_r = 1}^{n_0} k_0(x_{i_1}, x_1) \cdots k_0(x_{i_r}, x_r) c_{i_1, \ldots, i_r}
\]
where the coefficients $c_{i_1,\ldots,i_r} \in \mathbb{R}$ are the unique solution of the $n^r$ linear equations

$$
\sum_{j_1,\ldots,j_r=1}^{n_0} \left( k_0 \left(x_{i_1}^0, x_{j_1}^0 \right) \ldots k_0 \left(x_{i_r}^0, x_{j_r}^0 \right) + \left(\frac{n_0}{n_r}\right) \lambda_0^r \delta_{i_1 j_1} \ldots \delta_{i_r j_r} \right) c_{j_1,\ldots,j_r} = h \left(y_{i_1}^0, \ldots, y_{i_r}^0 \right).
$$

Also, for any $F \in \mathcal{H}_0^r$, write $\hat{\mathcal{E}}_{\text{reg}} (F)$ for the empirical regularised least-squares risk of $F$:

$$
\hat{\mathcal{E}}_{\text{reg}} (F) = \frac{1}{(n_0)^r} \sum \left( F \left(x_{i_1}^0, \ldots, x_{i_r}^0 \right) - h \left(y_{i_1}^0, \ldots, y_{i_r}^0 \right) \right)^2 + \lambda_0^1 \|F\|_{\mathcal{H}_0}^2,
$$

so that $\hat{F}_0 = \arg \min_{F \in \mathcal{H}_0^r} \hat{\mathcal{E}}_{\text{reg}} (F)$. We will show that $\hat{F}_0' = \hat{F}_0$. For any $F \in \mathcal{H}_0^r$, write $G = F - \hat{F}_0$. Then

$$
\hat{\mathcal{E}}_{\text{reg}} (F) = \frac{1}{(n_0)^r} \sum \left( F \left(x_{i_1}^0, \ldots, x_{i_r}^0 \right) - h \left(y_{i_1}^0, \ldots, y_{i_r}^0 \right) \right)^2 + \lambda_0^1 \|F\|_{\mathcal{H}_0}^2
$$

$$
= \frac{1}{(n_0)^r} \sum \left( F \left(x_{i_1}^0, \ldots, x_{i_r}^0 \right) - \hat{F}_0' \left(x_{i_1}^0, \ldots, x_{i_r}^0 \right) + \hat{F}_0' \left(x_{i_1}^0, \ldots, x_{i_r}^0 \right) - h \left(y_{i_1}^0, \ldots, y_{i_r}^0 \right) \right)^2 + \lambda_0^1 \|F\|_{\mathcal{H}_0}^2
$$

$$
= \hat{\mathcal{E}}_{\text{reg}} (\hat{F}_0') + \frac{1}{(n_0)^r} \sum G \left(x_{i_1}^0, \ldots, x_{i_r}^0 \right)^2 + \frac{2}{(n_0)^r} \sum G \left(x_{i_1}^0, \ldots, x_{i_r}^0 \right) \left( \hat{F}_0' \left(x_{i_1}^0, \ldots, x_{i_r}^0 \right) - h \left(y_{i_1}^0, \ldots, y_{i_r}^0 \right) \right)
$$

$$
+ \lambda_0^1 \|G\|_{\mathcal{H}_0}^2 + 2 \lambda_0^1 \langle G, \hat{F}_0' \rangle_{\mathcal{H}_0^r}
$$

$$
\geq \hat{\mathcal{E}}_{\text{reg}} (\hat{F}_0') - \frac{2}{(n_0)^r} \sum G \left(x_{i_1}^0, \ldots, x_{i_r}^0 \right) \left( h \left(y_{i_1}^0, \ldots, y_{i_r}^0 \right) - \hat{F}_0' \left(x_{i_1}^0, \ldots, x_{i_r}^0 \right) \right) + 2 \lambda_0^1 \langle G, \hat{F}_0' \rangle_{\mathcal{H}_0^r}
$$

$$
= \hat{\mathcal{E}}_{\text{reg}} (\hat{F}_0') - 2 \lambda_0^1 \sum G \left(x_{i_1}^0, \ldots, x_{i_r}^0 \right) c_{i_1,\ldots,i_r} + 2 \lambda_0^1 \sum_{i_1,\ldots,i_r=1}^{n_0} G \left(x_{i_1}^0, \ldots, x_{i_r}^0 \right) c_{i_1,\ldots,i_r}
$$

by the reproducing property and the definition of $c_{i_1,\ldots,i_r}$

$$
= \hat{\mathcal{E}}_{\text{reg}} (\hat{F}_0')
$$

Hence, $\hat{F}_0'$ minimises $\hat{\mathcal{E}}_{\text{reg}}$ in $\mathcal{H}_0^r$, and so $\hat{F}_0' = \hat{F}_0$ as required.

**Theorem 5.2.** Suppose $k_0^r$ is a bounded and universal kernel and that $\lambda_0^0$ decays at a slower rate than $O(n_0^{-1/2})$. Then as $n_0 \to \infty$,

$$
\mathbb{E} \left[ \left( \hat{F}_0 \left(X_1, \ldots, X_r \right) - F_0 \left(X_1, \ldots, X_r \right) \right)^2 \right] \overset{P}{\to} 0.
$$

**Proof.** Define

$$
F_{0,\lambda_0^0} = \arg \min_{F \in \mathcal{H}_0^r} \left\{ \mathbb{E} \left[ \left( F \left(X_1, \ldots, X_r \right) - F_0 \left(X_1, \ldots, X_r \right) \right)^2 \right] + \lambda_0^0 \|F\|_{\mathcal{H}_0^r}^2 \right\}.
$$

By the bias-variance decomposition, this also minimises

$$
\mathcal{E}_{\lambda_0^0} (F) = \mathbb{E} \left[ \left( F \left(X_1, \ldots, X_r \right) - h \left(Y_1, \ldots, Y_r \right) \right)^2 \right] + \lambda_0^0 \|F\|_{\mathcal{H}_0^r}^2.
$$

Denote the Hilbert space of $P_X^r$-square-integrable $\mathcal{X}^r \to \mathbb{R}$ functions by $L^2(\mathcal{X}^r, P_X^r)$, and define the inclusion operator

$$
\iota : \mathcal{H}_0^r \to L^2(\mathcal{X}^r, P_X^r).
$$

Then we see that

$$
F_{0,\lambda_0^0} = \arg \min_{F \in \mathcal{H}_0^r} \left\{ \|\iota(F) - F_0\|_2^2 + \lambda_0^0 \|F\|_{\mathcal{H}_0^r}^2 \right\}
$$

$$
\implies 0 = \iota^* (\iota(F_{0,\lambda_0^0}) - F_0) + \lambda_0^0 F_{0,\lambda_0^0}
$$
We consider the following decomposition:

\[ F_{0, \lambda_{n_0}^0} = \left( \iota^* \circ \iota + \lambda_{n_0}^0 I \right)^{-1} \iota^* F_0 \]

Now, for any \( x^0 = (x_1^0, \ldots, x_{n_0}^0)^T \in X_{n_0} \), define the sampling operator

\[ S_{x^0} : \mathcal{H}_r \to \mathbb{R}^{(r_0)}, \quad (S_{x^0}(F))_{i_1, \ldots, i_r} = \frac{1}{(n_0)^2} F\left( x_{i_1}^0, \ldots, x_{i_r}^0 \right), \{i_1, \ldots, i_r\} \subset \{1, \ldots, n_0\}, \]

with adjoint

\[ S_{x^0}^* (h) = \frac{1}{(n_0)^2} \sum k_0 \left( x_{i_1}^0, \ldots, x_{i_r}^0 \right) h_{i_1, \ldots, i_r}, \quad h \in \mathbb{R}^{(n_0)}. \]

Indeed, for any \( F \in \mathcal{H}_r \) and \( h \in \mathbb{R}^{(n_0)}, \)

\[ (S_{x^0}F, h)_{\mathbb{R}^{(n_0)}} = \frac{1}{(n_0)^2} \sum F\left( x_{i_1}^0, \ldots, x_{i_r}^0 \right) h_{i_1, \ldots, i_r} \]

\[ = \frac{1}{(n_0)^2} \sum \left( F, k_0 \left( x_{i_1}^0, \ldots, x_{i_r}^0 \right) \right)_{\mathcal{H}_r^0} h_{i_1, \ldots, i_r} \]

\[ = \left( F, \frac{1}{(n_0)^2} \sum k_0 \left( x_{i_1}^0, \ldots, x_{i_r}^0 \right) h_{i_1, \ldots, i_r} \right)_{\mathcal{H}_r^0}. \]

For \( y^0 \in \mathcal{Y}_{n_0}, \) write

\[ h \left( y^0 \right) = \in \mathbb{R}^{(n_0)}, \quad h \left( y^0 \right)_{i_1, \ldots, i_r} = h \left( y_i^0, \ldots, y_i^0 \right), \{i_1, \ldots, i_r\} \subset \{1, \ldots, n_0\}. \]

Then we see that

\[ \hat{F}_0 = \text{arg min}_{F \in \mathcal{H}_r^0} \left\{ \frac{1}{n_0} \left\| S_{x^0}(F) - \frac{1}{(n_0)^2} h \left( y^0 \right) \right\|^2 + \lambda_{n_0}^0 \| F \|_{\mathcal{H}_r^0}^2 \right\} \]

\[ \implies 0 = \left( \frac{n_0}{r} \right) S_{x^0}^* \left( S_{x^0} \left( \hat{F}_0 \right) - \frac{1}{(n_0)^2} h \left( y^0 \right) \right) + \lambda_{n_0}^0 \hat{F}_0 \]

\[ \implies \hat{F}_0 = \left( \frac{n_0}{r} \right) S_{x^0}^* \circ S_{x^0} + \lambda_{n_0}^0 I \right)^{-1} S_{x^0}^* h \left( y^0 \right). \]

We consider the following decomposition:

\[ \mathbb{E} \left[ \left( \hat{F}_0(X_1, \ldots, X_r) - F_0(X_1, \ldots, X_r) \right)^2 \right] = \left\| \iota \hat{F}_0 - \iota F_0 \right\|_2^2 \leq 2 \left\| \iota \hat{F}_0 - \iota F_{0, \lambda_{n_0}^0} \right\|_2^2 \]

\[ + 2 \left\| \iota F_{0, \lambda_{n_0}^0} - \iota F_0 \right\|_2^2. \]

We are done if we show that the terms (a) and (b) separately converge to 0 (in probability, for (a)).

(a) See that

\[ \hat{F}_0 - F_{0, \lambda_{n_0}^0} = \left( \frac{n_0}{r} \right) S_{x^0}^* \circ S_{x^0} + \lambda_{n_0}^0 I \right)^{-1} S_{x^0}^* h \left( y^0 \right) - F_{0, \lambda_{n_0}^0} \]

\[ = \left( \frac{n_0}{r} \right) S_{x^0}^* \circ S_{x^0} + \lambda_{n_0}^0 I \right)^{-1} \left( S_{x^0}^* h \left( y^0 \right) - \left( \frac{n_0}{r} \right) S_{x^0}^* \circ S_{x^0} F_{0, \lambda_{n_0}^0} + \iota^* \left( \iota F_{0, \lambda_{n_0}^0} - F_0 \right) \right). \]
By spectral theorem,
\[
\left\| \hat{F}_0 - F_{0,\lambda_{n_0}} \right\|_{\mathcal{H}} \leq \frac{1}{\lambda_{n_0}^0} \left\| S_{x^0}^* h \left( y^0 \right) - \left( \frac{n_0}{r} \right) S_{x^0}^* \circ S_{x^0} F_{0,\lambda_{n_0}}^0 + \tau^* \left( \iota F_{0,\lambda_{n_0}}^0 - F_0 \right) \right\|_{\mathcal{H}}.
\]

Using this inequality and Chebyshev's inequality, for any \( \epsilon > 0 \),
\[
P \left( \left\| \hat{F}_0 - F_{0,\lambda_{n_0}} \right\|_{\mathcal{H}} \geq \epsilon \right) \leq \frac{\left\| S_{x^0}^* h \left( y^0 \right) - \left( \frac{n_0}{r} \right) S_{x^0}^* \circ S_{x^0} F_{0,\lambda_{n_0}}^0 + \tau^* \left( F_0 - \iota F_{0,\lambda_{n_0}}^0 \right) \right\|_{\mathcal{H}}^2}{\epsilon^2}
\]
\[
\leq \frac{1}{(\lambda_{n_0}^0)^2 \epsilon^2} \mathbb{E} \left[ \left\| S_{x^0}^* h \left( y^0 \right) - \left( \frac{n_0}{r} \right) S_{x^0}^* \circ S_{x^0} F_{0,\lambda_{n_0}}^0 + \tau^* \left( F_0 - \iota F_{0,\lambda_{n_0}}^0 \right) \right\|_{\mathcal{H}}^2 \right]
\]
\[
\leq \frac{1}{(\lambda_{n_0}^0)^2 \epsilon^2} \mathbb{E} \left[ \left\| k_0 \left( x_1, \ldots, x_r \right) \ldots k_0 \left( x_1, \ldots, x_r \right) \left( h \left( y_{i_1}, \ldots, y_{i_r} \right) - F_{0,\lambda_{n_0}} \left( x_{i_1}, \ldots, x_{i_r} \right) \right) \right\|_{\mathcal{H}}^2 \right]
\]
\[
\to 0
\]
as \( n \to \infty \), since the kernel is bounded.

(b) Take an arbitrary \( \epsilon > 0 \). By the denseness of \( \mathcal{H}_0^\circ \) in \( L^2(X^r, \mathcal{P}^r_X) \), there exists some \( F_\epsilon \in \mathcal{H}_0^\circ \) with
\[
\left\| \iota F_\epsilon - F_0 \right\|_2^2 = \mathcal{E}(F_\epsilon) - \mathcal{E}(F_0) \leq \frac{\epsilon}{2}.
\]

Then
\[
\left\| \iota F_{0,\lambda_{n_0}} - F_0 \right\|_2^2 = \mathcal{E}(F_{0,\lambda_{n_0}}) - \mathcal{E}(F_0)
\]
\[
\leq \mathcal{E}_{\lambda_{n_0}^0}(F_{0,\lambda_{n_0}}) - \mathcal{E}(F_0)
\]
\[
= \mathcal{E}_{\lambda_{n_0}^0}(F_{0,\lambda_{n_0}}) - \mathcal{E}_{\lambda_{n_0}^0}(F_\epsilon) + \mathcal{E}_{\lambda_{n_0}^0}(F_\epsilon) - \mathcal{E}(F_\epsilon) + \mathcal{E}(F_\epsilon) - \mathcal{E}(F_0)
\]
\[
\leq \lambda_{n_0}^0 \left\| F_\epsilon \right\|_{\mathcal{H}_0^\circ}^2 + \frac{\epsilon}{2}.
\]

Now let \( n \) be large enough for
\[
\lambda_{n_0}^0 \left\| F_\epsilon \right\|_{\mathcal{H}_0^\circ}^2 \leq \frac{\epsilon}{2}
\]

to hold.