Abstract: Conditional mean embeddings (CME) have proven themselves to be a powerful tool in many machine learning applications. They allow the efficient conditioning of probability distributions within the corresponding reproducing kernel Hilbert spaces (RKHSs) by providing a linear-algebraic relation for the kernel mean embeddings of the respective probability distributions. Both centered and uncentered covariance operators have been used to define CMEs in the existing literature. In this paper, we develop a mathematically rigorous theory for both variants, discuss the merits and problems of each, and significantly weaken the conditions for applicability of CMEs. In the course of this, we demonstrate a beautiful connection to Gaussian conditioning in Hilbert spaces.

Keywords: conditional mean embedding, Gaussian measure, reproducing kernel Hilbert space.

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1. Introduction

Reproducing kernel Hilbert spaces (RKHSs) have long been popular tools in machine learning because of the powerful property — often called the “kernel trick” — that many problems posed in terms of the base set $\mathcal{X}$ of the RKHS $\mathcal{H}$ (e.g. classification into two or more classes) become linear-algebraic problems in $\mathcal{H}$ under the embedding of $\mathcal{X}$ into $\mathcal{H}$ induced by the reproducing kernel $k: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. This insight has been used to define the kernel mean embedding (KME; Berlinet and Thomas-Agnan, 2004; Smola et al., 2007) $\mu_X \in \mathcal{H}$ of an $\mathcal{X}$-valued random variable $X$ as the $\mathcal{H}$-valued mean of the embedded random variable $k(X, \cdot)$, and also the conditional mean embedding (CME; Fukumizu et al., 2004, Song et al., 2009), which seeks to perform conditioning of the original random variable $X$ through application of the Gaussian conditioning formula (also known as the Kalman update) to the embedded non-Gaussian random variable $k(X, \cdot)$. This article aims to provide rigorous mathematical foundations for this attractive but apparently naïve approach to conditional probability, and hence to Bayesian inference.

To be more precise, let us fix two RKHSs $\mathcal{H}$ and $\mathcal{G}$ over $\mathcal{X}$ and $\mathcal{Y}$ respectively, with reproducing kernels $k$ and $\ell$ and canonical feature maps $\varphi(x) := k(x, \cdot)$ and $\psi(y) := \ell(y, \cdot)$. Let $X$ and $Y$ be random variables taking values in $\mathcal{X}$ and $\mathcal{Y}$ respectively, and let $\mu_X$, $\mu_Y$, and $\mu_{Y|X=x}$ denote
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Figure 1.1: While conditioning of the probability distributions in the original spaces $X, Y$ is a possibly complicated, non-linear problem, the corresponding formula for their kernel mean embeddings reduces to elementary linear algebra — a common guiding theme when working with reproducing kernel Hilbert spaces.

the kernel mean embeddings (KMEs) of the distributions $P_X$ of $X$, $P_Y$ of $Y$, and $P_{Y|X=x}$ given by

$$
\mu_X := \mathbb{E}[\varphi(X)] \in \mathcal{H}, \quad \mu_Y := \mathbb{E}[\psi(Y)] \in \mathcal{G}, \quad \mu_{Y|X=x} := \mathbb{E}[\psi(Y)|X = x] \in \mathcal{G}.
$$

The **conditional mean embedding** (CME) offers a way to perform conditioning of probability distributions in the corresponding feature spaces $\mathcal{H}$ and $\mathcal{G}$, where it becomes a linear-algebraic transformation (Figure 1.1). Under the assumptions that $\mathbb{E}[g(Y)|X = \cdot]$ is an element of $\mathcal{H}$ and that $C_X$ is invertible, the well-known formula for the CME is given by

$$
\mu_{Y|X=x} = C_{Y|X}C_X^{-1}\varphi(x), \quad x \in X.
$$

(1.1)

Here, $C_X$ and $C_{Y|X}$ denote the kernel covariance and cross-covariance operators defined in (2.3). Note that there are in fact two theories of CMEs, one working with **centred** covariance operators (Fukumizu et al., 2004; Song et al., 2009) and the other with **uncentred** ones (Fukumizu et al., 2013). We will discuss both theories in detail, but let us focus for a moment on the centred case for which the above formula was originally derived (Song et al., 2009, Theorem 4).

In the trivial case where $X$ and $Y$ are independent, the CME should yield $\mu_{Y|X=x} = \mu_Y$. However, independence implies that $C_{XY} = 0$, and so (1.1) yields $\mu_{Y|X=x} = 0$, regardless of $x$. In order to understand what has gone wrong it is helpful to consider in turn the two cases in which the constant function $1_X: x \mapsto 1$ is, or is not, an element of $\mathcal{H}$.

- If $1_X \in \mathcal{H}$, then $C_X$ cannot be injective, since $C_X 1_X = 0$, and (1.1) is not applicable.
- If $1_X \notin \mathcal{H}$ and $X$ and $Y$ are independent, then the assumption $\mathbb{E}[g(Y)|X = x] \in \mathcal{H}$ cannot be fulfilled (except for those special elements $g \in \mathcal{H}$ for which $\mathbb{E}[g(Y)] = 0$ or if $\mathbb{E}[\psi(y, Y)] = 0$ for all $y \in \mathcal{Y}$, respectively).

In summary, (1.1) is never applicable for independent random variables except in certain degenerate cases. Note that this problem does not occur in the case of uncentred operators, where $aC_X$ is typically injective.

Therefore, this paper aims to provide a rigorous theory of CMEs that addresses not only the above-mentioned pathology but also substantially generalises the assumptions under which CME can be performed. We will treat both centred an uncentred (cross-)covariance operators,

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**Note:** The original document contains several mathematical expressions and diagrams. The text here has been simplified for clarity, and some details may have been omitted for the sake of readability. The full context and precision of the mathematical content can be found in the original document.
with particular emphasis on the centred case, and will also exhibit a connection to Gaussian conditioning in general Hilbert spaces.

1) The standard assumption \( \mathbb{E}[g(Y)|X = \cdot] \in \mathcal{H} \) (Assumption A) for CME is rather restrictive.\(^1\) For example, it does not hold in the case of independent random variables and Gaussian kernels; see Counterexample B.6. We show in Section 4 that this assumption can be significantly weakened in the case of centred kernel (cross-)covariance operators as defined in (2.3): only \( \mathbb{E}[g(Y)|X = \cdot] \) shifted by some constant function needs to lie in \( \mathcal{H} \) (Assumption B). In this setting, the correct expression of the CME formula is

\[
\mu_{Y|X=x} = \mu_Y + (C_X^\dagger C_{XY})^* (\varphi(x) - \mu_X) \quad \text{for } \mathbb{P}_X\text{-a.e. } x \in \mathcal{X},
\]

where \( A^* \) denotes the adjoint and \( A^\dagger \) the Moore–Penrose pseudo-inverse of a linear operator \( A \). As a first sanity check, note that this formula indeed yields \( \mu_{Y|X=x} = \mu_Y \) when \( X \) and \( Y \) are independent. Similarly, as shown in Section 5, for uncentred kernel (cross-)covariance operators as defined in (2.5), the more general CME formula is

\[
\mu_{Y|X=x} = (u C_X^\dagger u C_{XY})^* \varphi(x) \quad \text{for } \mathbb{P}_X\text{-a.e. } x \in \mathcal{X}.
\]

(2) Furthermore, the assumption \( \mathbb{E}[g(Y)|X = \cdot] \in \mathcal{H} \) is hard to check in most applications. To the best of our knowledge, the only verifiable condition that supposedly implies this assumption is given by Fukumizu et al. (2004, Proposition 4). However, this implication turns out to be incorrect; see Counterexamples B.5 and B.6. We will present weaker assumptions (Assumption B\(^*\)) for the applicability of CMEs which hold whenever the kernel \( k \) is characteristic.\(^2\) Characteristic kernels are well studied (see e.g. Sriperumbudur et al. (2010)) and therefore provide a verifiable condition as desired.

(3) The applicability of (1.1) requires the additional assumptions that \( C_X \) is injective and that \( \varphi(x) \) lies in the range of \( C_X \), which is also hard to verify in practice.\(^3\) We show that both assumptions can be avoided completely by replacing \( C_{Y|X} C_X^{-1} \) in (1.1) by \( (C_X^\dagger C_{XY})^* \) in (1.2) and (1.3), and this turns out to be a globally-defined and bounded operator under rather weak assumptions (Assumption C).

(4) The experienced reader will also observe that, modulo the replacement of \( C_{Y|X} C_X^{-1} \) by \( (C_X^\dagger C_{XY})^* \), (1.2) is identical to the familiar Sherman–Morrison–Woodbury / Schur complement formula for conditional Gaussian distributions, a connection on which we will elaborate in detail in Section 7. We call particular attention to the fact that the random variable \( (\psi(Y), \varphi(X)) \), which has no reason to be normally distributed, behaves very much like a Gaussian random variable in terms of its conditional mean.

\textbf{Remark 1.1.} Note that we stated (1.2) and (1.3) only for \( \mathbb{P}_X\text{-a.e. } x \in \mathcal{X} \). This is the best that one can generally hope for, since the regular conditional probability \( \mathbb{P}_{Y|X=x} \) is uniquely determined only for \( \mathbb{P}_X\text{-a.e. } x \in \mathcal{X} \) (Kallenberg, 2006, Theorem 5.3). The work on CMEs so far completely ignores the fact that conditioning (especially on events of the form \( X = x \)) is not trivial, requires certain assumptions and, in general, yields results only for \( \mathbb{P}_X\text{-a.e. } x \in \mathcal{X} \).

\(^1\) Fukumizu et al. (2013) themselves write “Note, however, that the assumptions […] may not hold in general; we can easily give counterexamples for the latter in the case of Gaussian kernels.”

\(^2\) A kernel \( k \) is called characteristic (Fukumizu et al., 2008) if the kernel mean embedding is injective as a function from \( \{Q \mid Q \text{ is a prob. meas. on } \mathcal{X} \text{ with } \int_X \|\varphi(x)\|_H \, dQ(x) < \infty \} \) into \( \mathcal{H} \); naturally, the KME cannot be injective as a function from the space of random variables on \( \mathcal{X} \) to \( \mathcal{H} \), since random variables with the same law embed to the same point of \( \mathcal{H} \).

\(^3\) Note that, typically, \( \dim \mathcal{H} = \infty \), in which case the compact operator \( C_X \) cannot possibly be surjective. To verify that \( \varphi(x) \in \text{ran} C_X \), one would need to compute a singular value decomposition \( C_X = \sum_n \sigma_n h_n^* \otimes h_n \) of \( C_X \) and check the Picard condition \( \sum_{n \in \mathbb{N}} \sigma_n^{-1} \|\varphi(x), h_n\|^2 < \infty \).
The rest of the paper is structured as follows. Section 2 establishes the notation and problem setting, and motivates some of the assumptions that are made. Section 3 discusses several critical assumptions for the applicability of the theory of CMEs and the relations among them. Section 4 proceeds to build a rigorous theory of CMEs using centred covariance operators, with the main results being Theorems 4.3 and 4.4, whereas Section 5 does the same for uncentred covariance operators, with the main result being Theorem 5.3. Section 6 reviews the established theory for the conditioning of Gaussian measures on Hilbert spaces, and this is then used in Section 7 to rigorously connect the theory of CMEs to the conditioning of Gaussian measures, with the main result being Theorem 7.1. We give some closing remarks in Section 8. Appendix A contains various auxiliary technical results and Appendix B gives counterexamples to some CME-related results of Fukumizu et al. (2004) and Alpay (2001).

2. Setup and Notation

Throughout this paper, when considering Hilbert-space valued random variables $U : \Omega \to \mathcal{G}$ and $V : \Omega \to \mathcal{H}$ defined over a probability space $(\Omega, \Sigma, \mathbb{P})$, the expected value $\mathbb{E}[U] := \int_{\Omega} U(\omega) \, d\mathbb{P}(\omega)$ is meant in the sense of a Bochner integral (Diestel, 1984), as are the uncentred and centred covariance operators

$$u \text{Cov}(U, V) := \mathbb{E}[U \otimes V], \quad \text{Cov}(U, V) := \mathbb{E}[(U - \mathbb{E}[U]) \otimes (V - \mathbb{E}[V])],$$

where, for $h \in \mathcal{H}$ and $g \in \mathcal{G}$, the outer product $h \otimes g : \mathcal{G} \to \mathcal{H}$ is the rank-one linear operator $(h \otimes g)(g') := (g, g')_G h$. Naturally, we write $u \text{Cov}[U]$ and $\text{Cov}[U]$ for $u \text{Cov}[U, U]$ and $\text{Cov}[U, U]$ respectively, and all of the above reduces to the usual definitions in the scalar-valued case.

Our treatment of conditional mean embeddings will operate under the following assumptions and notation:

**Assumption 2.1.**

(a) $(\Omega, \Sigma, \mathbb{P})$ is a probability space, $\mathcal{X}$ is a measurable space, and $\mathcal{Y}$ is a Borel space.\(^4\)

(b) $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ and $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ are symmetric and positive definite kernels, such that $k(x, \cdot)$ and $\ell(y, \cdot)$ are measurable functions for each $x \in \mathcal{X}$ and $y \in \mathcal{Y}$.

(c) $(\mathcal{H}, \langle \cdot, \cdot \rangle_\mathcal{H})$ and $(\mathcal{G}, \langle \cdot, \cdot \rangle_\mathcal{G})$ are the corresponding RKHSs, which we assume to be separable. Indeed, according to Owhadi and Scovel (2017), if the base sets $\mathcal{X}$ and $\mathcal{Y}$ are separable absolute Borel spaces or analytic subsets of Polish spaces, then separability of $\mathcal{H}$ and $\mathcal{G}$ follows from the measurability of their respective kernels and feature maps.

(d) $\varphi(x) := k(x, \cdot)$ and $\psi(y) := \ell(y, \cdot)$ are the corresponding canonical feature maps. Note that they satisfy the “reproducing properties” $\langle h, \varphi(x) \rangle_\mathcal{H} = h(x)$, $\langle g, \psi(y) \rangle_\mathcal{G} = g(y)$ for $x \in \mathcal{X}, y \in \mathcal{Y}, h \in \mathcal{H}, g \in \mathcal{G}$ and that $\varphi : \mathcal{X} \to \mathcal{H}$, $\psi : \mathcal{Y} \to \mathcal{G}$ are measurable by Steinwart and Christmann (2008, Lemma 4.25).

(e) $X : \Omega \to \mathcal{X}$ and $Y : \Omega \to \mathcal{Y}$ are random variables with distributions $\mathbb{P}_X$ and $\mathbb{P}_Y$ and joint distribution $\mathbb{P}_{XY}$. **Assumption 2.1(a)** and Kallenberg (2006, Theorem 5.3) ensure the existence of a $\mathbb{P}_X$-a.e.-unique regular version of the conditional probability distribution $\mathbb{P}_Y |_{X = x}$. We assume that

$$\mathbb{E}[\|\varphi(X)\|^2_\mathcal{H} + \|\psi(Y)\|^2_\mathcal{G}] < \infty \quad \text{and} \quad \mathbb{E}[\|\psi(Y)\|^2_\mathcal{G} | X = x] < \infty \quad \text{for } \mathbb{P}_X\text{-a.e. } x \in \mathcal{X},$$

\(^4\)A space $\mathcal{Y}$ is called **Borel space** if it is Borel isomorphic to a Borel subset of $[0, 1]$. In particular, $\mathcal{Y}$ is a Borel space if it is Polish, i.e. if it is separable and completely metrisable; see Kallenberg (2006, Chapter 1).
which guarantees that \( \mathcal{H} \subseteq \mathcal{L}^2(\mathbb{P}_X), \mathcal{G} \subseteq \mathcal{L}^2(\mathbb{P}_Y), \mathcal{G} \subseteq \mathcal{L}^2(\mathbb{P}_{Y|X=x}) \) since, by the reproducing property and the Cauchy–Schwarz inequality, for all \( h \in \mathcal{H} \),

\[
\|h\|_{\mathcal{L}^2(\mathbb{P}_X)}^2 = \int_X |h(x)|^2 \, d\mathbb{P}_X(x) = \int_X |\langle h, \varphi(x) \rangle_\mathcal{H}|^2 \, d\mathbb{P}_X(x) \\
\leq \int_X \|h\|_\mathcal{H}^2 \|\varphi(x)\|_\mathcal{H}^2 \, d\mathbb{P}_X(x) = \mathbb{E}[\|\varphi(X)\|_\mathcal{H}^2] \|h\|_\mathcal{H}^2
\]

(2.2)

and similarly for \( g \in \mathcal{G} \) and \( \mathbb{P}_Y, \mathbb{P}_{Y|X=x} \). It follows from (2.2) that the inclusions \( \iota_{\varphi, \mathbb{P}_X} : \mathcal{H} \hookrightarrow \mathcal{L}^2(\mathbb{P}_X), \iota_{\psi, \mathbb{P}_Y} : \mathcal{G} \hookrightarrow \mathcal{L}^2(\mathbb{P}_Y) \) and \( \iota_{\psi, \mathbb{P}_{Y|X=x}} : \mathcal{G} \hookrightarrow \mathcal{L}^2(\mathbb{P}_{Y|X=x}) \) are bounded linear operators.

(f) Observe that \( \langle f_1, f_2 \rangle := \text{Cov}[f_1(X), f_2(X)] \) defines a symmetric and positive-semidefinite bilinear form on \( \mathcal{L}^2(\mathbb{P}_X) \). Since it is invariant under \( \mathbb{P}_X \)-a.s. constant shifts of \( f_1 \) and \( f_2 \) and since \( \text{Cov}[f(X), f(X)] = \mathbb{V}[f(X)] = 0 \) if and only if \( f \) is \( \mathbb{P}_X \)-a.s. constant, we can make it positive definite (and thereby an inner product) by considering the quotient space\(^5\)

\( \mathcal{L}^2_\mathcal{C} := \mathcal{L}^2 / \mathcal{C} \), where

\[ \mathcal{C} := \{ f \in \mathcal{L}^2 | f \text{ is constant } \mathbb{P}_X\text{-a.s.} \}, \quad \langle [f_1], [f_2] \rangle_{\mathcal{L}^2_\mathcal{C}} := \text{Cov}[f_1(X), f_2(X)]. \]

Similarly, we define \( \mathcal{H}_\mathcal{C} := \mathcal{H} / (\mathcal{C} \cap \mathcal{H}) \) and identify \( \mathcal{H}_\mathcal{C} \) with a subset of \( \mathcal{L}_\mathcal{C}, \mathcal{H}_\mathcal{C} \subseteq \mathcal{L}_\mathcal{C} \).

(g) Since \( \varphi \) and \( \psi \) are measurable, \( Z = (\psi(Y), \varphi(X)) \) is a well-defined \( \mathcal{G} \oplus \mathcal{H} \)-valued random variable; (2.1) ensures that \( Z \) has finite second moment and its mean and covariance have the following block structure:

\[
\mu := \mathbb{E} \left[ \begin{pmatrix} \psi(Y) \\ \varphi(X) \end{pmatrix} \right] = \begin{pmatrix} \mu_Y \\ \mu_X \end{pmatrix}, \quad \Sigma := \text{Cov} \left[ \begin{pmatrix} \psi(Y) \\ \varphi(X) \end{pmatrix} \right] = \begin{pmatrix} C_Y & C_{XY} \\ C_{XY} & C_X \end{pmatrix},
\]

(2.3)

where the components

\[
\mu_Y := \mathbb{E}[\psi(Y)], \quad C_Y := \text{Cov}[\psi(Y)], \quad C_{XY} := \text{Cov}[\psi(Y), \varphi(X)], \\
\mu_X := \mathbb{E}[\varphi(X)], \quad C_{XY} := \text{Cov}[\varphi(X), \psi(Y)], \quad C_X := \text{Cov}[\varphi(X)]
\]

are called the kernel mean embeddings (KME) and kernel (cross-)covariance operators, respectively. Note that \( C_{XY}^* = C_{YX} \) and that the reproducing properties translate to the KMEs and covariance operators in the following way:

\[
\langle h, \mu_X \rangle_{\mathcal{H}} = \mathbb{E}[h(X)], \\
\langle h, C_X h' \rangle_{\mathcal{H}} = \text{Cov}[h(X), h'(X)], \\
\langle h, C_{XY} g \rangle_{\mathcal{H}} = \text{Cov}[h(X), g(Y)]
\]

and so on, for arbitrary \( h, h', h \in \mathcal{H} \) and \( g \in \mathcal{G} \). We are further interested in the conditional kernel mean embedding and the conditional kernel covariance operator given by

\[
\mu_{Y|X=x} = \mathbb{E}[\psi(Y)|X=x], \quad C_{Y|X=x} = \text{Cov}[\psi(Y)|X=x].
\]

(2.4)

Similarly, \( (Y, X) \) has the uncentred kernel covariance structure

\[
u_{C} := \nu_{\text{Cov}} \left[ \begin{pmatrix} \psi(Y) \\ \varphi(X) \end{pmatrix} \right] = \begin{pmatrix} u_{C_Y} & u_{C_{XY}} \\ u_{C_{XY}} & u_{C_X} \end{pmatrix},
\]

(2.5)

where \( u_{C_Y} := \nu_{\text{Cov}}[\psi(Y)] \) etc. Note that, for \( f_1, f_2 \in \mathcal{L}^2(\mathbb{P}_X) \), \( \nu_{\text{Cov}}(f_1(X), f_2(X)) = \langle f_1, f_2 \rangle_{\mathcal{L}^2(\mathbb{P}_X)} \), and similarly for functions of \( Y \).

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\(^5\)By the variational characterisation of variance, \( \| \cdot \|_{\mathcal{L}^2_\mathcal{C}} \) coincides with the norm induced on \( \mathcal{L}^2_\mathcal{C} \) by \( \| \cdot \|_{L^2} \):

\[
\|f\|_{\mathcal{L}^2_\mathcal{C}}^2 = \mathbb{V}[f(X)] = \mathbb{E}[(f(X) - \mathbb{E}[f(X)])^2] = \inf_{m \in \mathbb{R}} \mathbb{E}[(f(X) - m)^2] = \inf_{m \in \mathbb{C}} \|f - m\|^2_{L^2_\mathcal{C}}.
\]
(h) For $g \in G$ we let $f_g(x) := \mathbb{E}[g(Y)|X = x]$. These functions $f_g$ will be of particular importance since, for $g = \psi(y)$ and $y \in \mathcal{Y}$, we obtain $f_\psi(y)(x) = \mu_{Y|X=x}(y)$, our main object of interest. Note that $f_g \in L^2(\mathbb{P}_X)$ since by (2.1), (2.2), and the law of total expectation,

$$
\|f_g\|_{L^2(\mathbb{P}_X)} = \mathbb{E}[f_g(X)^2] = \mathbb{E}[\mathbb{E}[g(Y)|X]^2] \leq \mathbb{E}[\mathbb{E}[g(Y)^2|X]]
$$

and that, again by the law of total expectation,

$$
\mathbb{E}[f_g(X)] = \mathbb{E}[g(Y)], \quad \mathbb{E}[f_{\psi}(y)(X)] = \mu_{Y}(y). \quad (2.6)
$$

(i) For any linear operator $A$ between Hilbert spaces, $A^\dagger$ denotes its Moore–Penrose pseudo-inverse, i.e. the unique extension of $(A|_{(\ker A)^\perp})^{-1}$ to a (possibly unbounded) linear operator defined on $(\text{ran } A) \oplus (\text{ran } A)^\perp$ and such that $\ker A^\dagger = (\text{ran } A)^\perp$.

**Remark 2.2.** Measurability of $k(x, \cdot)$ and $\ell(y, \cdot)$ together with the separability of $\mathcal{H}$ and $\mathcal{G}$ guarantee the measurability of $\varphi$ and $\psi$ (Steinwart and Christmann, 2008, Lemma 4.25). Separability of $\mathcal{H}$ and $\mathcal{G}$ is also needed for Gaussian conditioning (see Owhadi and Scovel (2018) and Section 6), for the existence of a countable orthonormal basis of $\mathcal{H}$, and to ensure that weak (Pettis) and strong (Bochner) measurability of Hilbert–valued random variables coincide.

### 3. The Crucial Assumptions for CMEs

This section discusses the various versions of the assumption $f_g \in \mathcal{H}$ under which we are going to prove various versions of the CME formula.

**Assumption A.** For all $g \in G$ we have $f_g \in \mathcal{H}$.

**Assumption B.** For all $g \in G$ there exist a function $h_g \in \mathcal{H}$ and a constant $c_g \in \mathbb{R}$ such that $h_g = f_g - c_g \, \mathbb{P}_X$-a.e. in $\mathcal{X}$.

**Assumption C.** For all $g \in G$ there exists a function $h_g \in \mathcal{H}$ such that

$$
\text{Cov}[h_g(X) - f_g(X), h(X)] = 0 \quad \text{for all } h \in \mathcal{H}.
$$

In this case we denote $c_g := \mathbb{E}[f_g(X) - h_g(X)]$ (in conformity with Assumption B).

**Assumption $^{u}\text{C.}$** For all $g \in G$ there exists a function $h_g \in \mathcal{H}$ such that

$$
^{u}\text{Cov}[h_g(X) - f_g(X), h(X)] = \langle h_g - f_g, h \rangle_{L^2(\mathbb{P}_X)} = 0 \quad \text{for all } h \in \mathcal{H}.
$$

**Remark 3.1.** Note that $A \implies B \implies C$, $A \implies ^{u}\text{C}$, and that $C \implies B$ if $\mathcal{H}_C \subseteq L^2_{\text{loc}}(\mathbb{P}_X)$ is dense. In terms of the spaces $L_C$ and $\mathcal{H}_C$, Assumptions A–$^{u}\text{C}$ can be reformulated as follows:

(A) $f_g \in \mathcal{H}$ for $g \in G$.

(B) $[f_g] \in \mathcal{H}_C$ for $g \in G$.

(C) The orthogonal projection $P_{\tilde{f}_g \in L^2_C} f_g$ of $[f_g]$ onto $\mathcal{H}_C^{L^2}$ lies in $\mathcal{H}_C$ for $g \in G$.

($^{u}\text{C}$) The orthogonal projection $P_{\tilde{f}_g \in L^2} f_g$ of $[f_g]$ onto $\tilde{f}_g^{L^2}$ lies in $\mathcal{H}$ for $g \in G$. 

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A Rigorous Theory of Conditional Mean Embeddings

∃C > 0 ∀x₁, x₂ ∈ X, y₁, y₂ ∈ Y: µ_{Y|x=x₁}(y₁) µ_{Y|x=x₂}(y₂) ≤ C k(x₁, x₂) ℓ(x₁, x₂)

\[ H = \mathcal{L}^2(\mathbb{P}_X) \quad \Rightarrow \quad H_C = \mathcal{L}^2_{\mathcal{C}}(\mathbb{P}_X) \]

A: \[ f_g \in \mathcal{H} \text{ for } g \in \mathcal{G} \]

B: \[ [f_g] \in H_C \text{ for } g \in \mathcal{G} \]

C: \[ P_{\mathcal{C}} f_g \in \mathcal{H} \text{ for } g \in \mathcal{G} \]

\[ \mathcal{A}^*: f_{\psi(y)} \in \overline{\mathcal{H}}_{\mathcal{C}}^2 \text{ for } y \in \mathcal{Y} \]

\[ \mathcal{B}^*: [f_{\psi(y)}] \in \overline{\mathcal{H}}_{\mathcal{C}}^2 \text{ for } y \in \mathcal{Y} \]

\[ \mathcal{H} \text{ dense in } \mathcal{L}^2(\mathbb{P}_X) \quad \Rightarrow \quad H_C \text{ dense in } \mathcal{L}^2_{\mathcal{C}}(\mathbb{P}_X) \quad \leftarrow \quad k \text{ is characteristic} \]

Figure 3.1: A hierarchy of CME-related assumptions. Sufficient conditions for validity of the CME formula are indicated by shaded boxes, and Assumption B* is the most favorable one, since it is verifiable in practice, and in particular is fulfilled if the kernel is characteristic. Note that Assumptions C and C are not sufficient for valid CME but have several strong theoretical implications and Assumption C has a beautiful connection to Gaussian conditioning (Theorem 7.3). The incorrect CME condition and implication of Fukumizu et al. (2004, Proposition 4) is indicated in red while the new CME condition of the kernel being characteristic is marked green.

In contrast to Assumption A, Assumptions B and C do not require the unfavourable property \( \mathbb{1}_{\mathcal{X}} \in \mathcal{H} \) for independent random variables \( X \) and \( Y \). Instead, this case reduces to the trivial condition \( 0 \in \mathcal{H} \). At the same time, the proofs of the key properties of CMEs are not affected by replacing Assumption A with Assumption B as long as we work with centred operators (see Theorems 4.1 and 4.3 below). Therefore, it is surprising that this modification has not been considered earlier, even though the issues with independent random variables have been observed before (Fukumizu et al., 2013). One reason might be that, instead of centred (cross-) covariance operators, researchers started using uncentred ones, for which such a modification is not feasible.

Assumption C, on the other hand, is not strong enough for proving the main formula for CMEs (the last statement of Theorem 4.3). Clearly, this cannot be expected: If the RKHS \( \mathcal{H} \) is not rich enough, e.g. \( \mathcal{H} = \{0\} \) or \( \mathcal{H} = \text{span}(\mathbb{1}_{\mathcal{X}}) \), and \( \mathcal{G} \) is reasonably large, then no map from \( \mathcal{H} \) to \( \mathcal{G} \) can cover sufficiently many kernel mean embeddings, in particular the embeddings of the conditional probability \( \mathbb{P}_{Y|X=x} \) for various \( x \) (while Assumption C is trivially fulfilled for \( \mathcal{H} = \{0\} \) or \( \mathcal{H} = \text{span}(\mathbb{1}_{\mathcal{X}}) \)). The weakness of Assumption C lies in the fact that it only requires the vanishing of the orthogonal projection of \([h_g] - [f_g]\) onto \( \mathcal{H}_C \). Only if \( \mathcal{H}_C \) is rich enough (e.g. if it is dense in \( \mathcal{L}^2_{\mathcal{C}} \)) can this condition have useful implications.

While it is nice to have a weaker form of Assumption A, the Assumptions A, B and C remain hard to check in practice. Fukumizu et al. (2004, Proposition 4) provide a condition that is sufficient for Assumption A and often easier to check, but unfortunately it is incorrect; see Counterexamples B.5 and B.6 in Appendix B. Since characteristic kernels are well studied in
the literature, Lemma A.3 gives hope for a verifiable condition for the applicability of CMEs: it states that $\mathcal{H}_C$ is dense in $L^2_\psi(\mathbb{P}_X)$ whenever the kernel $k$ is characteristic. So, if the denseness of $\mathcal{H}_C$ in $L^2_\psi(\mathbb{P}_X)$ were sufficient for performing CMEs, then the condition that $k$ be characteristic would be sufficient as well, thus providing a favorable criterion for the applicability of formula (1.2). Unfortunately, neither condition implies Assumption B. Therefore, we will consider the following slightly weaker versions of Assumptions A and B, under which conditional mean embeddings can be performed if one allows for certain finite-rank approximations of the (cross-)covariance operators:

**Assumption A*. For each $y \in \mathcal{Y}$ we have $f_{\psi(y)} \in \mathcal{H}_C^{L^2_\psi}$.  

**Assumption B*. For each $y \in \mathcal{Y}$ we have $[f_{\psi(y)}] \in \mathcal{H}_C^{L^2_\psi}$.  

Note that Assumption C and Assumption A*C have no weaker versions, since they would become trivial if $\mathcal{H}_C$ were replaced by $\mathcal{H}_c^{L^2_\psi}$ and $\mathcal{H}$ by $\mathcal{H}$ respectively. In summary, we consider the hierarchy of assumptions illustrated in Figure 3.1. The main contributions of this paper are rigorous proofs of three versions of the CME formula under various assumptions:

- Theorem 4.3 uses Assumption B and centred operators.
- Theorem 4.4 uses Assumption B* and finite-rank approximations of centred operators.
- Theorem 5.3 uses Assumption A and uncentred operators.

Whether an analogue of Theorem 4.4 for the uncentred case can be proven under Assumption A* remains an open problem.

### 4. Theory for Centred Operators

In this section we will formulate and prove two versions of the CME formula (1.2) — the original one under Assumption B and a weaker version involving finite-rank approximations $C_{XY}^{(n)}$, $C_{XY}^{(n)}$ of the (cross-)covariance operators under Assumption B*. The following theorem demonstrates the importance of Assumption C (which follows from Assumption B). It implies that the range of $C_{XY}$ is contained in that of $C_X$, making the operator $C_X C_{XY}$ well defined. By Theorem A.1 it is even a bounded operator, which is a non-trivial result requiring the application of the closed graph theorem.

Similar considerations cannot be performed, in general, under Assumption B* alone: it can no longer be expected that $\text{ran} \ C_{XY} \subseteq \text{ran} \ C_X$, which is why we have to introduce the above-mentioned finite-rank approximations in order to guarantee that $\text{ran} \ C_{XY}^{(n)} \subseteq \text{ran} \ C_X^{(n)}$.

In summary, Assumption B allows for the simple CME formula (1.2) by Theorem 4.1, while under Assumption B* we have to make a detour using certain approximations. Note that this distinction is very similar to the theory of Gaussian conditioning in Hilbert spaces introduced by Owhadi and Scovel (2018) and recapped in Section 6 below, a connection that will be elaborated upon in detail in Section 7.

**Theorem 4.1.** Under Assumption 2.1, the following statements are equivalent:

(i) Assumption C holds.

(ii) For each $g \in \mathcal{G}$ there exists $h_g \in \mathcal{H}$ such that $C_X h_g = C_{XY} g$.

(iii) $\text{ran} \ C_{XY} \subseteq \text{ran} \ C_X$.

**Proof.** Note that (iii) is just a reformulation of (ii), so we only have to prove (i) $\iff$ (ii). Let $g \in \mathcal{G}$ and $h, h_g \in \mathcal{H}$. By Lemma A.5, $\text{Cov}[h(X), f_g(X)] = \langle h, C_{XY} g \rangle$, and so

$$\text{Cov}[h(X), h_g(X)] = \text{Cov}[h(X), f_g(X)] \ \forall h \in \mathcal{H} \iff \langle h, C_X h_g \rangle = \langle h, C_{XY} g \rangle \ \forall h \in \mathcal{H} \iff C_X h_g = C_{XY} g,$$
which completes the proof. ■

Note that Assumption C implies that \([h_g] \in \mathcal{H}_C\) is the orthogonal projection of \([f_g] \in \mathcal{L}^2_\mathcal{C}\) onto \(\mathcal{H}_C\) with respect to \(\langle \cdot, \cdot \rangle_{\mathcal{L}^2_\mathcal{C}}\) (see the reformulation of Assumption C in Remark 3.1). Therefore, there might be some ambiguity in the choice of \(h_g \in \mathcal{H}\) if \(\mathcal{H}\) contains constant functions. However, there is a particular choice of \(h_g\) that always works:

**Proposition 4.2.** Under Assumption 2.1, if Assumption B or Assumption C holds, then \(h_g\) may be chosen as

\[
h_g = C_X^\dagger C_{XY} g. \tag{4.1}
\]

More precisely, if Assumption C holds, then \(\text{Cov}[\langle C_X^\dagger C_{XY} g \rangle(X), f_g(X)] = 0\) for all \(h \in \mathcal{H}\) and \(g \in \mathcal{G}\); and if Assumption B holds, then for all \(g \in \mathcal{G}\) there exists a constant \(c_g \in \mathbb{R}\) such that \(\mathbb{P}_X\)-almost everywhere \(f_g = c_g + C_X^\dagger C_{XY} g\).

**Proof.** By Theorem 4.1, (4.1) is well defined. Under Assumption C, for all \(g \in \mathcal{G}\) and \(h \in \mathcal{H}\),

\[
\text{Cov}[h(X), \langle C_X^\dagger C_{XY} g \rangle(X)] = \langle h, C_X^\dagger C_{XY} g \rangle
\]

by Theorem 4.1

\[
= \langle h, C_X^\dagger g \rangle \quad \text{by Lemma A.5.}
\]

Under Assumption B, for all \(g \in \mathcal{G}\), there exist a function \(h_g' \in \mathcal{H}\) and a constant \(c_g' \in \mathbb{R}\) such that, \(\mathbb{P}_X\)-a.e. in \(\mathcal{X}\), \(h_g' = f_g - c_g'\). Theorem 4.1 implies that \(C_X h_g' = C_{XY} g\), and so Lemma A.4 implies that \(h_g' - C_X^\dagger C_{XY} g\) is constant \(\mathbb{P}_X\)-a.e. Therefore \(f_g - C_X^\dagger C_{XY} g\) is constant \(\mathbb{P}_X\)-a.e. ■

We now give our first main result, the rigorous statement of the CME formula for centred (cross-)covariance operators. In fact, we give two results: a “weak” result (4.2) in which the CME, as a function on \(\mathcal{X}\), holds only when tested against elements of \(\mathcal{H}\) in the \(\mathcal{L}^2(\mathbb{P}_X)\) inner product, and a “strong” result (4.3), an almost-sure equality in \(\mathcal{G}\).

**Theorem 4.3** (Centred CME). Under Assumptions 2.1 and C, \(C_X^\dagger C_{XY} : \mathcal{G} \rightarrow \mathcal{H}\) is a bounded operator and, for all \(y \in \mathcal{Y}\) and \(h \in \mathcal{H}\),

\[
\langle h, \mu_{y|X=x} \cdot (y) \rangle_{\mathcal{L}^2(\mathbb{P}_X)} = \left\langle h, \left(\mu_y + (C_X^\dagger C_{XY})^* (\varphi(\cdot) - \mu_X)\right)(y) \right\rangle_{\mathcal{L}^2(\mathbb{P}_X)}. \tag{4.2}
\]

If, in addition,

(i) the kernel \(k\) is characteristic or

(ii) \(\mathcal{H}_C\) is dense in \(\mathcal{L}^2(\mathbb{P}_X)\) or

(iii) Assumption B holds or

(iv) \([f_{\psi(y)}] \in \mathcal{H}_C\) for each \(y \in \mathcal{Y}\),

then, for \(\mathbb{P}_X\)-a.e. \(x \in \mathcal{X}\),

\[
\mu_{y|X=x} = \mu_y + (C_X^\dagger C_{XY})^* (\varphi(x) - \mu_X). \tag{4.3}
\]

**Proof.** Theorems 4.1 and A.1 imply that the operator \(C_X^\dagger C_{XY}\) is well defined and bounded and that, for each \(g \in \mathcal{G}\), we may choose the function \(h_g \in \mathcal{H}\) in Assumptions B and C to be \(h_g = C_X^\dagger C_{XY} g\) (by Proposition 4.2). Now (2.6), Lemma A.6, and the definition of \(c_g\) (see Assumption C) yield that, for \(x \in \mathcal{X}\) and \(y \in \mathcal{Y}\),

\[
h_{\psi(y)}(x) + c_{\psi(y)} = (\mu_y + (C_X^\dagger C_{XY})^* (\varphi(x) - \mu_X))(y). \tag{4.4}
\]
This yields (4.2) for each \( h \in \mathcal{H} \) via
\[
\langle h, (\mu_Y|_{X=x} - \mu_Y - (C_X^t C_{XY})^*(\varphi(\cdot) - \mu_X))(y) \rangle_{L^2(\mathcal{P}_X)} \\
= \langle h, f_{\psi}(y) - h_{\psi}(y) - c_{\psi}(y) \rangle_{L^2(\mathcal{P}_X)} \\
= \text{Cov}[h(X), (f_{\psi}(y) - h_{\psi}(y))(X)] + \mathbb{E}[h(X)](\mathbb{E}[f_{\psi}(y) - h_{\psi}(y)](X) - c_{\psi}(y)) = 0.
\]

If (i) or (ii) holds (note that, by Lemma A.3, (i) \( \implies \) (ii)), then (4.3) follows directly. If (iii) or (iv) holds, then (4.3) can be obtained from
\[
\mu_{Y|X=x}(y) = \mathbb{E}[\ell(y, Y)|X = x] = f_{\psi}(y)(x) \ast h_{\psi}(y)(x) + c_{\psi}(y) \\
= (\mu_Y + (C_X^t C_{XY})^*(\varphi(x) - \mu_X))(y),
\]
where the last equality follows from (4.4).

Note that step (\ast) in the proof of Theorem 4.3 genuinely requires that \([f_{\psi}(y)] \in \mathcal{H}_C\) (which follows from Assumption B), and Assumption C alone does not suffice. Again we see that \( \mathcal{H} \) needs to be rich enough. The reason that we get (4.2) in terms of the inner product of \( L^2(\mathcal{P}_X) \), and not its weaker version in \( L^2(\mathcal{P}_X) \), is that we took care of the shifting constant \( c_g := \mathbb{E}[f_g] - \mathbb{E}[h_g] \).

Motivated by the theory of Gaussian conditioning in Hilbert spaces (Owhadi and Scovel, 2018) presented in Section 6 and Theorem 6.2 in particular, we hope to generalise CMEs to the case where \( \text{ran} \ C_{XY} \subseteq \text{ran} \ C_X \) (i.e., by Theorem 4.1, Assumption C) does not necessarily hold. As mentioned above, this will require us to work with certain finite-rank approximations of the operators \( C_X \) and \( C_{XY} \). We are still going to need some assumption that guarantees that \( \mathcal{H} \) is rich enough to be able to perform the conditioning process in the RKHSs. For this purpose Assumption B will be replaced by its weaker version \( B^* \).

**Theorem 4.4** (Centred CME under finite-rank approximation). Let Assumption 2.1 hold. Further, let \((h_n)_{n \in \mathbb{N}}\) be complete orthonormal system of \( \mathcal{H} \) that is an eigenbasis of \( C_X \), let \( \mathcal{H}^{(n)} := \text{span}(h_1, \ldots, h_n) \), let \( \mathcal{F} := \mathcal{G} \oplus \mathcal{H} \), let \( P^{(n)} : \mathcal{F} \to \mathcal{F} \) be the orthogonal projection onto \( \mathcal{G} \oplus \mathcal{H}^{(n)} \), and let
\[
\begin{align*}
C & := \begin{pmatrix} C_Y & C_{XY} \\ C_{XY} & C_X \end{pmatrix}, \\
C^{(n)} & := P^{(n)} C P^{(n)} = \begin{pmatrix} C_Y & C_{XY}^{(n)} \\ C_{XY}^{(n)} & C_X^{(n)} \end{pmatrix}.
\end{align*}
\]

Then \( \text{ran} \ C_X^{(n)} \subseteq \text{ran} \ C_X \) and therefore \( h_{\psi|X}(n) := (C_X^{(n)})^t C_{XY} g \in \mathcal{H} \) is well defined for each \( g \in \mathcal{G} \). For each \( y \in \mathcal{Y} \) and \( h \in \mathcal{H} \),
\[
\langle h, \mu_{Y|X=x}(y) \rangle_{L^2(\mathcal{P}_X)} = \lim_{n \to \infty} \langle h, (\mu_Y + (C_X^{(n)})^t C_{XY}^{(n)})^*(\varphi(\cdot) - \mu_X))(y) \rangle_{L^2(\mathcal{P}_X)}.
\]

If, in addition,
(i) the kernel \( k \) is characteristic or
(ii) \( \mathcal{H}_C \) is dense in \( L^2(\mathcal{P}_X) \) or
(iii) Assumption \( B^* \) holds,
then, for \( \mathbb{P}_X \)-a.e. \( x \in \mathcal{X} \),
\[
\mu_{Y|X=x} = \mu_Y + \lim_{n \to \infty} (C_X^{(n)})^t C_{XY}^{(n)} (\varphi(x) - \mu_X). \tag{4.6}
\]
Proof. Note that, since $C$ is a trace-class operator, so is $C^{(n)}$. Furthermore, by Baker (1973, Theorem 1), $C^{(n)}_{XY} = (C^{(n)}_X)^{1/2}V^{1/2}C^{(n)}_{YX}$ for some bounded operator $V: \mathcal{G} \to \mathcal{H}$. Since $C^{(n)}_X$ has finite rank, this implies that $\text{ran} C^{(n)}_{XY} \subseteq \text{ran} C^{(n)}_X$. Similarly to the proof of Theorem 4.3, we define $\epsilon^{(n)}_g(x) := \mathbb{E}[(f_g - h^{(n)}_g)(x)]$ for $g \in \mathcal{G}$, $n \in \mathbb{N}$ and obtain by (2.6) and Lemma A.6 for $x \in \mathcal{X}$, $y \in \mathcal{Y}$ and $n \in \mathbb{N}$ that

$$h^{(n)}_{\psi(y)}(x) + \epsilon^{(n)}_{\psi(y)} = \left(\mu_Y + (C^{(n)}_X C^{(n)}_{XY})^*(\varphi(x) - \mu_X)\right)(y), \quad (4.7)$$

Identity (4.5) can be obtained similarly to (4.2) except that we additionally need to show that $\text{Cov}[h(X), f_g(X)] = \lim_{n \to \infty} \text{Cov}[h(X), h^{(n)}_g(X)]$ for all $h \in \mathcal{H}$, as proved in Lemma A.8(a).

In order to prove (4.6) we first note that $|h^{(n)}_g|$ is the $L^2_{\mathcal{C}}$-orthogonal projection of $|f_g|$ onto $\mathcal{H}^{(n)}_C := \mathcal{H}^{(n)}/(\mathcal{C} \cap \mathcal{H}^{(n)})$ for all $g \in \mathcal{G}$ by Lemma A.8(b). Now let $y \in \mathcal{Y}$ and $U = \bigcup_{n \in \mathbb{N}} \mathcal{H}^{(n)}_C$. Since $U^{\mathcal{H}_C} = \mathcal{H}_C$ and $|f_{\psi(y)}| \in \overline{U^{\mathcal{H}_C} L^2_{\mathcal{C}}}$ by assumption (note that, by Lemma A.3, (i) $\implies$ (ii) $\implies$ (iii)), we also have $|f_{\psi(y)}| \in U^{\mathcal{H}_C L^2_{\mathcal{C}}}$ (here we used that $\|\cdot\|_H$ is a stronger norm than $\|\cdot\|_{L^2}$ by (2.2)) and Lemma A.7 implies

$$\lim_{n \to \infty} \left\|h^{(n)}_{\psi(y)} - f_{\psi(y)}\right\|_{L^2_{\mathcal{C}}} = 0.$$ 

Therefore, by the definition of $c^{(n)}_g$, 

$$\lim_{n \to \infty} \left\|h^{(n)}_{\psi(y)} + c^{(n)}_{\psi(y)} - f_{\psi(y)}\right\|_{L^2_{\mathcal{C}}} = 0. \quad (4.8)$$

Let $\mu^{(n)}(x,y) := h^{(n)}_{\psi(y)}(x) + c^{(n)}_{\psi(y)}$. From (4.7) and Owhadi and Scovel (2018, Theorem 3.3) (or, alternatively, from Theorems 6.2 and 6.6 later on) we know that $\mu^{(n)}(x, \cdot)$ converges in $\mathcal{G}$ to some pointwise limit $\mu^*(x, \cdot)$ for $\mathbb{P}_X$-a.e. $x \in \mathcal{X}$. Therefore $\mu^{(n)}(x,y) \xrightarrow{n \to \infty} \mu^*(x,y)$ for every $y \in \mathcal{Y}$ and $\mathbb{P}_X$-a.e. $x \in \mathcal{X}$ and together with (4.8) this implies that $f_{\psi(y)}(x)$ (the $L^2$ limit of $\mu^{(n)}(\cdot, y)$) and $\mu^*(\cdot, y)$ (the pointwise limit of $\mu^{(n)}(\cdot, y)$) agree $\mathbb{P}_X$-a.e. Hence, $\mu^{(n)}(x, \cdot) \xrightarrow{n \to \infty} f_{\psi(.)}(x) = \mu_{Y|X=x}$ in $\mathcal{G}$ for $\mathbb{P}_X$-a.e. $x \in \mathcal{X}$. Invoking (4.7) another time proves (4.6).

5. Theory for Uncentred Operators

Starting with the work of Song et al. (2010a,b), uncentred (cross-)covariance operators became more commonly used than centred ones. This section shows how similar results to those of Section 4 can be obtained for uncentred operators. Roughly speaking, the same conclusions can be made as in Theorem 4.3 but under Assumption A in place of B. This observation suggests that centred operators are superior to uncentred ones in terms of generality. So far, the theoretical justification for CME using uncentred operators relies on Fukumizu et al. (2013, Theorems 1 and 2), which require rather strong assumptions. Our improvement can be summarised as follows:

- Since we use $uC^i_X$ instead of $uC^{-1}_X$ our theory can cope with non-injective operators $uC_X$. This is only a minor advance, since $uC_X$ is injective under rather mild conditions on $X$ and $k$ (see Fukumizu et al. (2013, Footnote 3)).
- In contrast to Fukumizu et al. (2013, Theorem 2), we do not require the assumption that $\varphi(x)$ lies in the range of $uC_X$. The reason for this is that the operator $(uC^i_X uC_{XY})^*$ in (4.3) is globally defined whereas $uC_{YX} uC^{-1}_X$ is not. This is an important improvement since the assumption that $\varphi(x) \in \text{ran} uC_X$ is typically hard to verify, as explained in Section 1.
As mentioned above, using centred operators instead of uncentred ones yields the important advantage of requiring only the weaker Assumption B (or even just B') in place of A.

**Theorem 5.1.** Under Assumption 2.1, the following statements are equivalent:

(i) Assume Assumption $\text{A}^\dagger$ holds.

(ii) For each $g \in G$ there exists $h_g \in H$ such that $^uC_X h_g = ^uC_{XY} g$.

(iii) $\text{ran}^uC_{XY} \subseteq \text{ran}^uC_X$.

**Proof.** The proof is identical to that of Theorem 4.1. □

Similar to Proposition 4.2, the element $h_g \in H$ in Assumption $\text{A}^\dagger$ can always be chosen as $h_g = ^uC_X^\dagger^uC_{XY} g$.

**Proposition 5.2.** Let Assumption 2.1 hold. If Assumption $\text{A}^\dagger$ holds, then $h_g$ may be chosen as

$$h_g = ^uC_X^\dagger^uC_{XY} g.$$  \hspace{1cm} (5.1)

More precisely, $^uCov[(^uC_X^\dagger^uC_{XY} g)(X) - f_g(X), h(X)] = 0$ for all $h \in H$ and $g \in G$. If Assumption A holds, then for every $g \in G$ the identity $f_g = ^uC_X^\dagger^uC_{XY} g$ holds $\mathbb{P}_X$-almost everywhere.

**Proof.** First note that (5.1) is well defined by Theorem 5.1. If Assumption $\text{A}^\dagger$ holds, then, by Theorem 5.1 and Lemma A.10, for all $g \in G$ and $h \in H$,

$$^uCov[h(X), (^uC_X^\dagger^uC_{XY} g)(X)] = \langle h, ^uC_X^\dagger^uC_{XY} g \rangle = \langle h, ^uC_{XY} g \rangle = ^uCov[h(X), f_g(X)] .$$

If Assumption A holds, then Lemma A.10 implies $^uC_X f_g = ^uC_{XY} g$ for all $g \in G$ and the claim follows from Lemma A.9. □

Let us now formulate and prove the analog of Theorem 4.3 for uncentred operators. Note that stronger assumptions are required than in the centred case.

**Theorem 5.3** (Uncentred CME). Under Assumption 2.1 and Assumption $\text{A}^\dagger$, the operator $^uC_X^\dagger^uC_{XY} : G \to H$ is bounded and, for all $y \in Y$ and $h \in H$,

$$\langle h, \mu_{Y|x=\cdot}(y) \rangle_{L^2(\mathbb{P}_X)} = \langle h, ((^uC_X^\dagger^uC_{XY}^*) \varphi(\cdot))(y) \rangle_{L^2(\mathbb{P}_X)} .$$  \hspace{1cm} (5.2)

If, in addition,

(i) $H$ is dense in $L^2(\mathbb{P}_X)$ or

(ii) Assumption A holds or

(iii) $f_{\varphi(y)} \in H$ for each $y \in Y$.

then this implies that, for $\mathbb{P}_X$-a.e. $x \in X$,

$$\mu_{Y|x=x} = (^uC_X^\dagger^uC_{XY}^*) \varphi(x).$$  \hspace{1cm} (5.3)

**Proof.** First note that by Theorems 5.1 and A.1 the operator $^uC_X^\dagger^uC_{XY}$ is well defined and bounded and that for each $g \in G$ we may choose the function $h_g \in H$ in Assumption $\text{A}^\dagger$ as $h_g = ^uC_X^\dagger^uC_{XY} g$ by Proposition 5.2. By Lemma A.6 we obtain, for all $x \in X$ and $y \in Y$,

$$h_{\varphi(y)}(x) = ((^uC_X^\dagger^uC_{XY}^*) \varphi(x))(y).$$

This yields (5.2) via

$$\langle h, (\mu_{Y|x=\cdot} - (^uC_X^\dagger^uC_{XY}^*) \varphi(\cdot))(y) \rangle_{L^2} = h, f_{\psi(y)} - h_{\psi(y)} \rangle_{L^2} = ^uCov[h(X), (f_{\psi(y)} - h_{\psi(y)})(X)] = 0,$$
which implies (5.3) under any of the three conditions stated in the theorem.

As a byproduct we obtain a generalization of Fukumizu et al. (2013, Theorem 2):

Corollary 5.4. Under the assumptions of Theorem 5.3 (including either of the additional ones) we have
\[ \mu_Y = (u^C_X u C_{XY})^* \mu_X. \]

Proof. By Theorems 5.1 and A.1, \( u^C_X u C_{XY} \) is a well-defined and bounded linear operator. Hence, by the law of total expectation,
\[ \mu_Y = E[\mu_Y | X] = E[(u^C_X u C_{XY})^* \varphi(X)] = (u^C_X u C_{XY})^* E[\varphi(X)] = (u^C_X u C_{XY})^* \mu_X, \]
as claimed.

6. Gaussian Conditioning in Hilbert spaces

This section gives a review of conditioning theory for Gaussian random variables in separable Hilbert spaces, summarising the work of Owhadi and Scovel (2018). Our only somewhat novel contribution here is the explicit characterisation of the essential operator \( \hat{Q}_{C,H} \) in terms of the Moore–Penrose pseudo-inverse, which appears as an exercise for the reader in Arias et al. (2008, Remark 2.3).

In the following let \( F = G \oplus H \) be the sum of two separable Hilbert spaces \( G \) and \( H \) and let \((U, V)\) be an \( F\)-valued jointly Gaussian random variable with mean \( \mu \in F \) and covariance operator \( C : F \to F \) given by the following block structures:
\[
\begin{pmatrix} U \\ V \end{pmatrix} \sim \mathcal{N}(\mu, C), \quad \mu = \begin{pmatrix} \mu_U \\ \mu_V \end{pmatrix}, \quad C = \begin{pmatrix} C_U & C_{UV} \\ C_{VU} & C_V \end{pmatrix} \geq 0
\]
with \( \mu_U \in G \), etc. We denote by \( L(F) \) the Banach algebra of bounded linear operators on \( F \) and by \( L_+(F) = \{ A \in L(F) \mid A \geq 0 \} \) the set of positive operators, i.e. those self-adjoint operators \( A \) for which \( \langle x, Ax \rangle \geq 0 \) for all \( x \in F \). The theory of Gaussian conditioning relies on the concept of so-called oblique projections:

Definition 6.1. Let \( F = G \oplus H \) be a direct sum of two Hilbert spaces \( G, H \) and \( C \in L_+(F) \) a positive operator. The set of (\( C \)-symmetric) oblique projections onto \( H \) is given by
\[ \mathcal{P}(C, H) = \{ Q \in L(F) \mid Q^2 = Q, \ \text{ran} \ Q = H, \ CQ = Q^*C \}. \]
The pair \((C, H)\) is said to be compatible if \( \mathcal{P}(C, H) \) is non-empty.

The first two conditions \( Q^2 = Q \) and \( \text{ran} \ Q = H \) imply that \( Q \) has the block structure
\[
Q = \begin{pmatrix} 0 & 0 \\ \hat{Q} & \text{Id}_H \end{pmatrix}, \quad \hat{Q} : G \to H.
\] (6.1)

Then, the condition \( CQ = Q^*C \) is equivalent to \( C_V \hat{Q} = C_{VU} \) (which follows from a straightforward blockwise multiplication, see Lemma 6.3) and implies in particular \( \text{ran} \ C_{VU} \subseteq \text{ran} \ C_V \).

The other way round, as we will see later on, the condition \( \text{ran} \ C_{VU} \subseteq \text{ran} \ C_V \) guarantees the existence of an oblique projection \( Q \in \mathcal{P}(C, H) \) and will provide a crucial link between the theory of Gaussian conditioning and conditional mean embeddings in Section 7.

The results on conditioning Gaussian measures can then be summarised as follows:
Theorem 6.2 (Owhadi and Scovel, 2018, Theorem 3.3, Corollary 3.4). If \((C, H)\) is compatible, then conditioning \(U\) on \(V = v \in H\) results in a Gaussian random variable on \(G\) with mean \(\mu_{U|V=v}\) and covariance operator \(C_{U|V=v}\) given by

\[
\begin{cases}
\mu_{U|V=v} = \mu_U + \hat{Q}^*(v - \mu_V), \\
C_{U|V=v} = C_U - C_{UV}\hat{Q}
\end{cases}
\]

(6.2)

for any oblique projection \(Q\) given in the form (6.1). Also, in this case, \(\mathcal{P}(C, H)\) contains a unique element

\[
Q_{C,H} = \begin{pmatrix} 0 & 0 \\ \hat{Q}_{C,H} & \text{Id}_H \end{pmatrix}
\]

that fulfills the properties (6.4) defined below.

If \((C, H)\) is incompatible, then conditioning \(U\) on \(V = v \in H\) still yields a Gaussian random variable on \(G\), but the corresponding formulas for the conditional mean \(\mu_{U|V=v}\) and covariance operator \(C_{U|V=v}\) are given by a limiting process using finite-rank approximations of \(C\) in the following way. Let \((h_n)_{n \in \mathbb{N}}\) be a complete orthonormal system of \(H\), \(P^{(n)} : F \rightarrow F\) denote the orthogonal projection on \(G \oplus \text{span}(h_1, \ldots, h_n)\) and \(C^{(n)} = P^{(n)}CP^{(n)}\). Then \((C^{(n)}, H)\) is compatible for each \(n \in \mathbb{N}\) and

\[
\begin{cases}
\mu_{U|V=v} = \mu_U + \lim_{n \to \infty} \hat{Q}^{(n)}_{C^{(n)}, H}(v - \mu_V), \\
C_{U|V=v} = C_U - \lim_{n \to \infty} C_{UV}\hat{Q}_{C^{(n)}, H}
\end{cases}
\]

(6.3)

where the second limit is in the trace norm.

In the following we will revisit some theory on oblique projections which will be necessary to establish the connection between Gaussian conditioning and conditional mean embeddings. We will also characterise the special oblique projection \(Q_{C,H} \in \mathcal{P}(C, H)\) by means of the Moore–Penrose pseudo-inverse, which is a new result.

Lemma 6.3. If there exists a bounded linear operator \(\hat{Q} : G \rightarrow H\) such that \(C_V\hat{Q} = C_{VU}\), then

\[
Q = \begin{pmatrix} 0 & 0 \\ \hat{Q} & \text{Id}_H \end{pmatrix} \in \mathcal{P}(C, H).
\]

In particular, the pair \((C, H)\) is compatible.

Proof. The properties \(Q^2 = Q\) and \(\text{ran} \ Q = H\) are clear from the definition of \(Q\) and a straightforward blockwise multiplication yields \(CQ = Q^*C\).

Proposition 6.4. In the setup of Definition 6.1, if \((C, H)\) is compatible, then there exists a unique bounded operator \(\hat{Q}_{C,H} : G \rightarrow H\) such that

\[
C_V\hat{Q}_{C,H} = C_{VU}, \quad \ker \hat{Q}_{C,H} = \ker C_{VU}, \quad \text{ran} \ \hat{Q}_{C,H} \subseteq \text{ran} \ C_V.
\]

(6.4)

By Lemma 6.3 the first property implies that

\[
Q_{C,H} = \begin{pmatrix} 0 & 0 \\ \hat{Q}_{C,H} & \text{Id}_H \end{pmatrix} \in \mathcal{P}(C, H).
\]
Proof. See Douglas (1966, Theorem 1) or Fillmore and Williams (1971, Theorem 2.1) for the existence and uniqueness of \( \hat{Q}_{C,H} \) and Corach et al. (2001) or Owhadi and Scovel (2018) for its connection to oblique projections.

If one follows the original construction of Douglas (1966, Theorem 1) or Fillmore and Williams (1971, Theorem 2.1), it is easy to see how this unique element can be characterised in terms of the Moore–Penrose pseudo-inverse \( C^\dagger \) of \( C \):

**Theorem 6.5.** If \( \text{ran} \ C_{VU} \subseteq \text{ran} \ C_V \), then
\[
\hat{Q} = C_{VU}^\dagger C_{VU} : \mathcal{G} \to \mathcal{H}
\]
is a well-defined and bounded operator which uniquely fulfils the conditions (6.4).

Proof. This is a direct application of Theorem A.1.

**Theorem 6.6.** In the setup of Definition 6.1, the following statements are equivalent

(i) \((C, \mathcal{H})\) is compatible.
(ii) \( \text{ran} \ C_{VU} \subseteq \text{ran} \ C_V \).

If either of these conditions holds, then the unique element \( Q_{C,H} \in \mathcal{P}(C, \mathcal{H}) \) in Proposition 6.4 is given by
\[
\hat{Q}_{C,H} = C_{VU}^\dagger C_{VU}.
\]

Proof. If \((C, \mathcal{H})\) is compatible, there exists an element \( \hat{Q}_{C,H} : \mathcal{G} \to \mathcal{H} \) with \( C_V \hat{Q}_{C,H} = C_{VU} \) by Proposition 6.4, which implies (ii). If \( \text{ran} \ C_{VU} \subseteq \text{ran} \ C_V \), then Theorem 6.5 and Lemma 6.3 imply (i). Theorem 6.5 and the uniqueness of \( \hat{Q}_{C,H} \) in Proposition 6.4 imply (6.5).

**Remark 6.7.** Lemma 6.3 and the equivalence part of Theorem 6.6 were already proved by Corach et al. (2001); we state them for the sake of readability. The second part of Theorem 6.6(ii) characterises the operator \( \hat{Q}_{C,H} \) in terms of the Moore–Penrose pseudo-inverse, without an assumption of closed range, as anticipated by Arias et al. (2008, Remark 2.3).

We also give an example of a covariance operator for which the above conditions do not hold:

**Example 6.8.** Let \( \mathcal{H} = \mathcal{G} \) be any (separable) infinite-dimensional Hilbert space with complete orthonormal basis \((e_j)_{j \in \mathbb{N}}\). Let
\[
C_U := \sum_{j \in \mathbb{N}} j^{-2} e_j \otimes e_j,
C_V := \sum_{j \in \mathbb{N}} j^{-4} e_j \otimes e_j,
C_{VU} = C_{UV} := C_U^{1/2} \text{Id}_H C_{V}^{1/2} = \sum_{j \in \mathbb{N}} j^{-3} e_j \otimes e_j.
\]
By Baker (1973, Theorem 2),
\[
C := \begin{pmatrix} C_U & C_{UV} \\ C_{UV} & C_V \end{pmatrix}
\]
is a legitimate positive definite covariance operator on \( \mathcal{F} = \mathcal{G} \oplus \mathcal{H} \). However,
\[
\text{ran} \ C_{VU} = \left\{ \sum_{j \in \mathbb{N}} \alpha_j e_j \ \bigg| \ (j^3 \alpha_j)_{j \in \mathbb{N}} \in \ell^2 \right\} \supsetneq \left\{ \sum_{j \in \mathbb{N}} \alpha_j e_j \ \bigg| \ (j^4 \alpha_j)_{j \in \mathbb{N}} \in \ell^2 \right\} = \text{ran} \ C_V.
\]
7. Connection between CME and Gaussian Conditioning

If we compare the theories of CMEs and Gaussian conditioning in Hilbert spaces, we make the following observations:

- Formula (4.3) for CME and formula (6.2) for Gaussian conditioning look very similar (in view of Theorem 6.6).
- The assumptions under which the conditioning process is “easy” — namely Assumption C (as long as Assumption B holds as well) and the compatibility of \((C, H)\) — are equivalent to the conditions that ran \(C_{XY} \subseteq \text{ran} C_X\) and ran \(C_{UY} \subseteq \text{ran} C_Y\) respectively (Theorems 4.1 and 6.6).

This motivates us to connect these two theories by working in the setup of Section 2 and introducing new jointly Gaussian random variables \(U\) and \(V\) that take values in the RKHSs \(G\) and \(H\) respectively, where the means \(\mu_U\) and \(\mu_V\) and (cross-)covariance operators\(^6\) \(C_U, C_{UV}, C_{VU},\) and \(C_V\) are chosen to coincide with the kernel mean embeddings \(\mu_Y\) and \(\mu_X\) and the kernel (cross-)covariance operators \(C_Y, C_{YX}, C_{XY},\) and \(C_X\) respectively:

\[
\begin{pmatrix} U \\ V \end{pmatrix} \sim \mathcal{N}(\mu, C), \quad \mu = \begin{pmatrix} \mu_U \\ \mu_V \end{pmatrix} = \begin{pmatrix} \mu_Y \\ \mu_X \end{pmatrix}, \quad C = \begin{pmatrix} C_U & C_{UV} \\ C_{VU} & C_V \end{pmatrix} = \begin{pmatrix} C_Y & C_{YX} \\ C_{XY} & C_X \end{pmatrix}. \tag{7.1}
\]

Note that the random variables \(W = (U, V)\) and \(Z = (\psi(Y), \varphi(X))\) do not coincide even though they have the same mean and covariance operator, since the latter will not in general be Gaussian. Surprisingly, their conditional means agree, as long as we condition on \(V = v = \varphi(x), X = x\), respectively. This is obvious when one compares (4.3) with (6.2) and (4.6) with (6.3) using Theorem 6.5. A natural question is whether a similar equality holds for the conditional covariance operator \(C_{Y|X=x}\). However, the covariance operator \(C_{U|V=v}\) obtained from Gaussian conditioning is independent of \(v\), a special property of Gaussian measures that cannot be expected of the conditional kernel covariance operator \(C_{Y|X=x}\). Instead, \(C_{U|V=v}\) equals the mean of \(C_{Y|X=x}\) when averaged over all possible outcomes \(x \in \mathcal{X}\).\(^7\) These insights are summarised in the following proposition and illustrated in Figure 7.1.

**Theorem 7.1.** Under Assumption 2.1 and Assumption B\(^*\) we have the following identities for the random variable \((U, V)\) defined by (7.1) and for \(v = \varphi(x)\) and \(x \in \mathcal{X}\):

\[
\mu_{U|V=v} = \mu_{Y|X=x}, \quad C_{U|V=v} = \mathbb{E}[C_{Y|X}|X] = \int_{\mathcal{X}} C_{Y|X=x} d\mathbb{P}(x).
\]

**Proof.** By Lemma A.11, \(\mathbb{E}[C_{Y|X}|X]\) is well defined. The identity \(\mu_{U|V=v} = \mu_{Y|X=x}\) follows directly from Theorems 4.3, 4.4, 6.2, and 6.5. For the second identity, using the notation of Theorem 4.4, note that \(\|h_{\psi(y)}^{(n)} + c_{\varphi(y)}^{(n)} - f_{\psi(y)}\|_{L^2} \xrightarrow{n \to \infty} 0\) by (4.8). Therefore, for \(y, y' \in \mathcal{Y}\), \(g = \psi(y)\), and \(g' = \psi(y')\),

\[
\text{Cov}[f_g(X), f_{g'}(X)] = \lim_{n \to \infty} \text{Cov}[h_g^{(n)}(X), h_{g'}^{(n)}(X)] = \lim_{n \to \infty} \langle C_X h_g^{(n)}, h_{g'}^{(n)} \rangle_H = \lim_{n \to \infty} \langle C_{XY} g, C_{XY}^{(n)} g' \rangle_g = \lim_{n \to \infty} \langle g, C_{VY} C_{UV}^{(n)} g' \rangle_g.
\]

\(^6\)The Gaussian random variable \((U, V)\) is well-defined in \(G \oplus H\), since condition (2.1) implies that \(C\) is a trace-class covariance operator.

\(^7\)This observation has already been made by Fukumizu et al. (2004, Proposition 5) under stronger assumptions and by Fukumizu et al. (2009, Proposition 3) in a weaker form.
Figure 7.1: A normally-distributed \( \mathcal{G} \oplus \mathcal{H} \)-valued normal random variable \((U, V)\) can be defined with the same mean and covariance structure as \((\psi(Y), \varphi(X))\). While the latter will typically fail to be normally distributed, surprisingly, the conditional means of the two random variables happen to agree! Since \(C_{U|V=v} \) does not depend on the realisation \(v\), a specific property of Gaussian random variables that cannot be expected from \(C_{Y|X=x}\), a similar agreement for the conditional covariance operators cannot be obtained. Instead, the identity provided by Theorem 7.1 holds, which is open to interpretation.

By the law of total covariance and (6.3), (6.5) this implies that, for \(g = \psi(y)\) and \(g' = \psi(y')\),

\[
\langle g, \mathbb{E}[C_{Y|X}]g' \rangle = \mathbb{E}\left[\text{Cov}(g(Y), g'(Y)) | X \right] \\
= \text{Cov}(g(Y), g'(Y)) - \text{Cov}(f_g(X), f_{g'}(X)) \\
= \langle g, C_{U|V}g' \rangle \mathbb{I} - \lim_{n \to \infty} \langle g, C_{UV}C_V^{(n)} C_{VU}^{(n)} g' \rangle \mathbb{I} \\
= \langle g, C_{U|V=v}g' \rangle.
\]

Since \(\text{span}\{\psi(y) \mid y \in \mathcal{Y}\}\) is dense in \(\mathcal{G}\), this finishes the proof.

**Remark 7.2.** Theorem 7.1 implies in particular that the posterior mean \(\mu_{U|V=v}\) of the \(U\)-component of a jointly Gaussian random variable \((U, V)\) in an RKHS \(\mathcal{G} \oplus \mathcal{H}\) is not just some element in \(\mathcal{G}\), but in fact the KME of some probability distribution on \(\mathcal{Y}\), as long as we condition on an event of the form \(V = v = \varphi(x)\).

As mentioned above, there is another analogy between CMEs and Gaussian conditioning, namely the assumption under which the formula for the conditional mean is particularly nice, i.e. does not require finite-rank approximations of the (cross-)covariance operators:

**Theorem 7.3.** Under Assumption 2.1 and with the random variable \((U, V)\) defined by (7.1), Assumption \(\mathcal{C}\) is equivalent to the compatibility of \((C, \mathcal{H})\).

**Proof.** By Theorems 4.1 and 6.6, both conditions are equivalent to \(\text{ran} C_{XY} \subseteq \text{ran} C_X\).

8. Closing Remarks

This article has demonstrated rigorous foundations for the method of conditional mean embedding in reproducing kernel Hilbert spaces. Mild and verifiable sufficient conditions have
been provided for the centred and uncentred variants of the CME formula to yield an element \( \mu_{Y|X=x} \) that is indeed the kernel mean embedding of the conditional distribution \( P_{Y|X=x} \) on \( Y \). The CME formula required a correction in the centred case but, modulo this correction, it is more generally applicable than its uncentred counterpart; we therefore think that it should be the preferred formulation in practice. We also demonstrated the precise relationship between CMES and well-established formulae for the conditioning of Gaussian random variables in Hilbert spaces.

Multiple natural directions for further research suggest themselves:

First, our results concern mostly, though not exclusively, the case of centred kernel (cross-)covariance operators. We do not, at present, have an analogue of Theorem 4.4 for uncentred operators under Assumption A*. Indeed, the analogues for uncentred operators of the necessary supporting results from Owhadi and Scovel (2018) appear to be highly non-trivial and would merit a paper in their own right.

Second, in practice, the kernel mean embeddings and kernel (cross-)covariance operators will often be estimated empirically from observed data. In the simplest setting, given \( N \in \mathbb{N} \) independent samples \((X_1, Y_1), \ldots, (X_N, Y_N) \sim P_{XY}\), we have the empirical estimators

\[
\mu_X \approx \hat{\mu}_X^{(N)} := \frac{1}{N} \sum_{n=1}^{N} \varphi(X_n),
\]

\[
C_{XY} \approx \hat{C}_{XY}^{(N)} := \frac{1}{N-1} \sum_{n=1}^{N} \left( \varphi(X_n) - \hat{\mu}_X^{(N)} \right) \otimes \left( \psi(Y_n) - \hat{\mu}_Y^{(N)} \right),
\]

and so on. Laws of large numbers for these empirical estimators have already been established — see e.g. Smola et al. (2007, Theorem 2) and Mollenhauer (2018, Lemma 5.8) — but the impact of this approximation error upon conditioning is, to the best of our knowledge, not yet fully quantified. That is, what is the quality of the approximation

\[
\mu_{Y|X=x} \approx \hat{\mu}_Y^{(N)} + \left( \hat{C}_{X}^{(N)\dagger} \hat{C}_{XY}^{(N)} \right)^* (\varphi(x) - \hat{\mu}_X^{(N)}) \quad \text{ for } x \in X? \tag{8.1}
\]

The question is not at all trivial, since the convergence of the finite-rank operators \( \hat{C}_{X}^{(N)} \) to \( C_X \) as \( N \to \infty \) is generally insufficient to ensure convergence of \( \hat{C}_{X}^{(N)\dagger} \) to \( C_X^\dagger \).

Third, when using CMES for inference, a remaining step might be to undo the kernel mean embedding, i.e. to explicitly recover the conditional distribution \( P_{Y|X=x} \) on \( Y \) from its embedding \( \mu_{Y|X=x} \in \mathcal{G} \). This is a particular instance of a non-parametric inverse problem and a principled solution, based upon Tikhonov regularisation, has been proposed in the context of the kernel conditional density operator by Schuster et al. (2019). The relationship between this KCDO approach and the sufficient conditions for CME that have been considered in this article remains to be precisely formulated; given the intimate relationship between Tikhonov regularisation and the Moore–Penrose pseudo-inverse, this should be a fruitful avenue of research.

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A. Technical Results

This section contains several technical results used in the proofs of the theorems given in the article. The following well-known result due to Douglas (1966, Theorem 1) (see also Fillmore and Williams (1971, Theorem 2.1)) is used several times:

**Theorem A.1.** Let \( \mathcal{H}, \mathcal{H}_1, \) and \( \mathcal{H}_2 \) be Hilbert spaces and let \( A: \mathcal{H}_1 \to \mathcal{H} \) and \( B: \mathcal{H}_2 \to \mathcal{H} \) be bounded linear operators with \( \text{ran} A \subseteq \text{ran} B \). Then \( Q := B^\dagger A: \mathcal{H}_1 \to \mathcal{H}_2 \) is a well-defined and bounded linear operator, where \( B^\dagger \) denotes Moore–Penrose pseudo-inverse of \( B \). It is the unique operator that satisfies the conditions

\[
A = BQ, \quad \text{ker} Q = \ker A, \quad \text{ran} Q \subseteq \text{ran} B^\dagger. \tag{A.1}
\]

**Remark A.2.** In the original work of Douglas (1966) only the existence of a bounded operator \( Q \) such that \( A = BQ \) was shown. However, the construction of \( Q \) in the proof is identical to that of \( B^\dagger \) (multiplied by \( A \)). This connection has been observed before by Arias et al. (2008, Corollary 2.2 and Remark 2.3), where it was proven in the case of closed range operators, leaving the proof of the general case to the reader.

The following results are used in the proofs of Sections 3, 4, and 7.

**Lemma A.3.** If \( k \) is a characteristic kernel, then, under Assumption 2.1, \( \mathcal{H}_C \) is dense in \( L^2_C(\mathbb{P}_X) \).

This statement is essentially one direction of Proposition 5 in Fukumizu et al. (2009), but does not require \( k \) to be bounded, which makes a separate proof necessary.

**Proof.** Assume \( \mathcal{H}_C \) is not dense in \( L^2_C(\mathbb{P}_X) \). Then there exists \( f \in L^2(\mathbb{P}_X) \) that is not \( \mathbb{P}_X \)-a.s. constant such that \( [f] \perp L^2_C(\mathbb{P}_X) \). Choose \( f := f - \mathbb{E}[f(X)] \) and

\[
Q_1(E) = \int_E |\tilde{f}| \, d\mathbb{P}_X, \quad Q_2(E) = \int_E |\tilde{f}| - \tilde{f} \, d\mathbb{P}_X
\]
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for every measurable subset \( E \subseteq \mathcal{X} \). Since \( \| \tilde{f} \|_{L^1(P_X)} \neq 0 \), we may assume without loss of generality \( \| \tilde{f} \|_{L^1(P_X)} = 1 \), making \( Q_1 \) and \( Q_2 \) two distinct probability distributions. Note that

\[
\langle \tilde{f}, h \rangle_{L^2(P_X)} = \langle f - E[f(X)], h \rangle_{L^2(P_X)} = \| f \|_{L^1(P_X)} = 0.
\]

Let \( Z_1 \sim Q_1 \) and \( Z_2 \sim Q_2 \) and \( x \in \mathcal{X} \). Since \( k(x, \cdot) \in \mathcal{H} \) we obtain

\[
\mu_{Z_1}(x) - \mu_{Z_2}(x) = \langle \tilde{f}, k(x, \cdot) \rangle_{L^2(P_X)} = 0,
\]

contradicting the assumption of \( k \) being characteristic. Note that \( \mu_{Z_1} \) and \( \mu_{Z_2} \) are well defined by Assumption 2.1 and the Cauchy–Schwarz inequality:

\[
E[\| \varphi(Z_1) \|_{\mathcal{H}}] = \int_{\mathcal{X}} \| \varphi(x) \|_{\mathcal{H}} \| \tilde{f}(x) \| dP_X(x) \leq E[\| \varphi(X) \|_{\mathcal{H}}^2]^{1/2} E[\tilde{f}(X)^2]^{1/2} < \infty
\]

and similarly for \( Z_2 \).

Lemma A.4. Under Assumption 2.1, \( \ker C_X = \{ h \in \mathcal{H} \mid h \text{ is } P_X\text{-a.s. constant in } \mathcal{X} \} \).

Proof. This is a direct consequence of the fact that \( \langle h, C_X h \rangle = V[h(X)] \).

Lemma A.5. Under Assumption 2.1, for all \( h \in \mathcal{H} \) and \( g \in \mathcal{G} \), \( \text{Cov}[h(X), f_g(X)] = \langle h, C_{XY}g \rangle \).

Proof. Let \( h \in \mathcal{H} \) and \( g \in \mathcal{G} \) be arbitrary. Then

\[
\text{Cov}[h(X), f_g(X)] = E[h(X)E[g(Y)|X]] - E[h(X)]E[E[g(Y)|X]]
\]

\[
= E[h(X)g(Y)] - E[h(X)]E[g(Y)]
\]

\[
= \text{Cov}[h(X), g(Y)]
\]

\[
= \langle h, C_{XY}g \rangle,
\]

as required.

Lemma A.6. Under Assumption 2.1, let \( A: \mathcal{G} \to \mathcal{H} \) be a bounded linear operator. Then, for all \( x \in \mathcal{X} \) and \( y \in \mathcal{Y} \),

\[
(A\psi(y))(x) = (A^*\varphi(x))(y), \quad E[(A\psi(y))(X)] = (A^*\mu_X)(y)
\]

Proof. The reproducing properties of \( \psi \), \( \varphi \), and \( \mu_X \) imply that

\[
(A\psi(y))(x) = (A\psi(y), \varphi(x))_{\mathcal{H}} = \langle \psi(y), A^*\varphi(x) \rangle_{\mathcal{G}} = (A^*\varphi(x))(y),
\]

and

\[
E[(A\psi(y))(X)] = (A\psi(y), \mu_X)_{\mathcal{H}} = \langle \psi(y), A^*\mu_X \rangle_{\mathcal{G}} = (A^*\mu_X)(y),
\]

as claimed.

Lemma A.7. Let \( V \) be a Hilbert space, let \( U_1 \subseteq U_2 \subseteq \cdots \) be an increasing sequence of closed subspaces \( U_n \subseteq V \), \( n \in \mathbb{N} \), and let \( U := \bigcup_{n \in \mathbb{N}} U_n \). Further, let \( P_{U_n}: V \to U_n \) denote be the orthogonal projection onto \( U_n \). Then, for all \( v \in U \),

\[
P_{U_n}v \xrightarrow{n \to \infty} v.
\]
Proof. Let $v \in \overline{U}$ and $\epsilon > 0$. Then there exists $u \in U$ such that $\|u - v\| < \epsilon$. Since the sequence $(U_n)_{n \in \mathbb{N}}$ is increasing and $U$ is its union, there exists an $n_0 \in \mathbb{N}$ such that $u \in U_{n_0}$ and thereby $P_{U_n} u = u$ for all $n \geq n_0$. We therefore obtain, for $n \geq n_0$,

$$
\|P_{U_n} v - v\| \leq \|P_{U_n} v - P_{U_n} u\| + \|P_{U_n} u - u\| + \|u - v\| \leq \|P_{U_n}\| \|v - u\| + \|u - v\| < 2\epsilon,
$$

by the triangle inequality and non-expansivity of orthogonal projection. \hfill \blacksquare

Lemma A.8. Let $\mathcal{H}^{(n)}$, $C^{(n)}$, and $h_g^{(n)}$ be as in Theorem 4.4, and let $f_g(x) := \mathbb{E}[g(Y)|X = x]$. Then

(a) $\text{Cov}[h(X), f_g(X)] = \lim_{n \to \infty} \text{Cov}[h(X), h_g^{(n)}(X)]$ for all $h \in \mathcal{H}$;

(b) $[h_g^{(n)}]$ is the $L^2$-orthogonal projection of $[f_g]$ onto $\mathcal{H}_C^{(n)} := \mathcal{H}^{(n)}/(C \cap \mathcal{H}^{(n)})$ for all $g \in \mathcal{G}$.

Proof. It is straightforward that $C^{(n)}$ converges to $C$ (in the strong and thereby in the weak sense) and that $C_X$ and $C_X^{(n)}$ agree on $\text{span}(h_1, \ldots, h_n) \supseteq h_g^{(n)}$. Using Lemma A.5 we obtain, for all $h \in \mathcal{H}$ and $h^{(n)} \in \mathcal{H}^{(n)}$,

$$
\text{Cov}[h(X), f_g(X)] = \langle h, C_{XY} g \rangle = \lim_{n \to \infty} \langle h, C_{XY}^{(n)} g \rangle = \lim_{n \to \infty} \langle h, C_X h_g^{(n)} \rangle = \lim_{n \to \infty} \text{Cov}[h(X), h_g^{(n)}(X)],
$$

which yields (a). Also, for arbitrary $h^{(n)} \in \mathcal{H}^{(n)}$,

$$
[\langle h^{(n)}, f_g \rangle]_{L^2} = \text{Cov}[h^{(n)}(X), f_g(X)] = [\langle h^{(n)}, C_{XY} g \rangle]_{\mathcal{H}} = [\langle C_{XY} h^{(n)}, g \rangle]_{\mathcal{G}} = [\langle C_{XY} h_g^{(n)}, g \rangle]_{\mathcal{G}} = [\langle h^{(n)}, C_X h_g^{(n)} \rangle]_{\mathcal{H}} = [\langle h^{(n)}, C_X h_g^{(n)} \rangle]_{\mathcal{H}} = \text{Cov}[h^{(n)}(X), h_g^{(n)}(X)] = [\langle h^{(n)}, h_g^{(n)} \rangle]_{L^2}.
$$

which yields (b). \hfill \blacksquare

Lemma A.9. Under Assumption 2.1, $\ker^\perp C_X = \{ h \in \mathcal{H} \mid h = 0 \; \mathbb{P}_X \text{-a.s. in } X \}$.

Proof. This is a direct consequence of the fact that $\langle h, C_X h \rangle = \|h\|_{L^2(\mathbb{P}_X)}$. \hfill \blacksquare

Lemma A.10. Under Assumption 2.1, for all $h \in \mathcal{H}$ and $g \in \mathcal{G}$,

$$
\text{uCov}[h(X), f_g(X)] = \langle h, C_{XY} g \rangle_{\mathcal{H}}.
$$
**Proof.** Let \( h \in \mathcal{H} \) and \( g \in \mathcal{G} \) be arbitrary. Then

\[
\text{Cov}[h(X), f_g(X)] = \mathbb{E}[h(X)g(Y)] = \mathbb{E}[h(X)]g(Y) = \text{Cov}[h(X), g(Y)] = \langle h, \text{C}_{XY} g \rangle_{\mathcal{H}},
\]

as claimed. 

\[ \blacksquare \]

**Lemma A.11.** Let Assumptions 2.1 and \( B^* \) hold. Then \( \mathbb{E}[C_{Y|X}] = \int_X C_{Y|X=x} \, d\mathbb{P}_X(x) \) is well defined as a strong (Bochner) integral, i.e. \( \int_X \|C_{Y|X=x}\| \, d\mathbb{P}_X(x) < \infty. \)

**Proof.** The Cauchy–Schwarz inequality and (2.2) imply that

\[
\|C_{Y|X=x}\| = \sup \|g\|_{\mathcal{L}^2(\mathbb{P}_{Y|X=x})} \|f_{\mathcal{G}}(\mathbb{P}_{Y|X=x})\| \leq \sup \|g\|_{\mathcal{L}^2(\mathbb{P}_{Y|X=x})} \|f_{\mathcal{G}}(\mathbb{P}_{Y|X=x})\| \leq \mathbb{E}[\|\psi(Y)\|^2 | X = x],
\]

which, by the law of total expectation and (2.1), yields that

\[
\mathbb{E}[\|C_{Y|X}\|] \leq \mathbb{E}[\mathbb{E}[\|\psi(Y)\|^2 | X]] = \mathbb{E}[\|\psi(Y)\|^2] < \infty,
\]

as claimed. \[ \blacksquare \]

**B. Counterexamples to Results of Fukumizu et al. (2004) and Alpay (2001)**

The condition expressed in Assumption A, that \( \mathbb{E}[g(Y)|X = \cdot] \in \mathcal{H} \) for all \( g \in \mathcal{G} \), can be hard to check in practice. For this reason, Fukumizu et al. (2004, Proposition 4) suggest a simpler criterion that allegedly guarantees this assumption:

**Proposition B.1.** Let \( \mathcal{H} \) and \( \mathcal{G} \) be RKHSs over measurable spaces \( \mathcal{X} \) and \( \mathcal{Y} \), respectively, with measurable kernels \( k \) and \( \ell \), and let \( (X, Y) \) be a random variable in \( \mathcal{X} \times \mathcal{Y} \) such that \( \mathbb{E}[k(X, X)] \) and \( \mathbb{E}[\ell(Y, Y)] \) are finite. If there exists a constant \( C > 0 \) such that

\[
\mathbb{E}[\ell(y_1, Y)|X = x_1]\mathbb{E}[\ell(y_2, Y)|X = x_2] \leq Ck(x_1, x_2)\ell(y_1, y_2) \tag{B.1}
\]

for all \( x_1, x_2 \in \mathcal{X} \) and \( y_1, y_2 \in \mathcal{Y} \), then Assumption A is fulfilled.

**Remark B.2.** Several comments have to be made concerning this proposition:

- It is easy to find counterexamples to Proposition B.1 by considering e.g. independent random variables and Gaussian kernels on bounded domains; see Counterexample B.6.
- The authors did not give a rigorous proof for this proposition, instead simply writing

  “See Theorem 2.3.13 in Alpay (2001).”

However, our attempts to obtain Proposition B.1 from the quoted theorem have failed so far. One such attempt (which we suppose to be the strategy envisioned by Fukumizu et al.) is provided below and has two “gaps”. 

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The result of Alpay (2001, Theorem 2.3.13) upon which Proposition B.1 allegedly rests is itself incorrect. Again, considering Gaussian kernels on bounded domains provides a simple counterexample (Counterexample B.7).

Alpay (2001) gives proofs of neither Theorem 2.3.13 nor of its supporting result Theorem 2.3.9, nor are references to proofs given. The lemma preceding these theorems (Alpay, 2001, Lemma 2.3.8) is taken from Donoghue (1974, Lemma 2, p. 142), but stated incompletely (the set $\mathbb{D}$ is assumed to be an open disc in the plane by Donoghue (1974), which is completely ignored by Alpay; it is not clear what an interval $I \subset \mathbb{D}$ is supposed to be).

In the following we present our supposition of how the proof of Proposition B.1 might have been envisioned by Fukumizu et al. (2004). As mentioned above, it is incomplete and the critical steps are marked in red and underlined. Before the proof attempt we state the result of Alpay (2001, Theorem 2.3.13) upon which Proposition B.1 appears to rest:

**Theorem B.3** (Alpay, 2001, Theorem 2.3.13). Let $K$ be a positive kernel on a set $Z$ and $n \in \mathbb{N}$. The function $f : Z \rightarrow \mathbb{C}^n$ belongs to the associated RKHS if and only if there exists $m > 0$ such that for $z_1, z_2 \in Z$

$$m^2 K(z_1, z_2) - f(z_1) f(z_2)^* \geq 0. \quad (B.2)$$

The RKHS norm of $f$ is then given by the smallest number $m$ such that this kernel is positive.

**Proof attempt of Proposition B.1 (incomplete).** Consider the RKHS tensor product $\mathcal{H} \otimes \mathcal{G}$ equipped with the kernel

$$K : (X \times Y)^2 \rightarrow \mathbb{R}, \quad K((x_1, y_1), (x_2, y_2)) := k(x_1, x_2) \ell(y_1, y_2).$$

Let $f(x, y) := \mathbb{E}[\ell(y, Y)|X = x]$. Then, by condition (B.1) and Theorem B.3, it follows that $f \in \mathcal{H} \otimes \mathcal{G}$. This implies that $f(\cdot, y) \in \mathcal{H}$ for all $y \in \mathcal{Y}$. Now let $g = \sum_{j=1}^{\infty} \alpha_j \psi(y_j)$ be an element of $\mathcal{G}$ and $g_j := \sum_{j=1}^{J} \alpha_j \psi(y_j)$. Then

$$\mathbb{E}[g_j(Y)|X = \cdot] = \sum_{j=1}^{J} \alpha_j \mathbb{E}[\ell(y_j, Y)|X = \cdot] = \sum_{j=1}^{J} \alpha_j f(\cdot, y_j) \in \mathcal{H},$$

and hence $\mathbb{E}[g(Y)|X = \cdot] = \lim_{J \rightarrow \infty} \mathbb{E}[g_j(Y)|X = \cdot] \in \mathcal{H}$. \hfill $\blacksquare$

Two problems now present themselves: the two missing steps in the above proof outline are highly non-trivial, and it in fact turns out that there are counterexamples to both Proposition B.1 itself and the supporting result Theorem B.3.

We first present two counterexamples to Proposition B.1 (i.e. to Fukumizu et al. (2004, Proposition 4)). The first is based on the RKHS $\mathcal{H}$ of constant functions, which is not “rich” enough to deal with dependencies between $X$ and $Y$. The second uses Gaussian kernels and independent random variables $X$ and $Y$ on bounded domains $\mathcal{X}$ and $\mathcal{Y}$ respectively. The independence implies that all functions $\mathbb{E}[g(Y)|X = \cdot]$ for $g \in \mathcal{G}$ are constant, but non-trivial constants do not lie in $\mathcal{H}$ by the following result:

**Theorem B.4** (Steinwart et al., 2006, Corollary 5; Steinwart and Christmann, 2008, Corollary 4.44). Let $X \subset \mathbb{R}^d$ have non-empty interior and let $\mathcal{H}$ be the RKHS of the radial Gaussian kernel $k(x, y) := \exp(-\|x - y\|^2/\gamma^2)$. If $f \in \mathcal{H}$ is constant on any $A \subseteq X$ of non-empty interior, then $f = 0$.

Using the same appeal to this property of Gaussian RKHSs, we can also give a counterexample to Theorem B.3 (i.e. to Alpay (2001, Theorem 2.3.13)).
Counterexample B.5 (to Proposition B.1). Let $\mathcal{X} = \mathcal{Y} := [0, 1]$, let $k(x_1, x_2) := 1$ be a constant kernel and let $\ell(y_1, y_2) := e^{-(y_1-y_2)^2}$ be a Gaussian kernel; let $\mathcal{H}$ and $\mathcal{G}$ be the RKHSs with kernels $k$ and $\ell$ respectively. Note that, by the usual Moore–Aronszajn characterisation of $\mathcal{H}$ as the completion of the linear span of $\{k(x_1, \cdot) \mid x_1 \in \mathcal{X}\}$, which consists only of constant functions, $\mathcal{H}$ itself consists only of constant functions.

Now let the $\mathcal{X} \times \mathcal{Y}$-valued random variable $(X, Y)$ have the (discrete) probability distribution

$$P_{XY}(\{(1, 0)\}) = P_{XY}(\{(0, 1)\}) = \frac{1}{2}$$

i.e. $P(X = 1, Y = 0) = P(X = 0, Y = 1) = \frac{1}{2}$.

Since both kernels are bounded above as well as away from zero, condition (B.1) is fulfilled, but for $g = \ell(1, \cdot)$ we have

$$E[g(Y)|X = x] = \begin{cases} 1 & \text{for } x = 1, \\ e^{-1} & \text{for } x = 0, \end{cases}$$

which is not constant and hence not an element of $\mathcal{H}$.

We remark here that this example can be easily adapted to almost any $X$ and $Y$ with a non-trivial dependence structure.

Counterexample B.6 (to Proposition B.1). Let $\mathcal{X} = \mathcal{Y} := [0, 1]$, let $k(x, y) = \ell(x, y) := e^{-(x-y)^2}$ be Gaussian kernels and $\mathcal{H} = \mathcal{G}$ the corresponding RKHSs. Let $X$ and $Y$ be any independent random variables on $\mathcal{X}$ and $\mathcal{Y}$ respectively (e.g. $X = Y = 0$ almost surely). Then, for $g := \ell(0, \cdot)$, $E[g(Y)|X = \cdot]$ is a positive constant and so, by Theorem B.4, does not lie in $\mathcal{H}$. On the other hand, if $X$ and $Y$ are independent, then condition (B.1) simplifies to

$$E[\ell(y_1, Y)] E[\ell(y_2, Y)] \leq C k(x_1, x_2) \ell(y_1, y_2),$$

which certainly holds for Gaussian kernels on bounded domains, since they are bounded above as well as away from zero.

Counterexample B.7 (to Theorem B.3). Let $K$ be a Gaussian kernel on $Z := [0, 1]$ and $f = 1$ be a constant function. Since $K$ is bounded away from zero, condition (B.2) is fulfilled. Yet, by Theorem B.4, $f$ does not belong to the associated RKHS.