A Measure-Theoretic Approach to Kernel Conditional Mean Embeddings

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Abstract

We present a new operator-free, measure-theoretic definition of the conditional mean embedding as a random variable taking values in a reproducing kernel Hilbert space. While the kernel mean embedding of marginal distributions has been defined rigorously, the existing operator-based approach of the conditional version lacks a rigorous definition, and depends on strong assumptions that hinder its analysis. Our definition does not impose any of the assumptions that the operator-based counterpart requires. We derive a natural regression interpretation to obtain empirical estimates, and provide a thorough analysis of its properties, including universal consistency. As natural by-products, we obtain the conditional analogues of the Maximum Mean Discrepancy and Hilbert-Schmidt Independence Criterion, and demonstrate their behaviour via simulations.

1 Introduction

The idea of embedding probability distributions into a reproducing kernel Hilbert space (RKHS), a space associated to a positive definite kernel, has received a lot of attention in the past decades (Berlinet and Thomas-Agnan, 2004; Smola et al., 2007), and has found a wealth of successful applications, such as independence testing (Gretton et al., 2008), two-sample testing (Gretton et al., 2012), learning on distributions (Muandet et al., 2012; Lopez-Paz et al., 2015; Szabó et al., 2016), goodness-of-fit testing (Chwiałkowski et al., 2016; Liu et al., 2016) and probabilistic programming (Schölkopf et al., 2015; Simon-Gabriel et al., 2016), among others – see review by Muandet et al. (2017). It extends the idea of kernelising linear methods by embedding data points into high- (and often infinite-)dimensional RKHSs, which has been applied, for example, in ridge regression, spectral clustering, support vector machines and principal component analysis among others (Schölkopf and Smola, 2002; Hofmann et al., 2008; Christmann and Steinwart, 2008).

Conditional distributions can also be embedded into RKHSs in a similar manner (Song et al., 2013; Muandet et al., 2017). Compared to marginal distributions, conditional distributions can represent more complicated relations between several random variables, and therefore conditional mean embeddings (CMEs) have the potential to unlock the whole arsenal of kernel mean embeddings to a much wider setting. Indeed, conditional mean embeddings have been applied successfully to dynamical systems (Song et al., 2009), inference on graphical models via belief propagation (Song et al., 2010), probabilistic inference via kernel sum and product rules (Song et al., 2013), reinforcement learning (Grünewälder et al., 2012; Nishiyama et al., 2012), kernelising the Bayes rule and applying it to nonparametric state-space models (Fukumizu et al., 2013) and causal inference (Mitrovic et al., 2018) to name a few.

Despite such progress, the current prevalent definition of the conditional mean embedding based on composing cross-covariance operators (Song et al., 2009) relies on some stringent assumptions, which are often violated and hinder its analysis. Klebanov et al. (2019) recently attempted to clarify and weaken some of these assumptions, but strong and hard-to-verify conditions still persist. Grünewälder et al. (2012) provided a regression interpretation, but here, only the existence of the CME is shown, without an explicit expression.
The main contribution of this paper is to provide a theoretically rigorous, operator-free definition of the
CME that requires drastically weaker assumptions, and comes in an explicit expression. We believe this will enable a more principled analysis of its theoretical properties, and open doors to new application areas. We
derive the empirical estimate based on vector-valued RKHS regression, and provide an in-depth analysis of its properties, including a universal consistency result of rate $O(n^{-1/2})$. In particular, we relax the assumption of Grünewälder et al. (2012) to allow for infinite-dimensional RKHSs.

As natural by-products, we obtain quantities that are extensions of the Maximum Mean Discrepancy (MMD) and the Hilbert-Schmidt Independence Criterion (HSIC) to the conditional setting, which we call the Maximum Conditional Mean Discrepancy (MCMD) and the Hilbert-Schmidt Conditional Independence Criterion (HSCIC). We demonstrate their properties through simulation experiments.

All proofs can be found in Appendix C.

2 Preliminaries

We take $(\Omega, \mathcal{F}, P)$ as the underlying probability space. Let $(\mathcal{X}, \mathcal{X})$, $(\mathcal{Y}, \mathcal{Y})$ and $(\mathcal{Z}, \mathcal{Z})$ be separable measurable spaces, and let $X : \Omega \to \mathcal{X}$, $Y : \Omega \to \mathcal{Y}$ and $Z : \Omega \to \mathcal{Z}$ be random variables with distributions $P_X$, $P_Y$ and $P_Z$. We will use $Z$ as the conditioning variable throughout.

2.1 Positive Definite Kernels and RKHS Embeddings

Let $\mathcal{H}_X$ be a vector space of real-valued functions on $\mathcal{X}$, endowed with the structure of a Hilbert space via an inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}_X}$. A symmetric function $k_X : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a reproducing kernel of $\mathcal{H}_X$ if and only if:
1. $\forall x \in \mathcal{X}$, $k_X(x, \cdot) \in \mathcal{H}_X$; 2. $\forall x \in \mathcal{X}$ and $\forall f \in \mathcal{H}_X$, $f(x) = \langle f, k_X(x, \cdot) \rangle_{\mathcal{H}_X}$. A Hilbert space of real-valued functions which possesses a reproducing kernel is called a reproducing kernel Hilbert space (RKHS) (Berlinet and Thomas-Agnan, 2004). A symmetric function $k_X : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a positive-definite function if its Gram matrix is positive definite. The Moore-Aronszajn Theorem (Aronszajn, 1950) shows that the set of positive-definite functions and the set of reproducing kernels on $\mathcal{X}$ are in fact identical.

Assuming $\int_X \sqrt{k_X(x,x)}dP_X(x) < \infty$, we define the kernel mean embedding of the distribution $P_X$ as $\mu_{P_X}(\cdot) := \int_X k_X(x, \cdot)dP_X(x)$. Note that the integrand $k_X(x, \cdot)$ is an element in a Hilbert space (and therefore a Banach space), so this integral is not a Lebesgue integral, but a Bochner integral (Dinculeanu, 2000, p.15, Definition 35). The square-root integrability assumption ensures that $k_X(X, \cdot)$ is indeed Bochner-integrable. We will generalise the following lemma to the conditional case later.

Lemma 2.1 (Smola et al. (2007)). For each $f \in \mathcal{H}_X$, $\int_X f(x) dP_X(x) = \langle f, \mu_{P_X} \rangle_{\mathcal{H}_X}$.

Next, suppose $\mathcal{H}_Y$ is an RKHS of functions on $\mathcal{Y}$ with kernel $k_Y$, and consider the tensor product RKHS $\mathcal{H}_X \otimes \mathcal{H}_Y$ (see Weidmann (1980, pp.47-48) for a definition of tensor product Hilbert spaces).

Theorem 2.2 (Berlinet and Thomas-Agnan (2004, p.31, Theorem 13)). The tensor product $\mathcal{H}_X \otimes \mathcal{H}_Y$ is generated by the functions $f \otimes g : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$, with $f \in \mathcal{H}_X$ and $g \in \mathcal{H}_Y$ defined by $(f \otimes g)(x, y) = f(x)g(y)$. Moreover, $\mathcal{H}_X \otimes \mathcal{H}_Y$ is an RKHS of functions on $\mathcal{X} \times \mathcal{Y}$ with kernel $\langle k_X \otimes k_Y \rangle((x_1, y_1), (x_2, y_2)) = k_X(x_1, x_2)k_Y(y_1, y_2)$.

Now let us impose a slightly stronger integrability condition:

$$\mathbb{E}_X[k_X(X, X)] < \infty, \quad \mathbb{E}_Y[k_Y(Y, Y)] < \infty. \quad (1)$$

This ensures that $k_X(X, \cdot) \otimes k_Y(Y, ::)$ is Bochner $P_{XY}$-integrable, and so $\mu_{P_{XY}} := \mathbb{E}_{XY}[k_X(X, \cdot) \otimes k_Y(Y, \cdot)] \in \mathcal{H}_X \otimes \mathcal{H}_Y$. The next lemma is analogous to Lemma 2.1:

Lemma 2.3 (Fukumizu et al. (2004, Theorem 1)). For each pair $f \in \mathcal{H}_X$, $g \in \mathcal{H}_Y$,

$$\langle f \otimes g, \mu_{P_{XY}} \rangle_{\mathcal{H}_X \otimes \mathcal{H}_Y} = \mathbb{E}_{XY}[f(X)g(Y)].$$
As a consequence, for any pair \( f \in \mathcal{H}_X \) and \( g \in \mathcal{H}_Y \), we have:

\[
\langle f \otimes g, \mu_{P_{XY}} - \mu_{P_X} \otimes \mu_{P_Y} \rangle_{\mathcal{H}_X \otimes \mathcal{H}_Y} = \text{Cov}_{XY}[f(X), g(Y)].
\]

There exists an isometric isomorphism \( \Phi : \mathcal{H}_X \otimes \mathcal{H}_Y \to \text{HS}(\mathcal{H}_X, \mathcal{H}_Y) \), where \( \text{HS}(\mathcal{H}_X, \mathcal{H}_Y) \) is the space of Hilbert-Schmidt operators from \( \mathcal{H}_X \) to \( \mathcal{H}_Y \). The cross-covariance operator is defined as \( \mathcal{C}_{XY} := \Phi(\mu_{P_{XY}} - \mu_{P_X} \otimes \mu_{P_Y}) \) (Fukumizu et al., 2004). It is straightforward to show that \( \langle g, \mathcal{C}_{XY} f \rangle_{\mathcal{H}_Y} = \text{Cov}_{XY}[f(X), g(Y)] \).

The notion of characteristic kernels is essential, since it tells us that the associated RKHSs are rich enough to enable us to distinguish different distributions from their embeddings.

**Definition 2.4** (Fukumizu et al. (2008)). A positive definite kernel \( k_X \) is characteristic to a set \( \mathcal{P} \) of probability measures defined on \( \mathcal{X} \) if the map \( \mathcal{P} \to \mathcal{H}_X : P \mapsto \mu_P \) is injective.

Sriperumbudur et al. (2010) discuss various characterisations of characteristic kernels and show that the well-known Gaussian and Laplacian kernels are characteristic. We then have a metric on \( \mathcal{P} \), and the existence in Dinculeanu (2000, pp.45-46, Theorems 39 and 50).

The HSIC is defined as the Hilbert-Schmidt norm of \( \mathcal{C}_{XY} \), or equivalently, \( \| \mu_{P_{XY}} - \mu_{P_X} \otimes \mu_{P_Y} \|_{\mathcal{H}_X \otimes \mathcal{H}_Y} \) (Gretton et al., 2005), i.e. the MMD between \( P_{XY} \) and \( P_X P_Y \). If \( k_X \otimes k_Y \) is characteristic, then HSIC = 0 if and only if \( X \perp Y \).

### 2.2 Conditioning

In this subsection, we briefly review the concept of conditioning in the formal measure-theoretic probability theory, in the context of Banach space-valued random variables. We consider a sub-\( \sigma \)-algebra \( \mathcal{E} \) of \( \mathcal{F} \) and a Banach space \( \mathcal{H} \).

**Definition 2.5** (Conditional Expectation, Dinculeanu (2000, p.45, Definition 38)). Suppose \( H \) is a Bochner \( P \)-integrable, \( \mathcal{H} \)-valued random variable. Then the **conditional expectation** of \( H \) given \( \mathcal{E} \) is any \( \mathcal{E} \)-measurable, Bochner \( P \)-integrable, \( \mathcal{H} \)-valued random variable \( H' \) such that \( \int_A H dP = \int_A H' dP \) for all \( A \in \mathcal{E} \). Any \( H' \) satisfying this condition is said to be a version of \( \mathbb{E}[H \mid \mathcal{E}] \). We write \( \mathbb{E}[H \mid Z] \) to mean \( \mathbb{E}[H \mid \sigma(Z)] \), where \( \sigma(Z) \) is the sub-\( \sigma \)-algebra of \( \mathcal{F} \) generated by the random variable \( Z \).

The (almost sure) uniqueness of the conditional expectation is shown in Dinculeanu (2000, p.44, Proposition 37), and the existence in Dinculeanu (2000, pp.45-46, Theorems 39 and 50).

**Definition 2.6** (Çınlar (2011, p.149)). For each \( A \in \mathcal{F} \), the **conditional probability** of \( A \) given \( \mathcal{E} \) is \( P(A \mid \mathcal{E}) = \mathbb{E}[1_A \mid \mathcal{E}] \).

Note that, in the unconditional case, the expectation is defined as the integral with respect to the measure, but in the conditional case, the expectation is defined first, and the measure is defined as the expectation of the identity.

For this definition of conditional probability to be useful, we require an additional property, called a “regular version”\(^1\). We first define the transition probability kernel\(^1\).

**Definition 2.7** (Çınlar (2011, p.37,40)). Let \( (\Omega_i, \mathcal{F}_i) \), \( i = 1, 2 \) be measurable spaces. A mapping \( K : \Omega_1 \times \mathcal{F}_2 \to [0, \infty] \) is a transition kernel from \( (\Omega_1, \mathcal{F}_1) \) to \( (\Omega_2, \mathcal{F}_2) \) if (i) \( \forall B \in \mathcal{F}_2, \omega \mapsto K(\omega, B) \) is \( \mathcal{F}_1 \)-measurable; (ii) \( \forall \omega \in \Omega_1, B \mapsto K(\omega, B) \) is a measure on \( (\Omega_2, \mathcal{F}_2) \). If \( K(\omega, \Omega_2) = 1 \) \( \forall \omega \in \Omega_1 \), \( K \) is said to be a transition probability kernel.

**Definition 2.8** (Çınlar (2011, p.150, Definition 2.4)). For each \( A \in \mathcal{F} \), let \( Q(A) \) be a version of \( P(A \mid \mathcal{E}) = \mathbb{E}[1_A \mid \mathcal{E}] \). Then \( Q : (\omega, A) \mapsto Q_\omega(A) \) is said to be a regular version of the conditional probability measure \( P(\cdot \mid \mathcal{E}) \) if \( Q \) is a transition probability kernel from \( (\Omega, \mathcal{E}) \) to \( (\Omega, \mathcal{F}) \).

\(^1\)Here, the term “kernel” must not be confused with the kernel associated to RKHSs.
The following theorem, proved in Appendix C, is the reason why a regular version is important. It means that, roughly speaking, the conditional expectation is indeed obtained by integration with respect to the conditional measure.

**Theorem 2.9** (Adapted from Çınlar (2011, p.150, Proposition 2.5)). *Suppose that \( P(\cdot \mid \mathcal{E}) \) admits a regular version \( Q \). Then \( QH : \Omega \to \mathcal{H} \) with \( \omega \mapsto Q_\omega H = \int_\Omega H(\omega')Q_\omega(d\omega') \) is a version of \( \mathbb{E}[H \mid \mathcal{E}] \) for every Bochner \( P \)-integrable \( H \).

Next, we define the conditional distribution.

**Definition 2.10** (Çınlar (2011, p.151)). Let \( X \) be a random variable taking values in a measurable space \((\mathcal{X}, \mathcal{F})\). Then the *conditional distribution* of \( X \) given \( \mathcal{E} \) is any transition probability kernel \( L : (\omega, B) \mapsto L_\omega(B) \) from \((\Omega, \mathcal{F})\) to \((\mathcal{X}, \mathcal{F})\) such that, for all \( B \in \mathcal{F} \), \( P(X \in B \mid \mathcal{E})(\omega) = \mathbb{E}[1_B \{ X \mid \mathcal{E} \}(\omega)] = L_\omega(B) \).

If \( P(\cdot \mid \mathcal{E}) \) has a regular version \( Q \), then letting
\[
P_{X|Z}(\omega)(B) = Q_\omega(X \in B)
\]
for \( \omega \in \Omega \), \( B \in \mathcal{F} \) defines a version \( P_{X|Z} \) of the conditional distribution of \( X \) given \( \mathcal{E} \). Unfortunately, a regular version of a conditional probability measure does not always exist. Also, it is not guaranteed that any version of the conditional distribution exists. The following definition and theorem tell us that, fortunately, these versions exist more often than not.

**Definition 2.11** (Çınlar (2011, p.11)). A measurable space \((E, \mathcal{E})\) is *standard* if it is isomorphic to \((F, \mathcal{B}_F)\), where \( F \) is some Borel subset of \( \mathbb{R} \) and \( \mathcal{B}_F \) is the Borel \( \sigma \)-algebra of \( F \).

**Theorem 2.12** (Çınlar (2011, p.151, Theorem 2.10)). *If \((\mathcal{X}, \mathcal{F})\) is a standard measurable space, then there exists a version of the conditional distribution of \( X \) given \( \mathcal{E} \). In particular, if \((\Omega, \mathcal{F})\) is a standard measurable space, then the conditional measure \( P(\cdot \mid \mathcal{E}) \) has a regular version.*

Examples of standard measurable spaces include \( \mathbb{R} \), \( \mathbb{R}^d \) and \( \mathbb{R}^\infty \) with their respective Borel \( \sigma \)-algebras, complete separable metric spaces with their Borel \( \sigma \)-algebra, Polish spaces with their Borel \( \sigma \)-algebras, separable Banach spaces with their Borel \( \sigma \)-algebras and separable Hilbert spaces with their Borel \( \sigma \)-algebras.

### 2.3 Vector-Valued RKHS Regression

In this subsection, we introduce the theory of vector-valued RKHS regression, based on operator-valued kernels. Let \( \mathcal{H} \) be a Hilbert space, which will be the output space of regression.

**Definition 2.13** (Carmeli et al. (2006, Definition 1)). An *\( \mathcal{H} \)-valued RKHS* on \( \mathbb{Z} \) is a Hilbert space \( \mathcal{G} \) such that 1. the elements of \( \mathcal{G} \) are functions \( \mathbb{Z} \to \mathcal{H} \); 2. \( \forall z \in \mathbb{Z} \) there exists \( C_z \geq 0 \) such that \( ||F(z)||_\mathcal{H} \leq C_z ||F||_\mathcal{G} \) for all \( F \in \mathcal{G} \).

For the next definition, we let \( \mathcal{L}(\mathcal{H}) \) denote the Banach space of bounded linear operators from \( \mathcal{H} \) into itself.

**Definition 2.14** (Carmeli et al. (2006, Definition 2)). A *\( \mathcal{H} \)-kernel of positive type* on \( \mathbb{Z} \times \mathbb{Z} \) is a map \( \Gamma : \mathbb{Z} \times \mathbb{Z} \to \mathcal{L}(\mathcal{H}) \) such that, for all \( N \in \mathbb{N} \), \( z_1, ..., z_N \in \mathbb{Z} \) and \( c_1, ..., c_N \in \mathbb{R} \), \( \sum_{i,j=1}^N c_i c_j \langle \Gamma(z_j, z_i) h, h \rangle_\mathcal{H} \geq 0 \) for all \( h \in \mathcal{H} \).

Analogously to the scalar case, it can be shown that any \( \mathcal{H} \)-valued RKHS \( \mathcal{G} \) possesses a *reproducing kernel*, which is an \( \mathcal{H} \)-kernel of positive type \( \Gamma \) satisfying, for any \( z, z' \in \mathbb{Z} \), \( h, h' \in \mathcal{H} \) and \( F \in \mathcal{G} \), \( \langle F(z), h \rangle_\mathcal{H} = \langle F, \Gamma(z, \cdot) h \rangle_\mathcal{G} \) and \( \langle h, \Gamma(z, z')(h') \rangle_\mathcal{H} = \langle \Gamma(\cdot, z)(h), \Gamma(\cdot, z')(h') \rangle_\mathcal{G} \). There is also an analogue of the Moore-Aronszajn Theorem:

**Theorem 2.15** (Carmeli et al. (2006, Proposition 1)). *Given an \( \mathcal{H} \)-kernel of positive type \( \Gamma : \mathbb{Z} \times \mathbb{Z} \to \mathcal{L}(\mathcal{H}) \), there is a unique \( \mathcal{H} \)-valued RKHS \( \mathcal{G} \) on \( \mathbb{Z} \) with reproducing kernel \( \Gamma \).*
Now suppose we want to perform regression with input space $Z$ and output space $H$, by minimising the following regularised loss functional:

$$\sum_{j=1}^{n} \|h_j - F(z_j)\|^2_H + \lambda \|F\|^2_{G},$$

where $\lambda > 0$ is a regularisation parameter and $\{(z_j, h_j) : j = 1, \ldots, n\} \subseteq Z \times H$. There is a corresponding representer theorem:

**Theorem 2.16** (Micchelli and Pontil (2005, Theorem 4.1)). If $\hat{F}$ minimises (4) in $G$, it is unique and has the form $\hat{F} = \sum_{j=1}^{n} \Gamma(z_j, z_j)(u_j)$ where the coefficients $\{u_j : j = 1, \ldots, n\} \subseteq H$ are the unique solution of the linear equations $\sum_{l=1}^{n} (\Gamma(z_j, z_l) + \lambda \delta_{jl})(u_l) = h_j, j = 1, \ldots, n$.

### 3 Conditional Mean Embedding

We are now ready to introduce a formal definition of the conditional mean embedding of $X$ given $Z$.

**Definition 3.1** (Conditional Mean Embedding (CME)). We define the **conditional mean embedding** of $X$ given $Z$ as

$$\mu_{P_{X|Z}} := \mathbb{E}_{X|Z}[k_X(X, \cdot) | Z].$$

This is a direct extension of the marginal kernel mean embedding, $\mu_{P_X} = \mathbb{E}_X[k_X(X, \cdot)]$, but instead of being a fixed element in $H_X$, $\mu_{P_{X|Z}}$ is a $Z$-measurable random variable taking values in $H_X$ (see Definition 2.5). Also, for $f \in H_X$, $E_{X|Z}[f(X) | Z]$ is a real-valued $Z$-measurable random variable. The following lemma is analogous to Lemma 2.1.

**Lemma 3.2.** Suppose $P(\cdot | Z)$ admits a regular version. Then for any $f \in H_X$,

$$\mathbb{E}_{X|Z}[f(X) | Z] = \langle f, \mu_{P_{X|Z}} \rangle_{H_X}$$

almost surely.

Next, we define $\mu_{P_{XY|Z}} := \mathbb{E}_{XY|Z}[k_X(X, \cdot) \otimes k_Y(Y, \cdot) | Z]$, a $Z$-measurable random variable taking values in $H_X \otimes H_Y$. The following lemma is an analogy of Lemma 2.3.

**Lemma 3.3.** Suppose that $P(\cdot | Z)$ admits a regular version. Then for each pair $f \in H_X$ and $g \in H_Y$,

$$\langle f \otimes g, \mu_{P_{XY|Z}} \rangle_{H_X \otimes H_Y} = \mathbb{E}_{XY|Z}[f(X)g(Y) | Z]$$

almost surely.

By Lemmas 3.2 and 3.3, for any pair $f \in H_X$ and $g \in H_Y$,

$$\langle f \otimes g, \mu_{P_{XY|Z}} - \mu_{P_{X|Z}} \otimes \mu_{P_{Y|Z}} \rangle_{H_X \otimes H_Y} = \mathbb{E}_{XY|Z}[f(X)g(Y) | Z] - \mathbb{E}_{X|Z}[f(X) | Z] \mathbb{E}_{Y|Z}[g(Y) | Z]$$

$$= \text{Cov}_{XY|Z}(f(X), g(Y) | Z)$$

almost surely. Hence, we define the **conditional cross-covariance operator** as $C_{Y|Z} := \Phi(\mu_{P_{XY|Z}} - \mu_{P_{X|Z}} \otimes \mu_{P_{Y|Z}})$ (see Section 2.1 for the definition of $\Phi$).

### 3.1 Comparison with Existing Definitions

As previously mentioned, the idea of CMEs and conditional cross-covariance operators is not a novel one, yet our development of the theory and definitions above differ significantly from the existing works. In this subsection, we review the previous approaches and compare them to ours.

The prevalent definition of CMEs in the literature is the one given in the following definition. We first need to endow the conditioning space $Z$ with a scalar kernel, say $k_Z : Z \times Z \to \mathbb{R}$, with corresponding RKHS $H_Z$. 

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Definition 3.4 (Song et al. (2009, Definition 3)). The conditional mean embedding of the conditional distribution \( P(X \mid Z) \) is the operator \( \mathcal{U}_{X|Z} : \mathcal{H}_Z \to \mathcal{H}_X \) defined by \( \mathcal{U}_{X|Z} = C_{XZ}C_{ZZ}^{-1} \), where \( C_{XZ} \) and \( C_{ZZ} \) are unconditional (cross-)covariance operators as defined in Section 2.1.

As noted by Song et al. (2009), the motivation for this comes from Theorem 2 in the appendix of Fukumizu et al. (2004), which states that if \( \mathbb{E}_{X|Z}[f(X) \mid Z = \cdot] \in \mathcal{H}_Z \), then for any \( f \in \mathcal{H}_X \), \( C_{ZZ}\mathbb{E}_{X|Z}[f(X) \mid Z = \cdot] = C_{XZ}f \). This relation can be used to prove the following theorem.

Theorem 3.5 (Song et al. (2009, Theorem 4)). Take any \( f \in \mathcal{H}_X \). Then assuming \( \mathbb{E}_{X|Z}[f(X) \mid Z = \cdot] \in \mathcal{H}_Z \), \( \mathcal{U}_{X|Z} \) satisfies: 1. \( \mu_{X|Z} := \mathbb{E}_{X|Z}[k_X(X, \cdot) \mid Z = z] = \mathcal{U}_{X|Z}k_Z(z, \cdot) \); 2. \( \mathbb{E}_{X|Z}[f(X) \mid Z = z] = \langle f, \mu_{X|Z} \rangle_{\mathcal{H}_X} \).

Now we highlight the key differences between this approach and ours. Firstly, this approach requires the endowment of a kernel \( k_Z \) on the conditioning space \( Z \), and subsequently defines the CME as an operator from \( \mathcal{H}_Z \) to \( \mathcal{H}_X \). By contrast, our definition did not consider any kernel or function on \( Z \), and defined the CME as a Bochner conditional expectation given \( \sigma(Z) \), i.e. a \( Z \)-measurable, \( \mathcal{H}_X \)-valued random variable. It seems more logical not to have to endow the conditioning space with a kernel, at least before the estimation stage. Secondly, the operator-based approach assumes that \( \mathbb{E}_{X|Z}[f(X) \mid Z = \cdot] \), as a function in \( z \), lives in \( \mathcal{H}_Z \). This is a severe restriction; it is stated in Song et al. (2009) that this assumption, while true for finite domains with characteristic kernels, is not necessarily true for continuous domains, and Fukumizu et al. (2013) gives a simple counterexample using the Gaussian kernel. Lastly, it also assumes that \( C_{ZZ}^{-1} \) exists, which is another severe restriction. Fukumizu et al. (2013) mentions that this assumption is too strong in many situations involving popular kernels, and gives a counterexample using the Gaussian kernel. The most common remedy is to resort to the regularised version \( C_{XZ}(C_{ZZ} + \lambda I)^{-1} \) and treat it as an approximation of \( \mathcal{U}_{X|Z} \). These assumptions have been clarified and slightly weakened in Klebanov et al. (2019), but strong and hard-to-verify conditions persist.

In contrast, our definitions extend the notions of kernel mean embedding, expectation operator and cross-covariance operator to the conditional setting simply by using the formal definition of conditional expectations (Definition 2.5), and only rely on the mild assumption that the conditional probability measure \( P(\cdot \mid Z) \) admits a regular version.

Grünewälder et al. (2012) gave a regression interpretation, by showing the existence, for each \( z \in Z \), of \( \mu(z) \in \mathcal{H}_X \) that satisfies \( \mathbb{E}[h(X) \mid Z = z] = \langle h, \mu(z) \rangle_{\mathcal{H}_X} \). However, the main drawback here is that there is no explicit expression for \( \mu(z) \), limiting its analysis and use. In contrast, our definition has an explicit expression \( \mu_{P_X|Z} = \mathbb{E}_{X|Z}[k_X(X, \cdot) \mid Z] \), with which it is easy to explore potential applications.

In Fukumizu et al. (2004), the conditional cross-covariance operator is defined, but in a significantly different way. It is defined as \( \Sigma_{YX|Z} := \Sigma_{YX} - \Sigma_{YZ}C_{ZZ}^{-1}\Sigma_{ZX} \), where \( C_{ZZ}^{-1} \) is the right inverse of \( C_{ZZ} \) on \( (\text{Ker}C_{ZZ})^\perp \). This has the property that, for all \( f \in \mathcal{H}_X \) and \( g \in \mathcal{H}_Y \), \( \langle \Sigma_{YX|Z}f, g \rangle_{\mathcal{H}_Y} = \mathbb{E}_Z[\text{Cov}_{YX|Z}(f(X), g(Y) \mid Z)] \). Note that this is different to our relation stated after Lemma 3.3; the conditional covariance is integrated out over \( Z \). In fact, this difference is explicitly noted by Song et al. (2009).

### 3.2 A Discrepancy Measure between Conditional Distributions

In this subsection, we propose a conditional analogue of the maximum mean discrepancy (MMD), and explore the role of characteristic kernels in the conditional case. Let \( X' : \Omega \to \mathcal{X}' \) be an additional random variable, satisfying \( \int_X \sqrt{k_X(x', x')} dP_{X'}(x') < \infty \).

Definition 3.6. We define the maximum conditional mean discrepancy (MCMD) between \( P_{X|Z} \) and \( P_{X'|Z} \) to be

\[
\text{MCMD}(X, X' \mid Z) := \| \mu_{P_{X|Z}} - \mu_{P_{X'|Z}} \|_{\mathcal{H}_X}.
\]

We note that MCMD is not a fixed value, but a real-valued, \( Z \)-measurable random variable.

The term MMD stems from the equality \( \| \mu_{P_X} - \mu_{P_{X'}} \|_{\mathcal{H}_X} = \sup_{f \in B_X} \mathbb{E}_X[f(X) - \mathbb{E}_{X'}[f(X')]] \) (Gretton et al., 2007; Sriperumbudur et al., 2010), where \( B_X := \{ f \in \mathcal{H}_X \mid \| f \|_{\mathcal{H}_X} \leq 1 \} \). The supremum is attained by the witness function,

\[
w_{XX'} := \frac{\mu_{P_X} - \mu_{P_{X'}}}{\| \mu_{P_X} - \mu_{P_{X'}} \|_{\mathcal{H}_X}}
\]
The analogous (a.s.) equality for the MCMD is:

$$\sup_{f \in B_X} |E_X|Z[f(X) \mid Z] - E_X|Z[f(X^*) \mid Z]| = \sup_{f \in B_X} |(\mu_{P_{X\mid Z}} - \mu_{P_{X^*\mid Z}}, f)_{\mathcal{H}_X}|$$

$$= \|\mu_{P_{X\mid Z}} - \mu_{P_{X^*\mid Z}}\|_{\mathcal{H}_X},$$

where we used Lemma 3.2. We define the conditional witness function as the $\mathcal{H}_X$-valued random variable

$$w_{XX'}|Z := \frac{\mu_{P_{X\mid Z}} - \mu_{P_{X^*\mid Z}}}{\|\mu_{P_{X\mid Z}} - \mu_{P_{X^*\mid Z}}\|_{\mathcal{H}_X}}.$$ 

Casting aside measure-theoretic issues arising from conditioning on an event of measure 0, we can informally think of the realisation of the MCMD at each $\omega \in \Omega$ with $z = Z(\omega)$ as “the MMD between $P_{X\mid Z=z}$ and $P_{X^*:\mid Z=z}$”, and $w_{XX'}|Z(\omega)$ as “the witness function between $P_{X\mid Z=z}$ and $P_{X^*:\mid Z=z}$”. The following theorem says that, with characteristic kernels, the MCMD can indeed act as a discrepancy measure between conditional distributions.

**Theorem 3.7.** Suppose $k_X$ is a characteristic kernel, and assume that $P(\cdot \mid Z)$ admits a regular version. Then $\text{MCMD}(X, X' \mid Z) = 0$ almost surely if and only if, almost surely, $P_{X\mid Z}(B \mid Z) = P_{X^*:\mid Z}(B \mid Z)$ for all $B \in \mathcal{X}$.

The MCMD is reminiscent of the conditional maximum mean discrepancy of Ren et al. (2016), defined as the Hilbert-Schmidt norm of the operator $\mathcal{U}_{X\mid Z} - \mathcal{U}_{X^*:\mid Z}$ (see Definition 3.4). However, due to strong assumptions previously discussed, $\mathcal{U}_{X\mid Z}$ and $\mathcal{U}_{X^*:\mid Z}$ often do not even exist, and/or do not have the desired properties of Theorem 3.5, so even at population level, $\mathcal{U}_{X\mid Z} - \mathcal{U}_{X^*:\mid Z}$ is often not an exact measure of discrepancy between conditional distributions. On the other hand, Theorem 3.7 with the MCMD is an exact mathematical statement at population level that is valid between any pair of conditional distributions.

The discussion on characteristic kernels in the conditional setting, and the precise meaning of an “injective embedding” of conditional distributions, has largely been absent in the existing literature. We suspect that this is because the operator-based definition is somewhat cumbersome to work with, and it is not immediately clear how to express such statements. The new, mathematically elegant definition of the CME can remedy that through Theorem 3.7. We conjecture that characteristic kernels will play a crucial role in many future applications of the CME.

### 3.3 A Criterion of Conditional Independence

In this subsection, we introduce a novel criterion of conditional independence, via a direct analogy with the HSIC.

**Definition 3.8.** We define the Hilbert-Schmidt Conditional Independence Criterion between $X$ and $Y$ given $Z$ to be

$$\text{HSCIC}(X, Y \mid Z) = \|\mu_{P_{XY\mid Z}} - \mu_{P_{X\mid Z}} \otimes \mu_{P_{Y\mid Z}}\|_{\mathcal{H}_X \otimes \mathcal{H}_Y}.$$ 

Note that HSCIC($X, Y \mid Z$) is an instance of the MCMD in the tensor product space $\mathcal{H}_X \otimes \mathcal{H}_Y$, and is a (real-valued) random variable. Again, casting aside measure-theoretic issues arising from conditioning on an event of probability 0, we can conceptually think of the realisation of the HSCIC at each $z = Z(\omega)$ as “the HSIC between $P_{X\mid Z=z}$ and $P_{Y\mid Z=z}$”. Since HSCIC is an instance of MCMD, the following theorem follows immediately from Theorem 3.7.

**Theorem 3.9.** Suppose $k_X \otimes k_Y$ is a characteristic kernel\(^2\) on $\mathcal{X} \times \mathcal{Y}$, and that $P(\cdot \mid Z)$ admits a regular version. Then $\text{HSCIC}(X, Y \mid Z) = 0$ a.s. if and only if $X \perp Y \mid Z$.

\(^2\)See Szabó and Sriperumbudur (2018) for a detailed discussion on characteristic tensor product kernels.
Concurrent and independent work by Sheng and Sriperumbudur (2019) proposes a similar criterion with the same nomenclature (HSCIC). However, they omit the discussion of CMEs entirely, and define the HSCIC as the usual HSIC between \( P_{X|Z} \) and \( P_{XZ} \), without considerations for conditioning on an event of measure 0. Their focus is more on investigating connections to distance-based measures (Wang et al., 2015; Sejdinovic et al., 2013). Fukumizu et al. (2008) propose \( I^{\text{COND}} \), defined as the squared Hilbert-Schmidt norm of the normalised conditional cross-covariance operator \( \gamma_{X|Z} := C_{YY}^{-1/2} \Sigma_{YX|Z} C_{XX}^{-1/2} \), where \( \tilde{X} := (X, Z) \) and \( \tilde{Y} := (Y, Z) \). As discussed, these operator-based definitions rely on a number of strong assumptions that will often mean that \( \gamma_{X|Z} \) does not exist, or it does not satisfy the conditions for it to be used as an exact criterion even at population level. On the other hand, the HSCIC defined as in Definition 3.8 is an exact mathematical criterion of conditional independence at population level. Note that \( I^{\text{COND}} \) is a single-value criterion, whereas the HSCIC is a random criterion.

4 Empirical Estimates

In this section, we discuss how we can obtain empirical estimates of \( \mu_{P_{X|Z}} = \mathbb{E}_{X|Z}[k_X(X, \cdot) \mid Z] \).

**Theorem 4.1.** Let \( Z \) be a random variable taking values in a measurable space \((\mathcal{Z}, \mathcal{F})\) with underlying probability space \((\Omega, \mathcal{F}, \mathbb{P})\), and let \( \mathcal{T} \) be a Hausdorff topological space, with its Borel \( \sigma \)-algebra \( \mathcal{B}(\mathcal{T}) \). A mapping \( V : \Omega \to \mathcal{T} \) is measurable with respect to \( \sigma(Z) \) and \( \mathcal{B}(\mathcal{T}) \) if and only if \( V = F \circ Z \) for some deterministic function \( F : \mathcal{Z} \to \mathcal{T} \), measurable with respect to \( \mathcal{F} \) and \( \mathcal{B}(\mathcal{T}) \).

Letting \( \mathcal{T} = \mathcal{H}_X \) and \( V = \mu_{P_{X|Z}} \), the upshot of Theorem 4.1 is that we can write

\[
\mu_{P_{X|Z}} = F_{P_{X|Z}} \circ Z,
\]

(5)

where \( F_{P_{X|Z}} : \mathcal{Z} \to \mathcal{H}_X \) is some deterministic, measurable function. Figure 1 depicts this relation. Hence, the problem of estimating \( \mu_{P_{X|Z}} \) boils down to estimating the function \( F_{P_{X|Z}} \), and this is exactly the setting for vector-valued regression discussed in Section 2.3, with input space \( \mathcal{Z} \) and output space \( \mathcal{H}_X \). In contrast to Grünewälder et al. (2012), where regression is motivated by applying the Riesz representation theorem conditioned on each value of \( z \in \mathcal{Z} \), we derive the CME as an explicit function of \( Z \), which we argue is a more principled way to motivate regression. Moreover, for continuous \( Z \), the event \( Z = z \) has measure 0 for each \( z \in \mathcal{Z} \), so it is not measure-theoretically rigorous to apply the Riesz representation theorem conditioned on \( Z = z \).

The natural optimisation problem is to minimise the loss

\[
\mathcal{E}_{X|Z}(F) := \mathbb{E}_Z[\|F_{P_{X|Z}}(Z) - F(Z)\|_{\mathcal{H}_X}^2]
\]

(6)

among all \( F \in \mathcal{G}_{X \mathcal{Z}} \), where \( \mathcal{G}_{X \mathcal{Z}} \) is a vector-valued RKHS of functions \( \mathcal{Z} \to \mathcal{H}_X \) endowed with a kernel \( l_{X \mathcal{Z}}(z, z') = k_Z(z, z') \text{Id} \), where \( k_Z(\cdot, \cdot) \) is a scalar kernel on \( \mathcal{Z} \).

We cannot minimise \( \mathcal{E}_{X|Z} \) directly, since we do not observe samples from \( \mu_{P_{X|Z}} = F_{P_{X|Z}}(Z) \), but only the pairs \((x_1, z_1), \ldots, (x_n, z_n)\) from \((X, Z)\). We bound this with a surrogate loss \( \tilde{\mathcal{E}}_{X|Z} \) that has a sample-based
There is no doubt that $k$ where we wrote $\lambda > 0$ is a regularisation parameter. We see that this loss functional has exactly the same form as in (4). Therefore, by Theorem 2.16, the minimiser $\hat{F}_{P_{X|Z}}(\cdot)$ of $\hat{E}_{X|Z,\lambda}$ has the form $\hat{F}_{X|Z,n,\lambda}(\cdot) = k^{(\lambda)}_Z(\cdot) f$, where we wrote $k_Z(\cdot) := \langle k_Z(z_1), \ldots, k_Z(z_n) \rangle^T$ and $f := (f_1, \ldots, f_n)^T$. By Theorem 2.16, the coefficients $f_i \in H_X$ are the unique solutions of the linear equations $(K_Z + \lambda I) f = k_X$, where $[K_Z]_{ij} := k_Z(z_i, z_j)$, $k_X := \langle k_X(x_1, \cdot), \ldots, k_X(x_n, \cdot) \rangle^T$ and $I$ is the $n \times n$ identity matrix. Hence, the coefficients are $f = (K_Z + \lambda I)^{-1} k_X = W_k X$, where we wrote $W = (K_Z + \lambda I)^{-1}$. Finally, substituting this into the expression for $\hat{F}_{P_{X|Z,\lambda}}(\cdot)$, we have

$$\hat{E}_{X|Z,\lambda}(\cdot) = k^{(\lambda)}_Z(\cdot) W_k X \in G_{X,\lambda}.$$  

Note that this expression is identical to those in Song et al. (2009) and Grünwälder et al. (2012).

4.1 Surrogate Loss, Universality and Consistency

There is no doubt that $E_{X|Z}$ in (6) is a more natural loss functional than the surrogate loss $\hat{E}_{X|Z}$. In this subsection, we investigate the meaning and consequences of using this surrogate loss, as well as the implications of using a universal kernel and the consistency properties of our algorithm.

Denote by $L^2(Z, P_Z; H_X)$ the Banach space of (equivalence classes of) measurable functions $F : Z \rightarrow H_X$ such that $\|F\|_2^2 = \int_Z \|F(z)\|^2_{H_X} dP_Z(z)$ is $P_Z$-integrable, with norm $\|F\|_2 = (\int_Z \|F(z)\|^2_{H_X} dP_Z(z))^{\frac{1}{2}}$. We can note that the true function $F_{P_{X|Z}}$ belongs to $L^2(Z, P_Z; H_X)$, because Theorem 4.1 tells us that $F_{P_{X|Z}}$ is indeed measurable, and

$$\int_Z \|F_{P_{X|Z}}(z)\|^2_{H_X} dP_Z(z) = \mathbb{E}_Z[\|E_{X|Z}[k_X(X, \cdot) | Z]\|_{H_X}^2] \leq \mathbb{E}_Z[\|E_{X|Z}[k_X(X, \cdot) | Z]\|_{H_X}^2] = \mathbb{E}_X[\|k_X(X, \cdot)\|_{H_X}^2] = \mathbb{E}_X[k_X(X, X)] < \infty,$$

by (1), where we used generalised conditional Jensen’s inequality again on the second line (Appendix A). The following theorem shows that the true function $F_{P_{X|Z}}$ is the unique minimiser in $L^2(Z, P_Z; H_X)$ of both $E_{X|Z}$ and $\hat{E}_{X|Z}$:

**Theorem 4.2.** $F_{P_{X|Z}}$ minimises both $\hat{E}_{X|Z}$ and $E_{X|Z}$ in $L^2(Z, P_Z; H_X)$. Moreover, it is almost surely equal to any other minimiser of the loss functionals.

Note the difference in the statement of Theorem 4.2 from Grünwälder et al. (2012, Theorem 3.1), who only consider the minimisation of the loss functionals in $G_X$, whereas we consider the larger space $L^2(Z, P_Z; H_X)$ in which to minimise our loss functionals.

Next, we discuss the concepts of universal kernels and universal consistency.
**Definition 4.3** (Carmeli et al. (2008, Definition 2)). An operator-valued reproducing kernel $l_{\mathcal{X}Z} : \mathcal{Z} \times \mathcal{Z} \rightarrow \mathcal{L}(\mathcal{H}_X)$ with associated RKHS $\mathcal{G}_{\mathcal{X}Z}$ is $C_0$ if $\mathcal{G}_{\mathcal{X}Z}$ is a subspace of $C_0(\mathcal{Z}, \mathcal{H}_X)$, the space of continuous functions $\mathcal{Z} \rightarrow \mathcal{H}_X$ vanishing at infinity. The kernel $l_{\mathcal{X}Z}$ is $C_0$-universal if $\mathcal{G}_{\mathcal{X}Z}$ is dense in $L^2(\mathcal{Z}, \mathcal{P}_Z; \mathcal{H}_X)$ for any measure $\mathcal{P}_Z$.

Recall that we are using the kernel $l_{\mathcal{X}Z}(\cdot, \cdot) = k_{\mathcal{Z}}(\cdot, \cdot)\text{Id}$. Carmeli et al. (2008, Example 14) show that $l_{\mathcal{X}Z}$ is $C_0$-universal if $k_{\mathcal{Z}}$ is a universal scalar kernel, which in turn is guaranteed if $k_{\mathcal{Z}}$ is Gaussian or Laplacian, for example (Steinwart, 2001).

The consistency result with optimal rate of $O(\log n / n)$ in Grünewälder et al. (2012) based on Caponnetto and De Vito (2006) imposes strong assumptions about the kernel $l_{\mathcal{X}Z}$, and finite-dimensional assumption on the output space $\mathcal{H}_X$. These are violated for many commonly used kernels such as the Gaussian kernel, and so we do not use this result in our paper (see Appendix B for more details). Fukumizu (2015) also shows consistency with rate slightly worse than $O(n^{-\frac{1}{2}})$ with weaker assumptions. We prove the following universal consistency result, which relies on even weaker assumptions and achieves a better rate of $O(n^{-\frac{1}{2}})$.

**Theorem 4.4.** Suppose $k_{\mathcal{X}}$ and $k_{\mathcal{Z}}$ are bounded kernels, i.e. for all $x_1, x_2 \in \mathcal{X}$, $k_{\mathcal{X}}(x_1, x_2) \leq B_{\mathcal{X}}$ for some $B_{\mathcal{X}} > 0$ and for all $z_1, z_2 \in \mathcal{Z}$, $k_{\mathcal{Z}}(z_1, z_2) \leq B_{\mathcal{Z}}$ for some $B_{\mathcal{Z}} > 0$. Then our learning algorithm that produces $\hat{F}_{\mathcal{X}Z}(x, \cdot)$ is universally consistent (in the surrogate loss $\tilde{\mathcal{E}}_{\mathcal{X}|Z}$), i.e. for any joint distribution $P_{\mathcal{X}Z}$ and constants $\epsilon > 0$ and $\delta > 0$,

$$P_{\mathcal{X}Z}(\tilde{\mathcal{E}}_{\mathcal{X}|Z}(\hat{F}_{\mathcal{X}Z}, n, \lambda) - \mathcal{E}_{\mathcal{X}|Z}(F_{\mathcal{X}Z}) > \epsilon) < \delta$$

for large enough $n$. The rate of convergence is $O(n^{-1/2})$.

The boundedness assumption is satisfied with many commonly used kernels, such as the Gaussian and Laplacian kernels, and hence is not a restrictive condition. The key observation is that the target values are all of the form $k_{\mathcal{X}}(x, \cdot)$ for $x \in \mathcal{X}$, so the target space is bounded if $k_{\mathcal{X}}$ is bounded (see Appendix B and the proof in Appendix C for details).

Theorem 4.4 is stated with respect to the surrogate loss, not the natural original loss $\mathcal{E}_{\mathcal{X}|Z}$. Let us now investigate is implications with respect to the original loss. Write $\eta = \tilde{\mathcal{E}}_{\mathcal{X}|Z}(F_{\mathcal{X}Z})$. Since $\tilde{\mathcal{E}}_{\mathcal{X}|Z}(\hat{F}_{\mathcal{X}Z}, n, \lambda) \geq \mathcal{E}_{\mathcal{X}|Z}(\hat{F}_{\mathcal{X}Z}, n, \lambda)$, a consequence of Theorem 4.4 is that

$$\lim_{n \rightarrow \infty} P_{\mathcal{X}Z}(\tilde{\mathcal{E}}_{\mathcal{X}|Z}(\hat{F}_{\mathcal{X}Z}, n, \lambda) > \epsilon + \eta) \leq \lim_{n \rightarrow \infty} P_{\mathcal{X}Z}(\tilde{\mathcal{E}}_{\mathcal{X}|Z}(\hat{F}_{\mathcal{X}Z}, n, \lambda) - \eta > \epsilon) = 0$$

by (8), for any $\epsilon > 0$. This shows that, in the limit as $n \rightarrow \infty$, the loss $\mathcal{E}_{\mathcal{X}|Z}(\hat{F}_{\mathcal{X}Z}, n, \lambda)$ is at most an arbitrarily small amount larger than $\eta$ with high probability. It remains to investigate what $\eta$ represents, and how large it is. The law of total expectation gives

$$\eta = \tilde{\mathcal{E}}_{\mathcal{X}|Z}(F_{\mathcal{X}Z}) = \mathbb{E}_{\mathcal{X},Z}[||k_{\mathcal{X}}(X, \cdot) - F_{\mathcal{X}Z}(Z)||^2_{\mathcal{H}_X}] = \mathbb{E}_Z[\mathbb{E}_{\mathcal{X}|Z}[||k_{\mathcal{X}}(X, \cdot) - F_{\mathcal{X}Z}(X, \cdot) | Z||^2_{\mathcal{H}_X} | Z]]$$

Here, the inner conditional expectation

$$\mathbb{E}_{\mathcal{X}|Z}[||k_{\mathcal{X}}(X, \cdot) - F_{\mathcal{X}Z}(X, \cdot) | Z||^2_{\mathcal{H}_X} | Z]$$

is the variance of $k_{\mathcal{X}}(X, \cdot)$ given $Z$ (see Bharucha-Reid (1972, p.24) for the definition of the variance of Banach-space valued random variables), and by integrating over $Z$ in the outer integral, $\eta$ represents the “mean variance” of $k_{\mathcal{X}}(X, \cdot)$ over $Z$.

Suppose $X$ is measurable with respect to $Z$, i.e. $F_{\mathcal{X}Z}$ has zero noise. Then we have $\mathbb{E}_{\mathcal{X}|Z}[k_{\mathcal{X}}(X, \cdot) | Z] = k_{\mathcal{X}}(X, \cdot)$, and consequently, $\eta = 0$. In this case, we have universal consistency in both the surrogate loss $\tilde{\mathcal{E}}_{\mathcal{X}|Z}$ and the original loss $\mathcal{E}_{\mathcal{X}|Z}$. On the other hand, $\eta$ will be large if information about $Z$ tells us little
which is precisely the variance of

\[ \text{witness function between } X \]

where \( \circ \) denotes elementwise multiplication of matrices. In this section, we carry out simulations to demonstrate the behaviour of the MCMD and HSCIC. In all simulations, we use the Gaussian kernel \( k(x, x') = k_{X}(x, x') = k_{Z}(x, x') = e^{-\frac{1}{2} \sigma_{X} \| x - x' \|^{2}} \) with hyperparameter \( \sigma_{X} = 0.1 \), and regularisation parameter \( \lambda = 0.01 \).

about \( X \), and subsequently \( k_{X}(X, \cdot) \in \mathcal{H}_{X} \). In the extreme case where \( X \) and \( Z \) are independent, we have

\[ \mathbb{E}_{X|Z}[k_{X}(X, \cdot) | Z] = \mathbb{E}_{X}[k_{X}(X, \cdot)], \]

and

\[ \eta = \mathbb{E}_{X}[\| k_{X}(X, \cdot) - \mathbb{E}_{X}[k_{X}(X, \cdot)] \|_{\mathcal{H}_{X}}^{2}], \]

which is precisely the variance of \( k_{X}(X, \cdot) \) in \( \mathcal{H}_{X} \). Hence, \( \eta \) represents the irreducible loss of the true function due to noise in \( X \), and the surrogate loss represents the loss functional taking noise into account, while the original loss measures the deviance from the true conditional expectation.

4.2 Empirical Estimates of MCMD and HSCIC

Recall that we defined the MCMD as \( \| \mu_{P_{X}\|Z} - \mu_{P_{X'}\|Z} \|_{\mathcal{H}_{X}} \) (Definition 3.6). By Theorem 4.1 (or directly using Çınlar (2011, Theorem I.4.4)), we can write MCMD\((X, X' \mid Z) = M_{XX'\mid Z} \circ Z \) for some function \( M_{XX'\mid Z} : Z \to \mathbb{R} \). Using samples \( \{(x_{i}, x'_{i}, z_{i})\}_{i=1}^{n} \) from the joint distribution \( P_{XX'Z} \), we can obtain a plug-in estimate of \( M_{XX'\mid Z} \) using (7): \( \hat{M}_{XX'\mid Z}(\cdot) = \| \hat{F}_{P_{X\mid Z},n,\lambda}(\cdot) - \hat{F}_{P_{X'\mid Z},n,\lambda}(\cdot) \|_{\mathcal{H}_{X}} \). To evaluate this norm, we take the square of it:

\[
\hat{M}_{XX'\mid Z}^{2}(\cdot) = \| \hat{F}_{P_{X\mid Z},n,\lambda}(\cdot) - \hat{F}_{P_{X'\mid Z},n,\lambda}(\cdot) \|_{\mathcal{H}_{X}}^{2} = k_{Z}^{T}(\cdot)W K_{X} W^{T} k_{Z}(\cdot) - 2k_{Z}^{T}(\cdot)W K_{XX'} W^{T} k_{Z}(\cdot) + k_{Z}^{T}(\cdot)W K_{X} W^{T} k_{Z}(\cdot),
\]

where \( [K_{X}]_{ij} := k_{X}(x_{i}, x_{j}) \), \( [K_{X'}]_{ij} := k_{X}(x'_{i}, x'_{j}) \) and \( [K_{XX'}]_{ij} := k_{X}(x_{i}, x'_{j}) \).

Similarly, we can write HSCIC\((X, Y \mid Z) = H_{X,Y\mid Z} \circ Z \) for some \( H_{X,Y\mid Z} : Z \to \mathbb{R} \). Writing \( [K_{Y}]_{ij} := k_{Y}(y_{i}, y_{j}) \), we obtain a closed-form estimate of \( H_{X,Y\mid Z}^{2}(\cdot) \) as follows:

\[
\hat{H}_{X,Y\mid Z}^{2}(\cdot) = k_{Z}^{T}(\cdot)W (K_{X} \odot K_{Y}) W^{T} k_{Z}(\cdot)
- 2k_{Z}^{T}(\cdot)W ((K_{X} W^{T} k_{Z}(\cdot)) \odot (K_{Y} W^{T} k_{Z}(\cdot)))
+ (k_{Z}^{T}(\cdot)W K_{X} W^{T} k_{Z}(\cdot))(k_{Z}^{T}(\cdot)W K_{Y} W^{T} k_{Z}(\cdot)),
\]

where \( \odot \) denotes elementwise multiplication of matrices.

4.3 Experiments

In this section, we carry out simulations to demonstrate the behaviour of the MCMD and HSCIC. In all simulations, we use the Gaussian kernel \( k_{X}(x, x') = k_{y}(x, x') = k_{Z}(x, x') = e^{-\frac{1}{2} \sigma_{X} \| x - x' \|^{2}} \) with hyperparameter \( \sigma_{X} = 0.1 \), and regularisation parameter \( \lambda = 0.01 \).
Figure 3: Behaviour of the HSCIC. We see that HSCIC($X, Y_{\text{noise}}|Z \simeq 0$ (left) and HSCIC($X, Y_{\text{ind}}|Z \simeq 0$ (right) for all $Z$, whereas HSCIC($X, Y_{\text{dep,add}}|Z > 0$, HSCIC($X, Y_{\text{dep,add}}|Z > 0$, HSCIC($X, Y_{\text{dep}}|Z > 0$. In particular, the dependence of $Y_{\text{dep,add}}$ and $Y_{\text{dep}}$, and is represented by larger values of HSCIC($X, Y_{\text{dep,add}}|Z$ and HSCIC($X, Y_{\text{dep}}|Z)$ compared to HSCIC($X, Y_{\text{dep}}|Z$ and HSCIC($X, Y_{\text{dep,add}}|Z$).

In Figure 2, we simulate 500 samples from $Z \sim N(0, 1)$, $X = X_{\text{same}} = e^{-0.5Z^2 \sin(2Z)} + N_X$ and $X_{\text{diff}} = Z + N_X$, where $N_X \sim 0.3N(0, 1)$ is the (additive) noise variable. The first plot shows simulated data, the second MCMC values against $Z$, and the heatmaps show the (unnormalised) conditional witness function, whose norm gives the MCMC.

In Figure 3, on the left, we simulate 500 samples from the additive noise model, $Z \sim N(0, 1)$, $X = e^{-0.5Z^2 \sin(2Z)} + N_X$, $Y_{\text{noise}} = N_Y$, $Y_{\text{dep,add}} = e^{-0.5Z^2 \sin(2Z)} + N_X + 0.2X$ and $Y_{\text{dep}} = e^{-0.5Z^2 \sin(2Z)} + N_X + 0.4X$, where $N_X \sim 0.3N(0, 1)$ is the (additive) noise variable. On the right, we simulate 500 samples from the multiplicative noise model, $Z \sim N(0, 1)$, $X = Y_{\text{ind}} = e^{-0.5Z^2 \sin(2Z)}N_X$, $Y_{\text{dep}} = e^{-0.5Z^2 \sin(2Z)}N_Y + 0.2X$ and $Y_{\text{dep}} = e^{-0.5Z^2 \sin(2Z)}N_Y + 0.4X$, where $N_X, N_Y \sim 0.3N(0, 1)$ are the (multiplicative) noise variables.

5 Conclusion

In this paper, we introduced a new definition of kernel conditional mean embedding, based on Bochner conditional expectation. It is mathematically elegant and measure-theoretically rigorous, and unlike the previous operator-based definition, does not rely on stringent assumptions that are often violated in common situations. Using this new approach for CMEs, we extended the notions of the MMD, witness function and HSIC to the conditional case. Finally, we discussed how to obtain empirical estimates via natural vector-valued regression, and established universal consistency with convergence rates of $O(n^{-1/2})$ under mild and intuitive assumptions. We believe that our new definition has the potential to unlock the powerful arsenal of kernel mean embeddings to the conditional setting, in a more convenient and rigorous manner than the previous approaches.

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A Generalised Jensen’s Inequality

In Section 4, we require a version of Jensen’s inequality generalised to (possibly) infinite-dimensional vector spaces, because our random variable takes values in $\mathcal{H}_X$, and our convex function is $\|\cdot\|^2_{\mathcal{H}_X} : \mathcal{H}_X \to \mathbb{R}$. Note that this square norm function is indeed convex, since, for any $t \in [0,1]$ and any pair $f,g \in \mathcal{H}_X$,

$$
\|tf + (1-t)g\|^2_{\mathcal{H}_X} \leq (t\|f\|_{\mathcal{H}_X} + (1-t)\|g\|_{\mathcal{H}_X})^2 \quad \text{by the triangle inequality}
$$

$$
\leq t\|f\|^2_{\mathcal{H}_X} + (1-t)\|g\|^2_{\mathcal{H}_X}, \quad \text{by the convexity of } x \mapsto x^2.
$$

The following theorem generalises Jensen’s inequality to infinite-dimensional vector spaces.

**Theorem A.1** (Generalised Jensen’s Inequality, (Perlman, 1974), Theorem 3.10). Suppose $\mathcal{T}$ is a real Hausdorff locally convex (possibly infinite-dimensional) linear topological space, and let $C$ be a closed convex subset of $\mathcal{T}$. Suppose $(\Omega, \mathcal{F}, P)$ is a probability space, and $V : \Omega \to \mathbb{R}$ a Pettis-integrable random variable such that $V(\Omega) \subseteq C$. Let $f : C \to [-\infty, \infty)$ be a convex, lower semi-continuous extended-real-valued function such that $\mathbb{E}_V[f(V)]$ exists. Then

$$
f(\mathbb{E}_V[V]) \leq \mathbb{E}_V[f(V)].
$$

We will actually apply generalised Jensen’s inequality with conditional expectations, so we need the following theorem.

**Theorem A.2** (Generalised Conditional Jensen’s Inequality). Suppose $\mathcal{T}$ is a real Hausdorff locally convex (possibly infinite-dimensional) linear topological space, and let $C$ be a closed convex subset of $\mathcal{T}$. Suppose $(\Omega, \mathcal{F}, P)$ is a probability space, and $V : \Omega \to \mathcal{X}$ a Pettis-integrable random variable such that $V(\Omega) \subseteq C$. Let $f : C \to [-\infty, \infty)$ be a convex, lower semi-continuous extended-real-valued function such that $\mathbb{E}_V[f(V)]$ exists. Suppose $\mathcal{E}$ is a sub-$\sigma$-algebra of $\mathcal{F}$. Then

$$
f(\mathbb{E}[V \mid \mathcal{E}]) \leq \mathbb{E}[f(V) \mid \mathcal{E}].
$$

**Proof.** Let $\mathcal{T}^*$ be the dual space of all real-valued continuous linear functionals on $\mathcal{T}$. The first part of the proof of Perlman (1974, Theorem 3.6) tells us that, for all $v \in \mathcal{T}$, we can write

$$
f(v) = \sup \{ m(v) \mid m \text{ affine, } m \leq f \text{ on } C \},
$$

where an affine function $m$ on $\mathcal{T}$ is of the form $m(v) = v^*(v) + \alpha$ for some $v^* \in \mathcal{T}^*$ and $\alpha \in \mathbb{R}$. If we define the subset $Q$ of $\mathcal{T}^* \times \mathbb{R}$ as

$$
Q := \{(v^*, \alpha) : v^* \in \mathcal{T}^*, \alpha \in \mathbb{R}, v^*(v) + \alpha \leq f(v) \text{ for all } v \in \mathcal{T}\},
$$

then we can rewrite $f$ as

$$
f(v) = \sup_{(v^*, \alpha) \in Q} \{ v^*(v) + \alpha \}, \quad \text{for all } v \in \mathcal{T}. \quad (9)
$$

See that, for any $(v^*, \alpha) \in Q$, we have

$$
\mathbb{E}[f(V) \mid \mathcal{E}] \geq \mathbb{E}[v^*(V) + \alpha \mid \mathcal{E}] \quad \text{almost surely, by assumption (*)}
$$

$$
= \mathbb{E}[v^*(V) \mid \mathcal{E}] + \alpha \quad \text{almost surely, by linearity (**).}
$$

Here, (*) and (**) use the properties of conditional expectation of vector-valued random variables given in Dinculeanu (2000, pp.45-46, Properties 43 and 40 respectively).

We want to show that $\mathbb{E}[v^*(V) \mid \mathcal{E}] = v^* \left( \mathbb{E}[V \mid \mathcal{E}] \right)$ almost surely, and in order to so, we show that the right-hand side is a version of the left-hand side. The right-hand side is clearly $\mathcal{E}$-measurable, since we have a
linear operator on an $\mathcal{E}$-measurable random variable. Moreover, for any $A \in \mathcal{E}$,

$$
\int_A v^* \left( \mathbb{E} \left[ V \mid \mathcal{E} \right] \right) dP = v^* \left( \int_A \mathbb{E} \left[ V \mid \mathcal{E} \right] dP \right)
$$

by Cohn (2013, p.403, Proposition E.11)

$$
= v^* \left( \int_A V dP \right)
$$

by the definition of conditional expectation

$$
= \int_A v^* (V) dP
$$

by Cohn (2013, p.403, Proposition E.11)

(here, all the equalities are almost-sure equalities). Hence, by the definition of the conditional expectation, we have that $\mathbb{E} \left[ v^*(V) \mid \mathcal{E} \right] = v^* \left( \mathbb{E} \left[ V \mid \mathcal{E} \right] \right)$ almost surely. Going back to our above work, this means that

$$
\mathbb{E} \left[ f(V) \mid \mathcal{E} \right] \geq v^* \left( \mathbb{E} \left[ V \mid \mathcal{E} \right] \right) + \alpha.
$$

Now take the supremum of the right-hand side over $Q$. Then (9) tells us that

$$
\mathbb{E} \left[ f(V) \mid \mathcal{E} \right] \geq f \left( \mathbb{E} \left[ V \mid \mathcal{E} \right] \right),
$$

as required.

In the context of Section 4, $\mathcal{H}_X$ is real and Hausdorff, and locally convex (because it is a normed space). We take the closed convex subset to be the whole space $\mathcal{H}_X$ itself. The function $\|\cdot\|_{2,\mathcal{H}_X} : \mathcal{H}_X \to \mathbb{R}$ is convex (as shown above) and continuous, and finally, since Bochner-integrability implies Pettis integrability, all the conditions of Theorem A.2 are satisfied.

## B Generalisation Error Bounds

Caponnetto and De Vito (2006) give an optimal rate of convergence of vector-valued RKHS regression estimators, and its results are quoted by Grünewälder et al. (2012) as the state of the art convergence rates, $O\left(\frac{\log n}{n}\right)$. In particular, this implies that the learning algorithm is consistent. However, the lower rate uses an assumption that the output space is a finite-dimensional Hilbert space (Caponnetto and De Vito, 2006, Theorem 2); and in our case, this will mean that $\mathcal{H}_X$ is finite-dimensional. This is not true if, for example, we take $k_X$ to be the Gaussian kernel; indeed, this is noted as a limitation by Grünewälder et al. (2012), stating that “It is likely that this (finite-dimension) assumption can be weakened, but this requires a deeper analysis”. In this paper, we do not want to restrict our attention to finite-dimensional $\mathcal{H}_X$. The upper bound would have been sufficient to guarantee consistency, but an assumption used in the upper bound requires the operator $l_{XZ,z} : \mathcal{H}_X \to \mathcal{G}_{XZ}$ defined by

$$
l_{XZ,z}(f)(z') = l_{XZ}(z,z')(f)
$$

to be Hilbert-Schmidt for all $z \in Z$. However, for each $z \in Z$, taking any orthonormal basis $\{\phi_i\}_{i=1}^{\infty}$ of $\mathcal{H}_X$, we see that

$$
\sum_{i=1}^{\infty} \langle l_{XZ,z}(\phi_i), l_{XZ,z}(\phi_i) \rangle_{\mathcal{G}_{XZ}} = \sum_{i=1}^{\infty} \langle k_Z(z,z'), k_Z(z,z') \rangle_{\mathcal{H}_X} = \sum_{i=1}^{\infty} \langle k_Z(z,z), \phi_i, \phi_i \rangle_{\mathcal{H}_X} = k_Z(z,z) \sum_{i=1}^{\infty} 1 = \infty,
$$

as required. \qed
meaning this assumption is not fulfilled with our choice of kernel either. Hence, results in Caponetto and De Vito (2006), used by Grünewälder et al. (2012), are not applicable to guarantee consistency in our context.

Kadri et al. (2016) address the problem of generalisability of function-valued learning algorithms. Let us write

$$D := \{(x_1, z_1), \ldots, (x_n, z_n)\}$$

for our training set of size \(n\) drawn i.i.d. from the distribution \(P_{XZ}\), and we denote by \(D^i = D \setminus (x_i, z_i)\) the set \(D\) from which the data point \((x_i, z_i)\) is removed. Further, we denote by \(F_{P_{X|Z}, D} = \hat{F}_{P_{X|Z}, n, \lambda}\) the estimate produced by our learning algorithm from the dataset \(D\) by minimising the loss \(\hat{\mathcal{E}}_{X|Z, n, \lambda}(F) = \sum_{i=1}^n \|k_X(x_i, \cdot) - F(z_i)\|_{H_X}^2 + \lambda\|F\|_{G_{XZ}}^2\)

The assumptions used in this paper, with notations translated to our context, are

1. There exists \(\kappa_1 > 0\) such that for all \(z \in Z\),
   $$\|l_{XZ}(z, z)\|_{\text{op}} = \sup_{f \in H_X} \frac{\|l_{XZ}(z, z)(f)\|_{H_X}}{\|f\|_{H_X}} \leq \kappa_1^2.$$

2. The real function \(Z \times Z \to \mathbb{R}\) defined by
   $$(z_1, z_2) \mapsto (l_{XZ}(z_1, z_2)f_1, f_2)_{H_X}$$
   is measurable for all \(f_1, f_2 \in H_X\).

3. The map \((f, F, z) \mapsto \|f - F(z)\|_{H_X}^2\) is \(\tau\)-admissible, i.e. convex with respect to \(F\) and Lipschitz continuous with respect to \(F(z)\), with \(\tau\) as its Lipschitz constant.

4. There exists \(\kappa_2 > 0\) such that for all \((z, f) \in Z \times H_X\) and any training set \(D\),
   $$\|f - \hat{F}_{P_{X|Z}, D}(z)\|_{H_X}^2 \leq \kappa_2.$$

The concept of uniform stability, with notations translated to our context, is defined as follows.

**Definition B.1** (Uniform algorithmic stability, Kadri et al. (2016, Definition 6)). For each \(F \in G_{XZ}\), define the function

$$\mathcal{R}(F) : Z \times H_X \to \mathbb{R}$$

$$(z, x) \mapsto \|k_X(x, \cdot) - F(z)\|_{H_X}^2.$$ A learning algorithm that calculates the estimate \(\hat{F}_{P_{X|Z}, D}\) from a training set has uniform stability \(\beta\) with respect to the squared loss if the following holds: for all \(n \geq 1\), all \(i \in \{1, \ldots, n\}\) and any training set \(D\) of size \(n\),

$$\|\mathcal{R}(\hat{F}_{P_{X|Z}, D}) - \mathcal{R}(\hat{F}_{P_{X|Z}, D})\|_{\infty} \leq \beta.$$

The next two theorems are quoted from Kadri et al. (2016).

**Theorem B.2** (Kadri et al. (2016, Theorem 7)). Under assumptions 1, 2 and 3, a learning algorithm that maps a training set \(D\) to the function \(\hat{F}_{P_{X|Z}, D} = \hat{F}_{P_{X|Z}, n, \lambda}\) is \(\beta\)-stable with

$$\beta = \frac{\tau^2 \kappa_1^2}{2\lambda n}.$$ 

**Theorem B.3** (Kadri et al. (2016, Theorem 8)). Let \(D \mapsto \hat{F}_{P_{X|Z}, D} = \hat{F}_{P_{X|Z}, n, \lambda}\) be a learning algorithm with uniform stability \(\beta\), and assume Assumption 4 is satisfied. Then, for all \(n \geq 1\) and any \(0 < \delta < 1\), the following bound holds with probability at least \(1 - \delta\) over the random draw of training samples:

$$\hat{\mathcal{E}}_{X|Z}(\hat{F}_{P_{X|Z}, n, \lambda}) \leq \frac{1}{n} \mathcal{E}_{X|Z, n}(\hat{F}_{P_{X|Z}, n, \lambda}) + 2\beta + (4n\beta + \kappa_2)\sqrt{\frac{\ln \frac{1}{\delta}}{2n}}.$$
Theorems B.2 and B.3 give us results about the generalisability of our learning algorithm. It remains to check whether the assumptions are satisfied.

Assumption 2 is satisfied thanks to our assumption that point embeddings are measurable functions, and Assumption 1 is satisfied if we assume that \( k_Z \) is a bounded kernel (i.e. there exists \( B_Z > 0 \) such that \( k_Z(z_1, z_2) \leq B_Z \) for all \( z_1, z_2 \in Z \)), because

\[
\|l_{XZ}(z, z)\|_{op} = \sup_{f \in \mathcal{H}_X, \|f\|_{\mathcal{H}_X} = 1} \|k_Z(z, z)(f)\|_{\mathcal{H}_X} \leq B_Z.
\]

In Kadri et al. (2016), a general loss function is used rather than the squared loss, and it is noted that Assumption 3 is in general not satisfied with the squared loss, which is what we use in our context. However, this issue can be addressed if we restrict the output space to a bounded subset. In fact, the only elements in \( \mathcal{H}_X \) that appear as the output samples in our case are \( k_X(x, \cdot) \) for \( x \in X \), so if we place the assumption that \( k_X \) is a bounded kernel (i.e. there exists \( B_X > 0 \) such that \( k_X(x_1, x_2) \leq B_X \) for all \( x_1, x_2 \in X \)), then

\[
\|k_X(x, \cdot)\|_{\mathcal{H}_X} = \sqrt{k_X(x, x)} \quad \text{by the reproducing property}
\]

\[
\leq \sqrt{B_X}.
\]

So it is no problem, in our case, to place this boundedness assumption. Kadri et al. (2016) tell us that Assumption 1 with this boundedness assumption imply Assumptions 3 and 4, thereby satisfying all the required assumptions.

C Proofs

Lemma 2.1. For each \( f \in \mathcal{H}_X \), \( \int_X f(x) dP_X(x) = \langle f, \mu_{P_X} \rangle_{\mathcal{H}_X} \).

Proof. Let \( L_P \) be a functional on \( \mathcal{H} \) defined by \( L_P(f) := \int_X f(x) dP(x) \). Then \( L_P \) is clearly linear, and moreover,

\[
|L_P(f)| = \left| \int_X f(x) dP(x) \right| \\
= \left| \int_X \langle f, k(x, \cdot) \rangle_{\mathcal{H}} dP(x) \right| \quad \text{by the reproducing property} \\
\leq \int_X |\langle f, k(x, \cdot) \rangle_{\mathcal{H}}| dP(x) \quad \text{by Jensen's inequality} \\
\leq \|f\|_{\mathcal{H}} \int_X \|k(x, \cdot)\|_{\mathcal{H}} dP(x) \quad \text{by Cauchy-Schwarz inequality}.
\]

Since the map \( x \mapsto k(x, \cdot) \) is Bochner \( P \)-integrable, \( L_P \) is bounded, i.e. \( L_P \in \mathcal{H}^* \). So by the Riesz Representation Theorem, there exists a unique \( h \in \mathcal{H} \) such that \( L_P(f) = \langle f, h \rangle_{\mathcal{H}} \) for all \( f \in \mathcal{H} \).

Choose \( f(\cdot) = k(x, \cdot) \) for some \( x \in X \). Then

\[
h(x) = \langle k(x, \cdot), h \rangle_{\mathcal{H}} \\
= L_P(k(x, \cdot)) \\
= \int_X k(x', x) dP(x'),
\]

which means \( h(\cdot) = \int_X k(x, \cdot) dP(x) = \mu_P(\cdot) \) (implicitly applying Dinculeanu (2000, Corollary 37)).

Lemma 2.3. For \( f \in \mathcal{H}_X \), \( g \in \mathcal{H}_Y \), \( \langle f \otimes g, \mu_{P_{XY}} \rangle_{\mathcal{H}_X \otimes \mathcal{H}_Y} = \mathbb{E}_{XY} [f(X)g(Y)] \).
Proof. For Bochner integrability, we see that

\[
E_{XY} \left[ \left\| k_X(X, \cdot) \otimes k_Y(Y, \cdot) \right\|_{H_X \otimes H_Y} \right] = E_{XY} \left[ \sqrt{\left( k_X(X,X) \right) \left( k_Y(Y,Y) \right)} \right] \\
\leq \sqrt{E_X \left[ k_X(X,X) \right]} \sqrt{E_Y \left[ k_Y(Y,Y) \right]},
\]

by Cauchy-Schwarz inequality. (1) now implies that \( k_X(X, \cdot) \otimes k_Y(Y, \cdot) \) is Bochner \( P_{XY} \)-integrable.

Let \( L_{P_{XY}} \) be a functional on \( H_X \otimes H_Y \) defined by \( L_{P_{XY}} \left( \sum_i f_i \otimes g_i \right) := E_{XY} \left[ \sum_i f_i(x)g_i(y) \right] \). Then \( L_{P_{XY}} \) is clearly linear, and moreover,

\[
\left| L_{P_{XY}} \left( \sum_i f_i \otimes g_i \right) \right| = \left| E_{XY} \left[ \sum_i f_i(x)g_i(y) \right] \right| \\
\leq E_{XY} \left[ \left| \sum_i f_i(x)g_i(y) \right| \right] \text{ by Jensen’s inequality} \\
= E_{XY} \left[ \left( \sum_i f_i \otimes g_i, k_X(X, \cdot) \otimes k_Y(Y, \cdot) \right)_{H_X \otimes H_Y} \right] \text{ by the reproducing property} \\
\leq \left\| \sum_i f_i \otimes g_i \right\|_{H_X \otimes H_Y} E_{XY} \left[ \left\| k_X(X, \cdot) \otimes k_Y(Y, \cdot) \right\|_{H_X \otimes H_Y} \right] \text{ by Cauchy-Schwarz inequality.}
\]

Hence, by Bochner integrability shown above, \( L_{P_{XY}} \in (H_X \otimes H_Y)^* \). So by the Riesz Representation Theorem, there exists \( h \in H_X \otimes H_Y \) such that \( L_{P_{XY}} \left( \sum_i f_i \otimes g_i \right) = \left( \sum_i f_i \otimes g_i, h \right)_{H_X \otimes H_Y} \) for all \( \sum_i f_i \otimes g_i \in H_X \otimes H_Y \).

Choose \( k_X(x, \cdot) \otimes k_Y(y, \cdot) \in H_X \otimes H_Y \) for some \( x \in \mathcal{X} \) and \( y \in \mathcal{Y} \). Then

\[
h(x,y) = \langle k_X(x, \cdot) \otimes k_Y(y, \cdot), h \rangle_{H_X \otimes H_Y} \text{ by the reproducing property} \\
= L_{P_{XY}} \left( k_X(x, \cdot) \otimes k_Y(y, \cdot) \right) \\
= E_{XY} \left[ k_X(X,x) \otimes k_Y(Y,y) \right] \\
= \mu_{P_{XY}}(x,y),
\]

as required. \( \square \)

Before we prove Theorem 2.9, we state the following definition and theorems related to measurable functions for Banach-space valued functions.

**Definition C.1** (Dinculeanu (2000, p.4, Definition 5)). A function \( H : \Omega \rightarrow \mathcal{H} \) is called an \( \mathcal{F} \)-simple function if it has the form \( H = \sum_{i=1}^H h_i1_{B_i} \), for some \( h_i \in \mathcal{H} \) and \( B_i \in \mathcal{F} \).

A function \( H : \Omega \rightarrow \mathcal{H} \) is said to be \( \mathcal{F} \)-measurable if there is a sequence \( (H_n) \) of \( \mathcal{H} \)-valued, \( \mathcal{F} \)-simple functions such that \( H_n \rightarrow H \) pointwise.

**Theorem C.2** (Dinculeanu (2000, p.4, Theorem 6)). If \( H : \Omega \rightarrow \mathcal{H} \) is \( \mathcal{F} \)-measurable, then there is a sequence \( (H_n) \) of \( \mathcal{H} \)-valued, \( \mathcal{F} \)-simple functions such that \( H_n \rightarrow H \) pointwise and \( |H_n| \leq |H| \) for every \( n \).

**Theorem C.3** (Dinculeanu (2000, p.19, Theorem 48), Lebesgue Convergence Theorem). Let \( (H_n) \) be a sequence in \( L^1_H(P) \), \( H : \Omega \rightarrow \mathcal{H} \) a \( P \)-measurable function, and \( g \in L^1_P \) such that \( H_n \rightarrow H \) \( P \)-almost everywhere and \( |H_n| \leq g \), \( P \)-almost everywhere, for each \( n \). Then \( H \in L^1_H(P) \) and \( H_n \rightarrow H \) in \( L^1_H(P) \), i.e. \( \int_{\Omega} H_n dP \rightarrow \int_{\Omega} H dP \).

**Theorem 2.9.** Suppose that \( P(\cdot \mid \mathcal{E}) \) admits a regular version \( Q \). Then \( QH : \Omega \rightarrow \mathcal{H} \) with \( \omega \mapsto Q_\omega H = \int_{\Omega} H(\omega')Q_\omega(d\omega') \) is a version of \( E[H \mid \mathcal{E}] \) for every Bochner \( P \)-integrable \( H \).

**Proof.** Suppose \( H \) is Bochner \( P \)-integrable. Since \( Q \) is a regular version of \( P(\cdot \mid \mathcal{E}) \), it is a probability transition kernel from \( (\Omega, \mathcal{E}) \) to \( (\Omega, \mathcal{F}) \).

We first show that \( QH \) is measurable with respect to \( \mathcal{E} \). The map \( Q : \Omega \rightarrow \mathcal{H} \) is well-defined, since, for each \( \omega \in \Omega \), \( Q_\omega H \) is the Bochner-integral of \( H \) with respect to the measure \( B \rightarrow Q_\omega(B) \). Since \( H \) is
We have $A_{2.9}$, the event $B$ holds has probability 1. Further, if we fix $f \in \mathcal{H}_X$, then by Theorem 2.9 (or by directly applying Cubilas (2011, p.150, Theorem 2.5)), the event $A_2 \in \mathcal{F}$ on which

$$
\int_X f(x) P_{X|Z}(\omega)(dx) = \int_{\Omega} f(X(\omega'))Q_{\omega}(d\omega') = \mathbb{E}_{X|Z}[f(X) | Z](\omega)
$$
holds also has probability 1. Then $P(A_1 \cap A_2) = 1$, and fixing $\omega \in A_1 \cap A_2$,

$$\langle f, \mu_{P_{X|Z}}(\omega) \rangle_{\mathcal{H}_X} = \langle f, \int_{\Omega} k_X(X(\omega'), \cdot) Q_\omega(d\omega') \rangle_{\mathcal{H}_X} \quad \text{since } \omega \in A_1$$

$$= \langle f, \int_X k_X(x, \cdot) P_{X|Z}(\omega)(dx) \rangle_{\mathcal{H}_X} \quad \text{by the definition of } P_{X|Z}$$

$$= \int_X f(x) P_{X|Z}(\omega)(dx) \quad \text{by Lemma 2.1}$$

$$= \mathbb{E}_{X|Z}[f(X) \mid Z](\omega) \quad \text{since } \omega \in A_2.$$ 

Hence $\langle f, \mu_{P_{X|Z}} \rangle_{\mathcal{H}_X} = \mathbb{E}_{X|Z}[f(X) \mid Z]$ almost surely.

\begin{lemma}
Suppose that the conditional probability $P(\cdot \mid Z)$ admits a regular version. Then for each pair $f \in \mathcal{H}_X$ and $g \in \mathcal{H}_Y$, $(f \otimes g, \mu_{P_{X|Y,Z}})_{\mathcal{H}_X \otimes \mathcal{H}_Y} = \mathbb{E}_{X|Y}[f(X)g(Y) \mid Z]$ almost surely.

\begin{proof}
Write $Q$ for a regular version of $P(\cdot \mid Z)$. Then in particular, $P_{X|Y,Z}$ defined by $P_{X|Y,Z}(\omega)(B) = Q_\omega((X,Y) \in B)$ for any measurable set $B \subseteq \mathcal{X} \times \mathcal{Y}$ is a version of the conditional distribution of $(X,Y)$ given $Z$. Then by Theorem 2.9, the event $A_1 \in \mathcal{F}$ on which

$$\mu_{P_{X|Y,Z}}(\omega) := \mathbb{E}_{X|Y}[k_X(X, \cdot) \otimes k_Y(Y, \cdot) \mid Z](\omega) = \int_{\Omega} k_X(X(\omega'), \cdot) \otimes k_Y(Y(\omega'), \cdot) Q_\omega(d\omega')$$

holds has probability 1. Further, if we fix $f \in \mathcal{H}_X$ and $g \in \mathcal{H}_Y$, then by Theorem 2.9 (or by directly applying Čınlar (2011, p.150, Theorem 2.5)), the event $A_2 \in \mathcal{F}$ on which

$$\int_{\mathcal{X} \times \mathcal{Y}} f(x) g(y) P_{X|Y,Z}(d(x,y)) = \int_{\Omega} f(X(\omega')) g(Y(\omega')) Q_\omega(d\omega') = \mathbb{E}_{X|Y}[f(X)g(Y) \mid Z]$$

holds has probability 1. Then $P(A_1 \cap A_2) = 1$, and fixing $\omega \in A_1 \cap A_2$,

$$\langle f \otimes g, \mu_{P_{X|Y,Z}}(\omega) \rangle_{\mathcal{H}_X \otimes \mathcal{H}_Y} = \langle f \otimes g, \int_{\Omega} k_X(X(\omega'), \cdot) \otimes k_Y(Y(\omega'), \cdot) Q_\omega(d\omega') \rangle_{\mathcal{H}_X \otimes \mathcal{H}_Y} \quad \text{since } \omega \in A_1$$

$$= \langle f \otimes g, \int_{\mathcal{X} \times \mathcal{Y}} k_X(x, \cdot) \otimes k_Y(y, \cdot) P_{X|Y,Z}(\omega)(d(x,y)) \rangle_{\mathcal{H}_X \otimes \mathcal{H}_Y} \quad \text{by the definition of } P_{X|Y,Z}$$

$$= \int_{\mathcal{X} \times \mathcal{Y}} f(X) g(Y) P_{X|Y,Z}(\omega)(d(x,y)) \quad \text{by Lemma 2.3}$$

$$= \mathbb{E}_{X|Y}[f(X)g(Y) \mid Z](\omega) \quad \text{since } \omega \in A_2.$$ 

Hence $\langle f \otimes g, \mu_{P_{X|Y,Z}} \rangle_{\mathcal{H}_X \otimes \mathcal{H}_Y} = \mathbb{E}_{X|Y}[f(X)g(Y) \mid Z]$ almost surely.
\end{proof}
\end{lemma}

\begin{theorem}
Suppose $k_X$ is a characteristic kernel, and assume that $P(\cdot \mid Z)$ admits a regular version. Then $\text{MCMD}(X, X' \mid Z) = 0$ almost surely if and only if, almost surely, $P_{X|Z}(B \mid Z) = P_{X'|Z}(B \mid Z)$ for all $B \in \mathcal{X}$.

\begin{proof}
Write $Q$ for a regular version of $P(\cdot \mid Z)$, and assume without loss of generality that the conditional distributions $P_{X|Z}$ and $P_{X'|Z}$ are given by $P_{X|Z}(\omega)(B) = Q_\omega(X \in B)$ and $P_{X'|Z}(\omega)(B) = Q_\omega(X' \in B)$ for $B \in \mathcal{X}$. By Theorem 2.9, there exists an event $A_1 \in \mathcal{F}$ with $P(A_1) = 1$ such that for all $\omega \in A_1$,

$$\mu_{P_{X|Z}}(\omega) := \mathbb{E}_{X|Z}[k_X(X, \cdot) \mid Z](\omega) = \int_{\Omega} k_X(X(\omega'), \cdot) Q_\omega(d\omega') = \int_X k_X(x, \cdot) P_{X|Z}(\omega)(dx),$$

and an event $A_2 \in \mathcal{F}$ with $P(A_2) = 1$ such that for all $\omega \in A_2$,

$$\mu_{P_{X'|Z}}(\omega) := \mathbb{E}_{X'|Z}[k_X(X', \cdot) \mid Z](\omega) = \int_{\Omega} k_X(X'(\omega'), \cdot) Q_\omega(d\omega') = \int_X k_X(x', \cdot) P_{X'|Z}(\omega)(dx').$$

This means that, for each $\omega \in A_1$, $\mu_{P_{X|Z}}(\omega)$ is the mean embedding of $P_{X|Z}(\omega)$, and for each $\omega \in A_2$, $\mu_{P_{X'|Z}}(\omega)$ is the mean embedding of $P_{X'|Z}(\omega)$.

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(⇒) Suppose first that MCMD\(\mathbb{X}, \mathbb{X}' \mid Z\) = \(\|\mu_{P_{X|Z}} - \mu_{P_{X'|Z}}\|_{\mathcal{H}} = 0\) almost surely, i.e., there exists \(A \in \mathcal{F}\) with \(P(A) = 1\) such that for all \(\omega \in A\), \(\|\mu_{P_{X|Z}}(\omega) - \mu_{P_{X'|Z}}(\omega)\|_{\mathcal{H}} = 0\). Then for any \(\omega \in A \cap A_1 \cap A_2\), since the kernel \(k_X\) is characteristic, our work above tells us that \(P_{X|Z}(\omega)\) and \(P_{X'|Z}(\omega)\) are the same distribution, i.e., for any \(B \in \mathbb{X}\), \(P_{X|Z}(\omega)(B) = P_{X'|Z}(\omega)(B)\). By countable intersection, we have \(P(A \cap A_1 \cap A_2) = 1\), so almost surely,
\[
P_{X|Z}(B) = P_{X'|Z}(B)
\]
for all \(B \in \mathbb{X}\).

(⇐) Now assume there exists \(A \in \mathcal{F}\) with \(P(A) = 1\) such that for each \(\omega \in A\), \(P_{X|Z}(\omega)(B) = P_{X'|Z}(\omega)(B)\) for all \(B \in \mathbb{X}\). Then for all \(\omega \in A \cap A_1 \cap A_2\),
\[
\begin{align*}
\|\mu_{P_{X|Z}}(\omega) - \mu_{P_{X'|Z}}(\omega)\|_{\mathcal{H}} &= \left\| \int_X k_X(x, \cdot)P_{X|Z}(\omega)(dx) - \int_X k_X(x', \cdot)P_{X'|Z}(\omega)(dx') \right\|_{\mathcal{H}} \\
&= \left\| \int_X k_X(x, \cdot)P_{X|Z}(\omega)(dx) - \int_X k_X(x', \cdot)P_{X'|Z}(\omega)(dx') \right\|_{\mathcal{H}} \\
&= 0,
\end{align*}
\]
and since \(P(A \cap A_1 \cap A_2) = 1\), \(\|\mu_{P_{X|Z}} - \mu_{P_{X'|Z}}\|_{\mathcal{H}} = 0\) almost surely.

\[\square\]

**Theorem 4.1.** Let \(Z\) be a random variable taking values in some measurable space \((\mathbb{Z}, \mathcal{Z})\), and let \(\mathcal{T}\) be a Hausdorff topological space, with its Borel \(\sigma\)-algebra \(\mathcal{B}(\mathcal{T})\). A mapping \(V : \Omega \to \mathcal{T}\) is measurable with respect to \(\sigma(Z)\) and \(\mathcal{B}(\mathcal{T})\) if and only if
\[
V = F \circ Z
\]
for some deterministic function \(F : \mathbb{Z} \to \mathcal{T}\), measurable with respect to \(\mathcal{Z}\) and \(\mathcal{B}(\mathcal{T})\).

**Proof.** (⇐) Suppose \(V = F \circ Z\) for some deterministic function \(F : \mathbb{Z} \to \mathcal{T}\), measurable with respect to \(\mathcal{Z}\) and \(\mathcal{B}(\mathcal{T})\). Since \(Z : \Omega \to \mathbb{Z}\) is measurable with respect to \(\sigma(Z)\) and \(\mathcal{Z}\), and since compositions of measurable functions are measurable ([Cınlar, 2011], page 7, Proposition 2.5), \(V\) is measurable with respect to \(\sigma(Z)\) and \(\mathcal{B}(\mathcal{T})\).

(⇒) Now suppose \(V : \Omega \to \mathcal{T}\) is \(\sigma(Z)\)-measurable. We want to define a function \(F : \mathbb{Z} \to \mathcal{T}\), measurable with respect to \(\mathcal{Z}\) and \(\mathcal{B}(\mathcal{T})\), such that \(V = F \circ Z\).

We can assume that, for every \(z \in \mathbb{Z}\), \(z = Z(\omega)\) for some \(\omega \in \Omega\); indeed, if not, then restrict the space \((\mathbb{Z}, \mathcal{Z})\) to the image \(Z(\Omega)\). Then for a given \(z \in \mathbb{Z}\), \(Z^{-1}(z) \subseteq \Omega\). Suppose for contradiction that there are two distinct elements \(\omega_1, \omega_2 \in Z^{-1}(z)\) such that \(V(\omega_1) \neq V(\omega_2)\). Since \(T\) is Hausdorff, there are disjoint open neighbourhoods \(N_1\) and \(N_2\) of \(V(\omega_1)\) and \(V(\omega_2)\) respectively. By definition of a Borel \(\sigma\)-algebra, we have \(N_1, N_2 \in \mathcal{B}(\mathcal{T})\), and since \(V\) is \(\sigma(Z)\)-measurable,
\[
V^{-1}(N_1), V^{-1}(N_2) \in \sigma(Z),
\]
Furthermore, \(V^{-1}(N_1)\) and \(V^{-1}(N_2)\) are neighbourhoods of \(\omega_1\) and \(\omega_2\) respectively, and are disjoint.

(i) For any \(B \in \mathcal{Z}\) with \(z \in B\), since \(Z(\omega_1) = z = Z(\omega_2)\), we have \(\omega_1, \omega_2 \in Z^{-1}(B)\). So \(Z^{-1}(B) \neq V^{-1}(N_1)\) and \(Z^{-1}(B) \neq V^{-1}(N_2)\), as \(\omega_2 \notin V^{-1}(N_1)\) and \(\omega_1 \notin V^{-1}(N_2)\).

(ii) For any \(B \in \mathcal{Z}\) with \(z \notin B\), we have \(\omega_1 \notin Z^{-1}(B)\) and \(\omega_2 \notin Z^{-1}(B)\). So \(Z^{-1}(B) \neq V^{-1}(N_1)\) and \(Z^{-1}(B) \neq V^{-1}(N_2)\).
Moreover, it is almost surely unique, i.e. it is almost surely equal to any other minimiser of the objective $F$.

Recall that we have $E\sigma(Z) \in L^2(Z, P_Z; \mathcal{H}_X)$ minimises both $\hat{E}_{X|Z}$ and $E_{X|Z}$, i.e.

$$F_{P_{X|Z}} = \arg\min_{F \in L^2(Z, P_Z; \mathcal{H}_X)} E_{X|Z}(F) = \arg\min_{F \in L^2(Z, P_Z; \mathcal{H}_X)} \hat{E}_{X|Z}(F).$$

Moreover, it is almost surely unique, i.e. it is almost surely equal to any other minimiser of the objective functionals.

**Proof.** Recall that we have

$$E_{X|Z}(F) := E_Z \left[ \|F_{P_{X|Z}}(Z) - F(Z)\|_{\mathcal{H}_X}^2 \right].$$

So clearly, $E_{X|Z}(F_{P_{X|Z}}) = 0$, meaning $F_{P_{X|Z}}$ minimises $E_{X|Z}$ in $L^2(Z, P_Z; \mathcal{H}_X)$. So it only remains to show that $\hat{E}_{X|Z}$ is minimised in $L^2(Z, P_Z; \mathcal{H}_X)$ by $F_{P_{X|Z}}$.

Let $F$ be any element in $L^2(Z, P_Z; \mathcal{H}_X)$. Then we have

$$\hat{E}_{X|Z}(F) - \hat{E}_{X|Z}(F_{P_{X|Z}}) = E_{X, Z} \left[ \|k_X(X, \cdot) - F(Z)\|_{\mathcal{H}_X}^2 \right] - E_{X, Z} \left[ \|k_X(X, \cdot) - F_{P_{X|Z}}(Z)\|_{\mathcal{H}_X}^2 \right]$$

$$= E_Z \left[ \|F(Z)\|_{\mathcal{H}_X}^2 \right] - 2 E_{X, Z} \left[ \langle k_X(X, \cdot), F(Z) \rangle_{\mathcal{H}_X} \right]$$

$$+ 2 E_{X, Z} \left[ \langle k_X(X, \cdot), F_{P_{X|Z}}(Z) \rangle_{\mathcal{H}_X} \right] - E_Z \left[ \|F_{P_{X|Z}}(Z)\|_{\mathcal{H}_X}^2 \right].$$

(11)

Here,

$$E_{X, Z} \left[ \langle k_X(X, \cdot), F(Z) \rangle_{\mathcal{H}_X} \right] = E_Z \left[ E_{X|Z} \left[ F(Z)(X) \mid Z \right] \right]$$

by the reproducing property

$$= E_Z \left[ (F(Z), \mu_{P_{X|Z}})_{\mathcal{H}_X} \right]$$

by Lemma 3.2

$$= E_Z \left[ (F(Z), F_{P_{X|Z}}(Z))_{\mathcal{H}_X} \right]$$

since $\mu_{P_{X|Z}} = F_{P_{X|Z}} \circ Z$ and similarly,

$$E_{X, Z} \left[ \langle k_X(X, \cdot), F_{P_{X|Z}}(Z) \rangle_{\mathcal{H}_X} \right] = E_Z \left[ E_{X|Z} \left[ F_{P_{X|Z}}(Z)(X) \mid Z \right] \right]$$

by the reproducing property

$$= E_Z \left[ (F_{P_{X|Z}}(Z), F_{P_{X|Z}}(Z))_{\mathcal{H}_X} \right]$$

by Lemma 3.2

$$= E_Z \left[ \|F_{P_{X|Z}}(Z)\|_{\mathcal{H}_X}^2 \right].$$

Substituting these expressions back into (11), we have

$$\hat{E}_{X|Z}(F) - \hat{E}_{X|Z}(F_{P_{X|Z}}) = E_Z \left[ \|F(Z)\|_{\mathcal{H}_X}^2 \right] - 2 E_Z \left[ \langle F(Z), F_{P_{X|Z}}(Z) \rangle_{\mathcal{H}_X} \right] + E_Z \left[ \|F_{P_{X|Z}}(Z)\|_{\mathcal{H}_X}^2 \right]$$

$$= E_Z \left[ \|F(Z) - F_{P_{X|Z}}(Z)\|_{\mathcal{H}_X}^2 \right]$$

$$\geq 0.$$
Hence, $F_{P_{X|Z}}$ minimises $\hat{\mathcal{E}}_{X|Z}$ in $L^2(\mathcal{Z}, P_Z; \mathcal{H}_X)$. The minimiser is further more $P_Z$-almost surely unique; indeed, if $F' \in L^2(\mathcal{Z}, P_Z; \mathcal{H}_X)$ is another minimiser of $\hat{\mathcal{E}}_{X|Z}$, then the calculation in (11) shows that

$$\mathbb{E}_Z \left[ \left\| F_{P_{X|Z}}(Z) - F'(Z) \right\|_{\mathcal{H}_X}^2 \right] = 0,$$

which immediately implies that $\left\| F_{P_{X|Z}}(Z) - F'(Z) \right\|_{\mathcal{H}_X} = 0$ $P_Z$-almost surely, which in turn implies that $F_{P_{X|Z}} = F'$ $P_Z$-almost surely.

\textbf{Theorem 4.4.} Suppose $k_X$ and $k_Z$ are bounded kernels, i.e. for all $x_1, x_2 \in \mathcal{X}$, $k_X(x_1, x_2) \leq B_X$ for some $B_X > 0$ and for all $z_1, z_2 \in \mathcal{Z}$, $k_Z(z_1, z_2) \leq B_z$ for some $B_Z > 0$. Then our learning algorithm that produces $\hat{F}_{P_{X|Z}, n, \lambda}$ is universally consistent (in the surrogate loss $\hat{\mathcal{E}}_{X|Z}$), i.e. for any joint distribution $P_{XZ}$ and constants $\epsilon > 0$ and $\delta > 0$,

$$P_{XZ}(\hat{\mathcal{E}}_{X|Z}(\hat{F}_{P_{X|Z}, n, \lambda}) - \hat{\mathcal{E}}_{X|Z}(F_{P_{X|Z}}) > \epsilon) < \delta$$

for large enough $n$. The rate of convergence is $\mathcal{O}(n^{-1/2})$.

\textbf{Proof.} Fix $\epsilon > 0$ and $\delta > 0$. Define $\hat{\mathcal{E}}_{X|Z, n}(F) = \frac{1}{n} \sum_{i=1}^{n} \left\| F(z_i) - k_X(x_i, \cdot) \right\|_{\mathcal{H}_X}^2$ for $F \in \mathcal{G}_{XZ}$, and define the real-valued random variable $\xi$ by

$$\xi := \left\| F_{P_{X|Z}}(Z) - k_X(X, \cdot) \right\|_{\mathcal{H}_X}^2.$$

Then we have

$$\hat{\mathcal{E}}_{X|Z, n}(F_{P_{X|Z}}) := \frac{1}{n} \sum_{i=1}^{n} \left\| F_{P_{X|Z}}(z_i) - k_X(x_i, \cdot) \right\|_{\mathcal{H}_X}^2 = \frac{1}{n} \sum_{i=1}^{n} \xi_i,$$

$$\hat{\mathcal{E}}_{X|Z, n, \lambda}(F_{P_{X|Z}}) = \frac{1}{n} \sum_{i=1}^{n} \left\| F_{P_{X|Z}}(z_i) - k_X(x_i, \cdot) \right\|_{\mathcal{H}_X}^2 + \lambda \left\| F_{P_{X|Z}} \right\|_{\mathcal{G}_{XZ}}^2 = \frac{1}{n} \sum_{i=1}^{n} \xi_i + \lambda \left\| F_{P_{X|Z}} \right\|_{\mathcal{G}_{XZ}}^2,$$

and

$$\hat{\mathcal{E}}_{X|Z}(F_{P_{X|Z}}) = \mathbb{E}_{X, Z} \left[ \left\| F_{P_{X|Z}}(Z) - k_X(X, \cdot) \right\|_{\mathcal{H}_X}^2 \right] = \mathbb{E}_{X, Z}[\xi],$$

where we recalled the definitions of $\hat{\mathcal{E}}_{X|Z, n, \lambda}$ and $\hat{\mathcal{E}}_{X|Z}$ from Section 4. Define $\sigma^2 = \text{Var}(\xi)$ ($\text{Var}(\xi)$ is bounded because $F_{P_{X|Z}} \in L^2(\mathcal{Z}, P_Z; \mathcal{H}_X)$ from Section 4.1 and $k_X$ is bounded by assumption). Then by Chebyshev’s inequality, we have

$$P_{XZ} \left( \left\| \hat{\mathcal{E}}_{X|Z, n}(F_{P_{X|Z}}) - \hat{\mathcal{E}}_{X|Z}(F_{P_{X|Z}}) \right\| \geq \frac{\epsilon}{2} \right) \leq \frac{4\sigma^2}{n\epsilon^2}. \quad (*)$$

Moreover, from Appendix B, we have

$$P_{XZ} \left( \left| \hat{\mathcal{E}}_{X|Z}(\hat{F}_{P_{X|Z}, n, \lambda}) - \hat{\mathcal{E}}_{X|Z, n}(\hat{F}_{P_{X|Z}, n, \lambda}) \right| \geq 2\beta + (4n\beta + \kappa_2) \sqrt{\frac{\ln \frac{2}{\delta}}{2n}} \right) \leq \frac{\delta}{2}, \quad (**)$$

where $\beta = \frac{\epsilon^2 \kappa_1^2}{2mn}$. Hence, if $n$ is large enough to ensure

$$\frac{4\sigma^2}{n\epsilon^2} \leq \frac{\delta}{2}, \quad (\dagger)$$

and

$$2\beta + (4n\beta + \kappa_2) \sqrt{\frac{\ln \frac{2}{\delta}}{2n}} \leq \frac{\epsilon}{2}, \quad (\dagger\dagger)$$

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then
\[ P_{X|Z} \left( \tilde{X} \mid Z(\hat{F}_{P_X|Z,n,\lambda}) - \tilde{X} \mid Z(F_{P_X|Z}) < \epsilon \right) \]
\[ \leq P_{X|Z} \left( \tilde{X} \mid Z(\hat{F}_{P_X|Z,n,\lambda}) - \tilde{X} \mid Z, n(\hat{F}_{P_X|Z,n,\lambda}) > \frac{\epsilon}{2} \right) \]
\[ + P_{X|Z} \left( \tilde{X} \mid Z,n(\hat{F}_{P_X|Z,n,\lambda}) - \tilde{X} \mid Z(F_{P_X|Z}) > \frac{\epsilon}{2} \right) \]
\[ \leq \frac{\delta}{2} + P_{X|Z} \left( \tilde{X} \mid Z,n(\hat{F}_{P_X|Z,n,\lambda}) - \tilde{X} \mid Z(F_{P_X|Z}) > \frac{\epsilon}{2} \right) \]
\[ \leq \frac{\delta}{2} + P_{X|Z} \left( \tilde{X} \mid Z,n,\lambda(\hat{F}_{P_X|Z,n,\lambda}) - \tilde{X} \mid Z, n(\hat{F}_{P_X|Z,n,\lambda}) > \frac{\epsilon}{2} \right) \]
\[ \leq \frac{\delta}{2} + \frac{\delta}{2} \]
\[ = \delta, \]
as required. \qed