Reproducing kernel Hilbert $C^*$-module and kernel mean embeddings

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Abstract

Kernel methods have been among the most popular techniques in machine learning, where learning tasks are solved using the property of reproducing kernel Hilbert space (RKHS). In this paper, we propose a novel data analysis framework with reproducing kernel Hilbert $C^*$-module (RKHM) and kernel mean embedding (KME) in RKHM. Since RKHM contains richer information than RKHS or vector-valued RKHS (vv RKHS), analysis with RKHM enables us to capture and extract structural properties in multivariate data, functional data and other structured data. We show a branch of theories for RKHM to apply to
data analysis, including the representer theorem, and the injectivity and universality of the proposed KME. We also show RKHM generalizes RKHS and vv RKHS. Then, we provide concrete procedures for employing RKHM and the proposed KME to data analysis.

**Keywords:** reproducing kernel Hilbert C*-module, kernel mean embedding, structured data, kernel PCA, interaction effects

1. Introduction

Kernel methods have been among the most popular techniques in machine learning (Schölkopf and Smola, 2001), where learning tasks are solved using the property of reproducing kernel Hilbert space (RKHS). RKHS is the space of complex-valued functions equipped with an inner product determined by a positive-definite kernel. One of the important tools with RKHS is kernel mean embedding (KME). In KME, a probability distribution (or measure) is embedded as a function in an RKHS (Smola et al., 2007; Muandet et al., 2017; Sriperumbudur et al., 2011), which enables us to analyze distributions in RKHSs.

Whereas much of the classical literature on RKHS approaches has focused on complex-valued functions, RKHSs of vector-valued functions, i.e., vector-valued RKHSs (vv RKHSs), have also been proposed (Micchelli and Pontil, 2005; Álvarez et al., 2011; Lim et al., 2015; Minh et al., 2016; Kadri et al., 2016). This allows us to learning vector-valued functions rather than complex-valued functions.

In this paper, we develop a branch of theories on reproducing kernel Hilbert C*-module (RKHM) and propose a generic framework for data analysis with RKHM. RKHM is a generalization of RKHS and vv RKHS in terms of C*-algebra, and we show RKHM is a powerful tool to analyze structural properties in multivariate data, functional data and other structured data. An RKHM is constructed by a C*-algebra-valued positive definite kernel and characterized by a C*-algebra-valued inner product (see Definition 3.2). The theory of C*-algebra has been discussed in mathematics, especially in operator algebra theory. An important example of C*-algebra is $L^\infty(\Omega)$, where $\Omega$ is a compact measure space. Another important example is $B(W)$, which denotes the space of bounded linear operators on a Hilbert space $W$. Note that $B(W)$ coincides with the space of matrices $C^{m \times m}$ if the Hilbert space $W$ is finite dimensional.

Although there are several advantages for studying RKHM compared with RKHS and vv RKHS, those can be summarized into two as in the following: First, an RKHM is a “Hilbert C*-module”, which is mathematically more general than a “Hilbert space”. An inner product in an RKHM is C*-algebra-valued, which captures more information than a complex-valued one in an RKHS or vv RKHS and enables us to extract richer information. For example, if we set $L^\infty(\Omega)$ as a C*-algebra, we can regard multi-variable functional data as functions of a single variable. Also, if we set $B(W)$ as a C*-algebra, we can encode distributions at all the points in a two-dimensional space into a vector in an RKHM. This cannot be achieved, in principle, by RKHSs and vv-RKHSs since their inner products are complex-valued, where such information is degenerated into one complex value, and therefore we cannot reconstruct the information from a vector in an RKHS or vv RKHS. Second, RKHM generalizes RKHS and vv RKHS. That is, it can be shown that we can reconstruct RKHSs and vv RKHSs from RKHMs. This implies that existing algorithms with RKHSs and vv RKHSs are reconstructed by using the framework of RKHM.
The theory of RKHM has been studied in mathematical physics and pure mathematics (Itoh, 1990; Heo, 2008; Szafraniec, 2010). On the other hand, to the best of our knowledge, as for the application of RKHM to data analysis, we can find the only literature by Ye (2017), where only the case of setting the space of matrices as a $C^*$-algebra is discussed. In this paper, we develop a branch of theories on RKHM and propose a generic framework for data analysis with RKHM. We show a theoretical property on minimization with respect to orthogonal projections and give the representer theorem in RKHMs. These are fundamental for data analysis that have been investigated and applied in the cases of RKHS and vv RKHS, which has made RKHS and vv RKHS widely-accepted tools for data analysis (Schölkopf et al., 2001). Moreover, we define a KME in an RKHM, and provide theoretical results about the injectivity of the proposed KME and the connection with universality of RKHM. Note that, as is well known for RKHSs, these two properties have been actively studied to theoretically guarantee the validity of kernel-based algorithms (Steinwart, 2001; Gretton et al., 2007; Fukumizu et al., 2008; Sriperumbudur et al., 2011). Then, we apply the developed theories to generalize kernel PCA (Schölkopf and Smola, 2001) and to apply to the analysis of interaction effects in finite or infinite dimensional data.

The remainder of this paper is organized as follows. First, in Section 2, we briefly review RKHS, vv RKHS, and mathematical notions and definitions required to discuss RKHM. In Section 3, we show some fundamental properties of RKHM for data analysis. In Sections 4, we propose a KME in RKHMs, and show the connection between the injectivity of the KME and the universality of RKHM. Then, in Section 5, we discuss applications of the developed results to kernel PCA and the analysis of interaction effects in finite or infinite dimensional data. Finally, in Section 6, we discuss the connection of RKHMs and the proposed KME with the existing notions, and conclude the paper in Section 7.

**Notations** Lowercase letters denote $\mathcal{A}$-valued coefficients (often by $a, b, c, d$), vectors in a Hilbert $C^*$-module $\mathcal{M}$ (often by $p, q, u, v$), or vectors in a Hilbert space $\mathcal{W}$ (often by $w, h$). Lowercase Greek letters denote measures (often by $\mu, \nu, \lambda$) or complex-valued coefficients (often by $\alpha, \beta$). Calligraphic capital letters denote sets. And, bold lowercase letters denote vectors in $\mathcal{A}^n$ for $n \in \mathbb{N}$ (a finite dimensional Hilbert $C^*$-module). Also, we use $\sim$ for objects related to RKHSs. Moreover, an inner product, an absolute value, and a norm in a space or a module $\mathcal{S}$ (see Definitions 2.12 and 2.13) are denoted as $\langle \cdot, \cdot \rangle_{\mathcal{S}}, | \cdot |_{\mathcal{S}},$ and $\| \cdot \|_{\mathcal{S}}$, respectively.

The typical notations in this paper are listed in Table 1.

### 2. Background

We briefly review RKHS and vv RKHS in Subsections 2.1 and 2.2, respectively. Then, we review $C^*$-algebra and $C^*$-module in Subsection 2.3, and Hilbert $C^*$-module in Subsection 2.4.

#### 2.1 Reproducing kernel Hilbert space (RKHS)

We review the theory of RKHS. An RKHS is a useful case of Hilbert spaces that can be used to extract nonlinearity or higher-order moments of data (Schölkopf and Smola, 2001; Saitoh and Sawano, 2016).
Table 1: Notation table

| Symbol | Description |
|--------|-------------|
| $\mathcal{A}$ | A $C^*$-algebra |
| $1_{\mathcal{A}}$ | The multiplicative identity in $\mathcal{A}$ |
| $\mathcal{A}_+$ | The subset of $\mathcal{A}$ composed of all positive elements in $\mathcal{A}$ |
| $\leq_{\mathcal{A}}$ | For $c, d \in \mathcal{A}$, $c \leq_{\mathcal{A}} d$ means $d - c$ is positive. |
| $<_{\mathcal{A}}$ | For $c, d \in \mathcal{A}$, $c < d$ means $d - c$ is strictly positive, i.e., $d - c$ is positive and invertible. |
| $L^\infty(\Omega)$ | The space of complex-valued $L^\infty$ functions on a measure space $\Omega$ |
| $\mathcal{B}(\mathcal{W})$ | The space of bounded linear operators on a Hilbert space $\mathcal{W}$ |
| $\mathbb{C}^{m \times m}$ | A set of all complex-valued $m \times m$ matrices |
| $\mathcal{M}$ | A Hilbert $\mathcal{A}$-module |
| $\mathcal{X}$ | A nonempty set for data |
| $n$ | A natural number that represents the number of samples |
| $k$ | An $\mathcal{A}$-valued positive definite kernel |
| $\phi$ | The feature map endowed with $k$ |
| $\mathcal{M}_k$ | The RKHM associated with $k$ |
| $\mathcal{S}^\mathcal{X}$ | The set of all functions from a set $\mathcal{X}$ to a space $\mathcal{S}$ |
| $\tilde{k}$ | A complex-valued positive definite kernel |
| $\tilde{\phi}$ | The feature map endowed with $\tilde{k}$ |
| $\mathcal{H}_{\tilde{k}}$ | The RKHS associated with $\tilde{k}$ |
| $\mathcal{H}_{k}$ | The vv RKHS associated with $k$ |
| $\mathcal{D}(\mathcal{X}, \mathcal{A})$ | The set of all $\mathcal{A}$-valued finite regular Borel measures |
| $\Phi$ | The proposed KME in an RKHM |
| $\delta_x$ | The $\mathcal{A}$-valued Dirac measure defined as $\delta_x(E) = 1_{\mathcal{A}}$ for $x \in E$ and $\delta_x(E) = 0$ for $x \notin E$ |
| $\tilde{\delta}_x$ | The complex-valued Dirac measure defined as $\tilde{\delta}_x(E) = 1$ for $x \in E$ and $\tilde{\delta}_x(E) = 0$ for $x \notin E$ |
| $\mathcal{C}_0(\mathcal{X}, \mathcal{A})$ | The space of all continuous $\mathcal{A}$-valued functions on $\mathcal{X}$ vanishing at infinity |
| $\mathbf{G}$ | The $\mathcal{A}$-valued Gram matrix defined as $\mathbf{G}_{i,j} = k(x_i, x_j)$ for given samples $x_1, \ldots, x_n \in \mathcal{X}$ |
| $p_j$ | The $j$-th principal axis generated by kernel PCA with an RKHM |
| $r$ | A natural number that represents the number of principal axes |
| $Df_c$ | The Gâteaux derivative of a function $f : \mathcal{M} \to \mathcal{A}$ at $c \in \mathcal{M}$ |
| $\nabla f_c$ | The gradient of a function $f : \mathcal{M} \to \mathcal{A}$ at $c \in \mathcal{M}$ |

We begin by a positive definite kernel. Let $\mathcal{X}$ be a non-empty set for data, and $\tilde{k}$ be a positive definite kernel, which is defined as follows:

...
Definition 2.1 (Positive definite kernel) A map \( \hat{k} : \mathcal{X} \times \mathcal{X} \to \mathbb{C} \) is called a positive definite kernel if it satisfies the following conditions:

1. \( \hat{k}(x, y) = \hat{k}(y, x) \) for \( x, y \in \mathcal{X} \),
2. \( \sum_{i,j=1}^{n} \alpha_i \alpha_j \hat{k}(x_i, x_j) \geq 0 \) for \( n \in \mathbb{N} \), \( \alpha_i \in \mathbb{C} \), \( x_i \in \mathcal{X} \).

Let \( \tilde{\phi} : \mathcal{X} \to \mathbb{C}^{\mathcal{X}} \) be a map defined as \( \tilde{\phi}(x) = \hat{k}(\cdot, x) \). With \( \tilde{\phi} \), the following space as a subset of \( \mathbb{C}^{\mathcal{X}} \) is constructed:

\[
\mathcal{H}_{\hat{k},0} := \left\{ \sum_{i=1}^{n} \alpha_i \tilde{\phi}(x_i) \mid n \in \mathbb{N}, \alpha_i \in \mathbb{C}, x_i \in \mathcal{X} \right\}.
\]

Then, a map \( \langle \cdot, \cdot \rangle_{\mathcal{H}_{\hat{k}}} : \mathcal{H}_{\hat{k},0} \times \mathcal{H}_{\hat{k},0} \to \mathbb{C} \) is defined as follows:

\[
\left\langle \sum_{i=1}^{n} \alpha_i \tilde{\phi}(x_i), \sum_{j=1}^{l} \beta_j \tilde{\phi}(y_j) \right\rangle_{\mathcal{H}_{\hat{k}}} := \sum_{i=1}^{n} \sum_{j=1}^{l} \alpha_i \beta_j \hat{k}(x_i, y_j).
\]

By the properties in Definition 2.1 of \( \hat{k} \), \( \langle \cdot, \cdot \rangle_{\mathcal{H}_{\hat{k}}} \) is well-defined, satisfies the axiom of inner products, and has the reproducing property, that is,

\[
\langle \tilde{\phi}(x), v \rangle_{\mathcal{H}_{\hat{k}}} = v(x),
\]

for \( v \in \mathcal{H}_{\hat{k},0} \) and \( x \in \mathcal{X} \).

The completion of \( \mathcal{H}_{\hat{k},0} \) is called the RKHS associated with \( \hat{k} \) and denoted as \( \mathcal{H}_{\hat{k}} \). It can be shown that \( \langle \cdot, \cdot \rangle_{\mathcal{H}_{\hat{k}}} \) is extended continuously to \( \mathcal{H}_{\hat{k}} \) and the map \( \mathcal{H}_{\hat{k}} \ni v \mapsto \langle \tilde{\phi}(x), v \rangle_{\mathcal{H}_{\hat{k}}} \in \mathbb{C}^{\mathcal{X}} \) is injective. Thus, \( \mathcal{H}_{\hat{k}} \) is regarded to be a subset of \( \mathbb{C}^{\mathcal{X}} \) and has the reproducing property. Also, by the Moore-Aronszajn theorem, \( \mathcal{H}_{\hat{k}} \) is determined uniquely.

The map \( \tilde{\phi} \) maps data into \( \mathcal{H}_{\hat{k}} \), whose dimension is generally higher (often infinite dimensional) than that of \( \mathcal{X} \), and is called the feature map. Since the dimension of \( \mathcal{H}_{\hat{k}} \) is higher than that of \( \mathcal{X} \), complicated behaviors of data in \( \mathcal{X} \) are expected to be transformed into simple ones in \( \mathcal{H}_{\hat{k}} \) (Schölkopf and Smola, 2001).

2.2 Vector-valued RKHS (vv RKHS)

We review the theory of vv RKHS. Complex-valued functions in RKHSs are generalized to vector-valued functions in vv RKHSs. Similar to the case of RKHS, we begin by a positive definite kernel. Let \( \mathcal{X} \) be a non-empty set for data and \( \mathcal{W} \) be a Hilbert space. In addition, let \( k \) be an operator-valued positive definite kernel, which is defined as follows:

Definition 2.2 (Operator-valued positive definite kernel) A map \( k : \mathcal{X} \times \mathcal{X} \to \mathcal{B}(\mathcal{W}) \) is called an operator-valued positive definite kernel if it satisfies the following conditions:

1. \( k(x, y) = k(y, x)^* \) for \( x, y \in \mathcal{X} \),
2. \( \sum_{i,j=1}^{n} \langle w_i, k(x_i, x_j) w_j \rangle_{\mathcal{W}} \geq 0 \) for \( n \in \mathbb{N} \), \( w_i \in \mathcal{W} \), \( x_i \in \mathcal{X} \).

Here, \( * \) represents the adjoint.
Let $\phi : X \to \mathcal{B}(W)^X$ be a map defined as $\phi(x) = k(\cdot, x)$. With $\phi$, the following space as a subset of $W^X$ is constructed:

$$\mathcal{H}_{k,0}^\nu := \left\{ \sum_{i=1}^{n} \phi(x_i)w_i \bigg| \ n \in \mathbb{N}, \ w_i \in W, \ x_i \in X \right\}.$$  

Then, a map $\langle \cdot, \cdot \rangle_{\mathcal{H}_{k,0}^\nu} : \mathcal{H}_{k,0}^\nu \times \mathcal{H}_{k,0}^\nu \to \mathbb{C}$ is defined as follows:

$$\langle \sum_{i=1}^{n} \phi(x_i)w_i, \sum_{j=1}^{l} \phi(y_j)h_j \rangle_{\mathcal{H}_{k}^\nu} := \sum_{i=1}^{n} \sum_{j=1}^{l} \langle w_i, k(x_i, y_j)h_j \rangle_W.$$  

By the properties in Definition 2.2 of $k$, $\langle \cdot, \cdot \rangle_{\mathcal{H}_{k}^\nu}$ is well-defined, satisfies the axiom of inner products, and has the reproducing property, that is,

$$\langle \phi(x)w, u \rangle_{\mathcal{H}_{k}^\nu} = \langle w, u(x) \rangle_W, \quad (1)$$

for $u \in \mathcal{H}_{k,0}^\nu$, $x \in X$, and $w \in W$.

The completion of $\mathcal{H}_{k,0}^\nu$ is called the $vv$ RKHS associated with $k$ and denoted as $\mathcal{H}_{k}^\nu$. Note that since an inner product in $\mathcal{H}_{k}^\nu$ is defined with the complex-valued inner product in $W$, it is complex-valued.

### 2.3 $C^*$-algebra and Hilbert $C^*$-module

A $C^*$-algebra and a $C^*$-module are generalizations of the space of complex numbers $\mathbb{C}$ and a vector space, respectively. In this paper, we denote a $C^*$-algebra by $\mathcal{A}$ and a $C^*$-module by $\mathcal{M}$, respectively. As we see below, many complex-valued notions can be generalized to $\mathcal{A}$-valued.

A $C^*$-algebra is defined as a Banach space equipped with a product structure and an involution $(\cdot)^* : \mathcal{A} \to \mathcal{A}$. We denote the norm of $\mathcal{A}$ by $\| \cdot \|_\mathcal{A}$.

**Definition 2.3 (C*-algebra)**  A set $\mathcal{A}$ is called a $C^*$-algebra if it satisfies the following conditions:

1. $\mathcal{A}$ is an algebra over $\mathbb{C}$, and there exists a bijection $(\cdot)^* : \mathcal{A} \to \mathcal{A}$ that satisfies the following conditions for $\alpha, \beta \in \mathbb{C}$ and $c, d \in \mathcal{A}$:
   - $(\alpha c + \beta d)^* = \alpha c^* + \beta d^*$,
   - $(cd)^* = d^*c^*$,
   - $(c^*)^* = c$

2. $\mathcal{A}$ is a norm space with $\| \cdot \|_\mathcal{A}$, and for $c, d \in \mathcal{A}$, $\| cd \|_\mathcal{A} \leq \| c \|_\mathcal{A} \| d \|_\mathcal{A}$ holds. In addition, $\mathcal{A}$ is complete with respect to $\| \cdot \|_\mathcal{A}$.

3. For $c \in \mathcal{A}$, $\| ce \|_\mathcal{A} = \| c \|_\mathcal{A}^2$ holds.

**Definition 2.4 (Multiplicative identity and unital C*-algebra)**  The multiplicative identity of $\mathcal{A}$ is the element $a \in \mathcal{A}$ which satisfies $ac = ca = c$ for any $c \in \mathcal{A}$. We denote by $1_\mathcal{A}$ the multiplicative identity of $\mathcal{A}$. If a $C^*$-algebra $\mathcal{A}$ has the multiplicative identity, then it is called a unital $C^*$-algebra.
In this paper, we focus on a special type of $C^*$-algebras called von Neumann-algebra because several important properties for data analysis are available for von Neumann-algebra. For example, the Riesz representation theorem (Proposition 4.13) is available.

**Definition 2.5 (von Neumann-algebra)** A $C^*$-algebra $A$ is called a von Neumann-algebra if $A$ is isomorphic to the dual Banach space of some Banach space.

**Example 2.6** Important examples of (unital) von Neumann-algebras are $L^\infty(\Omega)$ and $B(W)$, i.e., the space of complex-valued $L^\infty$ functions on a compact measure space $\Omega$ and the space of bounded linear operators on a Hilbert space $W$, respectively.

1. For $A = L^\infty(\Omega)$, the product of two functions $c,d \in A$ is defined as $(cd)(t) = c(t)d(t)$ for any $t \in \Omega$, the involution is defined as $c(t) = \overline{c(t)}$, the norm is the $L^\infty$-norm, and the multiplicative identity is the constant function whose value is 1 at almost everywhere $t \in \Omega$.

2. For $A = B(W)$, the product structure is the product (the composition) of operators, the involution is the adjoint, the norm $\| \cdot \|_A$ is the operator norm, and the multiplicative identity is the identity map.

The positiveness is also important in $C^*$-algebras.

**Definition 2.7 (Positive)** An element $c$ of $A$ is called positive if there exists $d \in A$ such that $c = d^*d$ holds. If a positive element $c \in A$ is invertible, i.e., there exists $d \in A$ such that $cd = dc = 1_A$, then $c$ is called strictly positive. For $c,d \in A$, we denote $c \leq_A d$ if $d - c$ is positive and $c <_A d$ if $d - c$ is strictly positive. We denote by $A_+$ the subset of $A$ composed of all positive elements in $A$.

**Example 2.8** 1. For $A = L^\infty(\Omega)$, a function $c \in A$ is positive if and only if $c(t) \geq 0$ for almost everywhere $t \in \Omega$, and strictly positive if and only is $c(t) > 0$ for almost everywhere $t \in \Omega$.

2. For $A = B(W)$, the positiveness is equivalent to the positive semi-definiteness of operators and the strictly positiveness is equivalent to the positive definiteness of operators.

The positiveness provides us the (pre) order in $A$ and, thus, enables us to consider optimization problems in $A$.

**Definition 2.9 (Supremum and infimum)** 1. For a subset $S$ of $A$, $a \in A$ is said to be an upper bound with respect to the order $\leq_A$, if $d \leq_A a$ for any $d \in S$. Then, $c \in A$ is said to be a supremum of $S$, if $c \leq_A a$ for any upper bound $a$ of $S$.

2. For a subset $S$ of $A$, $a \in A$ is said to be a lower bound with respect to the order $\leq_A$, if $a \leq_A d$ for any $d \in S$. Then, $c \in A$ is said to be an infimum of $S$, if $a \leq_A c$ for any lower bound $a$ of $S$.

We now introduce a $C^*$-module over $A$, which is a generalization of the vector space.

**Definition 2.10 (Right multiplication)** Let $M$ be an abelian group with operation $+$. For $c,d \in A$ and $u,v \in M$, if an operation $\cdot : M \times A \to M$ satisfies
1. \((u + v) \cdot c = u \cdot c + v \cdot c\),
2. \(u \cdot (c + d) = u \cdot c + u \cdot d\)
3. \(u \cdot (cd) = (u \cdot d) \cdot c\)
4. \(u \cdot 1_A = u\),

then, \(\cdot\) is called a (right) \(A\)-multiplication. The multiplication \(u \cdot c\) is usually denoted as \(uc\).

**Definition 2.11 \((C^*)\)-module** Let \(\mathcal{M}\) be an abelian group with operation \(+\). If \(\mathcal{M}\) has the structure of a (right) \(A\)-multiplication, \(\mathcal{M}\) is called a (right) \(C^*\)-module over \(A\).

In this paper, we consider column vectors rather than row vectors for representing \(A\)-valued coefficients, and column vectors act on the right. Therefore, we consider right multiplications. However, considering row vectors and left multiplications instead of column vectors and right multiplications is also possible.

### 2.4 Hilbert \(C^*\)-module

A Hilbert \(C^*\)-module is a generalization of a Hilbert space. We first consider an \(A\)-valued inner product, which is a generalization of a complex-valued inner product and, then, introduce the definition of a Hilbert \(C^*\)-module.

**Definition 2.12 \((A\text{-valued inner product})\)** A map \(\langle \cdot, \cdot \rangle_M : \mathcal{M} \times \mathcal{M} \to A\) is called an \(A\)-valued inner product if it satisfies the following properties for \(u, v, p \in \mathcal{M}\) and \(c, d \in A\):

1. \(\langle u, vc + pd \rangle_M = \langle u, v \rangle_M c + \langle u, p \rangle_M d\)
2. \(\langle v, u \rangle_M = \langle u, v \rangle_M^*\)
3. \(\langle u, u \rangle_M \geq_A 0\)
4. If \(\langle u, u \rangle_M = 0\) then \(u = 0\)

**Definition 2.13 \((A\text{-valued absolute value and norm})\)** For \(u \in \mathcal{M}\), the \(A\)-valued absolute value \(|u|_M\) on \(\mathcal{M}\) is defined by the positive element \(|u|_M\) of \(A\) such that \(|u|_M^2 = \langle u, u \rangle_M\). The (real-valued) norm \(\|\cdot\|_M\) on \(\mathcal{M}\) is defined by \(\|u\|_M = \| |u|_M \|_A\).

Since the absolute value \(|\cdot|_M\) takes values in \(A\), it behaves more complicatedly, but provides us with more information than the norm \(\|\cdot\|_M\) (which are real-valued).

**Definition 2.14 \((Hilbert C^*\text{-module})\)** Let \(\mathcal{M}\) be a (right) \(C^*\)-module over \(A\) equipped with an \(A\)-valued inner product defined in Definition 2.12. If \(\mathcal{M}\) is complete with respect to the norm \(\|\cdot\|_M\), it is called a Hilbert \(C^*\)-module over \(A\) or Hilbert \(A\)-module.

**Example 2.15** A simple example of Hilbert \(C^*\) modules over \(A\) is \(A^n\) for a natural number \(n\). The \(A\)-valued inner product between \(c = [c_1, \ldots, c_n]^T\) and \(d = [d_1, \ldots, d_n]^T\) is defined as \(\langle c, d \rangle_{A^n} = \sum_{i=1}^n c_i^* d_i\). The absolute value and norm in \(A^n\) are given as \(|c|_{A^n}^2 = \sum_{i=1}^n c_i^* c_i\) and \(\|c\|_{A^n} = \| \sum_{i=1}^n c_i^* c_i \|_A^{1/2}\).
Similar to the case of Hilbert spaces, the following Cauchy–Schwarz inequality for $A$-valued inner products is available (Lance, 1995, Proposition 1.1).

**Lemma 2.16 (Cauchy–Schwarz inequality)** For $u, v \in \mathcal{M}$, the following inequality holds:

$$|\langle u, v \rangle_{\mathcal{M}}|^2_A \leq \|u\|_A^2 \langle v, v \rangle_{\mathcal{M}}.$$

An important property associated with an inner product is the orthonormality. The orthonormality plays an important role in data analysis because, for example, an orthonormal basis constructs orthogonal projections and an orthogonally projected vector minimizes the deviation from its original vector in the projected space. Therefore, we also introduce the orthonormality in Hilbert $C^*$-module. See, for example, Definition 1.2 in (Bakić and Guljaš, 2001) for more details.

**Definition 2.17 (Normalized)** A vector $q \in \mathcal{M}$ is normalized if $0 \neq \langle q, q \rangle_{\mathcal{M}} = \langle q, q \rangle_{\mathcal{M}}^2$. Note that in the case of a general $C^*$-valued-inner product, for a normalized vector $q$, $\langle q, q \rangle_{\mathcal{M}}$ is not always equal to the identity of $A$ in contrast to the case of a complex-valued inner product.

**Definition 2.18 (Orthonormal system and basis)** Let $\mathcal{I}$ be an index set. A set $\mathcal{S} = \{q_i\}_{i \in \mathcal{I}} \subseteq \mathcal{M}$ is called an orthonormal system (ONS) of $\mathcal{M}$ if $q_i$ is normalized for any $i \in \mathcal{I}$ and $\langle q_i, q_j \rangle_{\mathcal{M}} = 0$ for $i \neq j$. We call $\mathcal{S}$ an orthonormal basis (ONB) if $\mathcal{S}$ is an ONS and dense in $\mathcal{M}$.

In Hilbert $C^*$-modules, $A$-linear is often used instead of $C$-linear.

**Definition 2.19 ($A$-linear operator)** Let $\mathcal{M}_1, \mathcal{M}_2$ be Hilbert $A$-modules. A linear map $L : \mathcal{M}_1 \to \mathcal{M}_2$ is referred to as $A$-linear if it satisfies $L(uc) = (Lu)c$ for any $u \in \mathcal{M}$ and $c \in A$.

**Definition 2.20 ($A$-linearly independent)** The set $\mathcal{S}$ of $\mathcal{M}$ is said to be $A$-linearly independent if it satisfies the following condition: For any finite subset $\{v_1, \ldots, v_n\}$ of $\mathcal{S}$, if $\sum_{i=1}^n v_ic_i = 0$ for $c_i \in A$, then $c_i = 0$ for $i = 1, \ldots, n$.

For further details about $C^*$-algebra, $C^*$-module, and Hilbert $C^*$-module, refer to Murphy (1990); Lance (1995).

3. RKHM for data analysis

We first review the theory of RKHM in Subsection 3.1, and then develop theories for the validity to apply it to data analysis in Subsection 3.2. Also, we investigate the connection of RKHM with RKHS and vv RKHS in Subsection 3.3.

Here, we set $\mathcal{A}$ as a unital von Neumann-algebra (see Definitions 2.4, 2.5, and Example 2.6) to derive useful properties of RKHM for data analysis.

**Assumption 3.1** We assume $\mathcal{A}$ is a unital von Neumann-algebra throughout this paper.
3.1 Reproducing kernel Hilbert $C^*$-module (RKHM)

We summarize the theory of RKHM, which is discussed, for example, in Heo (2008). We give proofs for the Lemmas and Propositions in this section in Appendix A.

Similar to the case of RKHS, we begin by an $A$-valued generalization of a positive definite kernel on a non-empty set $\mathcal{X}$ for data.

**Definition 3.2 (A-valued positive definite kernel)** An $A$-valued map $k : \mathcal{X} \times \mathcal{X} \to A$ is called a positive definite kernel if it satisfies the following conditions:

1. $k(x, y) = k(y, x)^* \quad \text{for } x, y \in \mathcal{X},$
2. $\sum_{i,j=1}^n c_i^* k(x_i, x_j) c_j \geq_A 0 \quad \text{for } n \in \mathbb{N}, \ c_i \in A, \ x_i \in \mathcal{X}.$

**Example 3.3** 1. Let $\mathcal{X} = C([0, 1]^m).$ Let $A = L^\infty([0, 1])$ and let $k : \mathcal{X} \times \mathcal{X} \to A$ be defined as $k(x, y)(t) = \int_{[0, 1]^m} (t-x(s))(t-y(s))ds$ for $t \in [0, 1].$ Then, for $x_1, \ldots, x_n \in \mathcal{X}, \ c_1, \ldots, c_n \in A$ and $t \in [0, 1],$ we have

$$\sum_{i,j=1}^n c_i^* k(x_i, x_j)(t)c_j(t) = \int_{[0, 1]^m} \sum_{i,j=1}^n c_i(t)^* (t-x_i(s))(t-x_j(s))c_j(t)ds$$

$$= \int_{[0, 1]^m} \sum_{i=1}^n (t-x_i(s)) \sum_{j=1}^n (t-x_j(s))ds \geq 0,$$

for $t \in [0, 1].$ Thus, $k$ is an $A$-valued positive definite kernel.

2. Let $A = L^\infty([0, 1])$ and $k : \mathcal{X} \times \mathcal{X} \to A$ be defined such that $k(x, y)(t)$ is a complex-valued positive definite kernel for any $t \in [0, 1].$ Then, $k$ is an $A$-valued positive definite kernel.

3. Let $\mathcal{W}$ be a separable Hilbert space and let $\{e_i\}_{i=1}^\infty$ be an orthonormal basis of $\mathcal{W}.$ Let $A = \mathcal{B}(\mathcal{W})$ and let $k : \mathcal{X} \times \mathcal{X} \to A$ be defined as $k(x, y)e_i = k_i(x, y)e_i,$ where $k_i : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ is a complex-valued positive definite kernel for any $i = 1, 2, \ldots.$ Then, for $x_1, \ldots, x_n \in \mathcal{X}, \ c_1, \ldots, c_n \in A$ and $w \in \mathcal{W},$ we have

$$\left\langle w, \left( \sum_{i,j=1}^n c_i^* k(x_i, x_j)c_j \right) w \right\rangle_{\mathcal{W}} = \sum_{i,j=1}^n \sum_{l=1}^\infty \langle \alpha_i e_l, k(x_i, x_j)\alpha_j e_l \rangle_{\mathcal{W}}$$

$$= \sum_{l=1}^\infty \sum_{i,j=1}^n \overline{\alpha_i} \alpha_j k_l(x_i, x_j) \geq 0,$$

where $c_i w = \sum_{l=1}^\infty \alpha_i e_l$ is the expansion with respect to $\{e_i\}_{i=1}^\infty.$ Thus, $k$ is an $A$-valued positive definite kernel.

We remark that in the case of $A = \mathcal{B}(\mathcal{W}),$ Definition 3.2 is equivalent to the operator valued positive definite kernel (Definition 2.2) for the theory of vv-RKHSs.

**Lemma 3.4 (Connection between Definition 3.2 and Definition 2.2)** If $A = \mathcal{B}(\mathcal{W}),$ then, the $A$-valued positive definite kernel defined in Definition 3.2 is equivalent to the operator valued positive definite kernel defined in Definition 2.2.

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Let $\phi : \mathcal{X} \to A^\mathcal{X}$ be the feature map associated with $k$, which is defined as $\phi(x) = k(\cdot, x)$ for $x \in \mathcal{X}$. Similar to the case of RKHS, we construct the following $C^*$-module composed of $A$-valued functions by means of $\phi$:

$$\mathcal{M}_{k,0} := \left\{ \sum_{i=1}^{n} \phi(x_i)c_i \Big| n \in \mathbb{N}, \ c_i \in A, \ x_i \in \mathcal{X} \right\}.$$

An $A$-valued map $\langle \cdot, \cdot \rangle_{\mathcal{M}_k} : \mathcal{M}_{k,0} \times \mathcal{M}_{k,0} \to A$ is defined as follows with $k$:

$$\langle \sum_{i=1}^{n} \phi(x_i)c_i, \sum_{j=1}^{l} \phi(y_j)d_j \rangle_{\mathcal{M}_k} := \sum_{i=1}^{n} \sum_{j=1}^{l} c^*_i k(x_i, y_j)d_j.$$

By the properties in Definition 3.2 of $k$, $\langle \cdot, \cdot \rangle_{\mathcal{M}_k}$ is well-defined and has the reproducing property

$$\langle \phi(x), v \rangle_{\mathcal{M}_k} = v(x),$$

for $v \in \mathcal{M}_{k,0}$ and $x \in \mathcal{X}$. Also, it satisfies the properties in Definition 2.12. As a result, $\langle \cdot, \cdot \rangle_{\mathcal{M}_k}$ is shown to be an $A$-valued inner product.

The reproducing kernel Hilbert $A$-module (RKHM) associated with $k$ is defined as the completion of $\mathcal{M}_{k,0}$. We denote by $\mathcal{M}_k$ the RKHM associated with $k$. Similar to the cases of RKHSs, $\langle \cdot, \cdot \rangle_{\mathcal{M}_k}$ is extended continuously to the RKHM and has the reproducing property. Also, the RKHM is uniquely determined.

**Proposition 3.5** The map $\langle \cdot, \cdot \rangle_{\mathcal{M}_k}$ defined on $\mathcal{M}_{k,0}$ is extended continuously to $\mathcal{M}_k$ and the map $\mathcal{M}_k \ni v \mapsto x \mapsto \langle \phi(x), v \rangle_{\mathcal{M}_k} \in A^\mathcal{X}$ is injective. Thus, $\mathcal{M}_k$ is regarded to be the subset of $A^\mathcal{X}$ and has the reproducing property.

**Proposition 3.6** Assume a Hilbert $C^*$-module $\mathcal{M}$ over $A$ and a map $\psi : \mathcal{X} \to \mathcal{M}$ satisfy the following conditions:

1. $\forall x, y \in \mathcal{X}, \langle \psi(x), \psi(y) \rangle_{\mathcal{M}} = k(x, y)$
2. $\left\{ \sum_{i=1}^{n} \psi(x_i)c_i \Big| x_i \in \mathcal{X}, \ c_i \in A \right\} = \mathcal{M}$

Then, there exists a unique $A$-linear bijection map $\Psi : \mathcal{M}_k \to \mathcal{M}$ that preserves the inner product and satisfies the following commutative diagram:

$$\begin{align*}
\mathcal{M}_k & \xrightarrow{\psi} \mathcal{M} \\
\phi \downarrow & \quad \downarrow \circ \Psi \\
\mathcal{X} & \xrightarrow{\psi} \mathcal{M}
\end{align*}$$

**3.2 Some theories on RKHM for data analysis**

We now develop some theories for the validity to apply RKHM to data analysis. First, we show a minimization property of orthogonal projection operators, which is a fundamental property in Hilbert spaces, is also available in Hilbert $C^*$-modules.
Proof Since Troitsky, 2000, Proposition 2.5.4), i.e.,

\[ 2 \times A \]

Let Theorem 3.8 (Representer theorem) \( C \) from an original vector in \( V \). Proposition 3.7 shows the orthogonally projected vector uniquely minimizes the deviation which implies \( |v - u|_M^2 \leq |v - u_1|_M^2 \). Therefore, setting \( u_1 = u \) holds and the uniqueness of \( u_1 \) has been proved.

Moreover, if there exists \( u' \in V \) such that \( |u - u_1|_M^2 = |u - u'|_M^2 \), letting \( v = u' \) in Eq. (3) derives \( |u - u'|_M^2 = |u_2|_M^2 + |u_1 - u'|_M^2 \), which implies \( |u_1 - u'|_M^2 = 0 \). As a result, \( u_1 = u' \) holds and the uniqueness of \( u_1 \) has been proved.

Proposition 3.7 shows the orthogonally projected vector uniquely minimizes the deviation from an original vector in \( V \). Thus, we can generalize methods related to orthogonal projections in Hilbert spaces to Hilbert \( C^* \)-modules.

Next, we show the representer theorem in RKHMs.

Theorem 3.8 (Representer theorem) Let \( x_1, \ldots, x_n \in X \) and \( a_1, \ldots, a_n \in A \). Let \( h : X \times A^2 \to A_+ \) be an error function and let \( g : A_+ \to A_+ \) satisfy \( g(c) \leq_A g(d) \) for \( c \leq_A d \). Then, any \( u \in M_k \) minimizing \( \sum_{i=1}^n h(x_i, a_i, u(x_i)) + g(|u|_{M_k}) \) admits a representation of the form \( \sum_{i=1}^n \phi(x_i)c_i \) for some \( c_1, \ldots, c_n \in A \).

Proof Let \( V \) be the space spanned by \( \{\phi(x_i)\}_{i=1}^n \). Since \( V \) is orthogonally complemented, \( u \in M_k \) is decomposed into \( u = u_1 + u_2 \), where \( u_1 \in V, u_2 \in V^\perp \). By the reproducing property of \( M_k \), the following equalities are derived for \( i = 1, \ldots, n \):

\[ u(x_i) = \langle \phi(x_i), u \rangle_{M_k} = \langle \phi(x_i), u__{M_k} = \langle \phi(x_i), u_1 \rangle_{M_k} + \langle \phi(x_i), u_2 \rangle_{M_k}. \]

Thus, \( \sum_{i=1}^n h(x_i, a_i, u(x_i)) \) is independent of \( u_2 \). As for the term \( g(|u|_{M_k}) \), since \( g \) satisfies \( g(c) \leq_A g(d) \) for \( c \leq_A d \), we have

\[ g(|u|_{M_k}) = g(|u_1 + u_2|_{M_k}) = g\left(\left(|u_1|_{M_k}^2 + |u_2|_{M_k}^2\right)^{1/2}\right) \geq_A g(|u_1|_{M_k}). \]

Therefore, setting \( u_2 = 0 \) does not affect the term \( \sum_{i=1}^n h(x_i, a_i, u(x_i)) \), while strictly reducing the term \( g(|u|_{M_k}) \), which implies any minimizer must have \( u_2 = 0 \). As a result, any minimizer takes the form \( \sum_{i=1}^n \phi(x_i)c_i \).
3.3 Connection with RKHSs and vv RKHSs

We show that the framework of RKHM is more general than those of RKHS and vv RKHS. Let \( \hat{k} \) be a complex-valued positive definite kernel and let \( \mathcal{H}_{\hat{k}} \) be the RKHS associated with \( \hat{k} \). In addition, let \( k \) be an \( \mathcal{A} \)-valued positive definite kernel and \( \mathcal{M}_{k} \) be the RKHM associated with \( k \). The following proposition is derived by the definitions of RKHSs and RKHMs.

**Proposition 3.9 (Connection between RKHMs with RKHSs)** If \( \mathcal{A} = \mathbb{C} \) and \( k = \hat{k} \), then \( \mathcal{H}_{\hat{k}} = \mathcal{M}_{k} \).

Let \( \mathcal{A} = \mathcal{B}(W) \) and let \( \mathcal{H}_{k}^{v} \) be the vv RKHS associated with \( k \). To investigate the connection between vv RKHSs and RKHMs, we introduce the notion of interior tensor (Lance, 1995, Chapter 4).

**Proposition 3.10** Let \( \mathcal{M} \) be a Hilbert \( \mathcal{B}(W) \)-module. The map \( \langle \cdot, \cdot \rangle_{\mathcal{M} \otimes W} : \mathcal{M} \otimes W \times \mathcal{M} \otimes W \rightarrow \mathbb{C} \) defined as
\[
\langle v \otimes w, u \otimes h \rangle_{\mathcal{M} \otimes W} = \langle w, \langle v, u \rangle_{\mathcal{M}} h \rangle_{W},
\]
is a complex-valued pre inner product on \( \mathcal{M} \otimes W \).

**Definition 3.11 (Interior tensor)** The completion of \( \mathcal{M} \otimes W \) with respect to the pre inner product \( \langle \cdot, \cdot \rangle_{\mathcal{M} \otimes W} \) is referred to as the interior tensor between \( \mathcal{M} \) and \( W \), and denoted as \( \mathcal{M} \otimes_{\mathcal{B}(W)} W \).

Note that \( \mathcal{M} \otimes_{\mathcal{B}(W)} W \) is a Hilbert space. We now show vv RKHSs are reconstructed by the interior tensor between RKHMs and \( W \).

**Theorem 3.12 (Connection between RKHMs and vv RKHSs)** If \( \mathcal{A} = \mathcal{B}(W) \), then two Hilbert spaces \( \mathcal{H}_{k}^{v} \) and \( \mathcal{M} \otimes_{\mathcal{B}(W)} W \) are isomorphic.

Theorem 3.12 is derived by the following lemma.

**Lemma 3.13** There exists a unique unitary map \( U : \mathcal{M}_{k} \otimes_{\mathcal{B}(W)} W \rightarrow \mathcal{H}_{k}^{v} \) such that \( U(\phi(x)c \otimes w) = \phi(x)(cw) \) holds for all \( x \in \mathcal{X}, c \in \mathcal{B}(W) \) and \( w \in W \).

**Proof** First, we show that
\[
\left\langle \sum_{i=1}^{n} \phi(x_{i})c_{i} \otimes w_{i}, \sum_{j=1}^{l} \phi(y_{j})d_{j} \otimes h_{j} \right\rangle_{\mathcal{M}_{k} \otimes W} = \left\langle \sum_{i=1}^{n} \phi(x_{i})(c_{i}w_{i}), \sum_{j=1}^{l} \phi(y_{j})(d_{j}h_{j}) \right\rangle_{\mathcal{H}_{k}^{v}}
\]
holds for all \( \sum_{i=1}^{n} \phi(x_{i})c_{i} \otimes w_{i}, \sum_{j=1}^{l} \phi(y_{j})d_{j} \otimes h_{j} \in \mathcal{M}_{k} \otimes_{\mathcal{B}(W)} W \). This follows from the straightforward calculation. Indeed, we have
\[
\left\langle \sum_{i=1}^{n} \phi(x_{i})c_{i} \otimes w_{i}, \sum_{j=1}^{l} \phi(y_{j})d_{j} \otimes h_{j} \right\rangle_{\mathcal{M}_{k} \otimes W} = \sum_{i=1}^{n} \sum_{j=1}^{l} \langle w_{i}, \phi(x_{i})c_{i}, \phi(y_{j})d_{j} \rangle_{\mathcal{M}_{k}} h_{j} \rangle_{W} \]
\[
= \sum_{i=1}^{n} \sum_{j=1}^{l} \langle w_{i}, c_{i}^{*}k(x_{i}, y_{j})d_{j}h_{j} \rangle_{W} = \sum_{i=1}^{n} \sum_{j=1}^{l} \langle c_{i}w_{i}, k(x_{i}, y_{j})d_{j}h_{j} \rangle_{W} \]
\[
= \left\langle \sum_{i=1}^{n} \phi(x_{i})(c_{i}w_{i}), \sum_{j=1}^{l} \phi(y_{j})(d_{j}h_{j}) \right\rangle_{\mathcal{H}_{k}^{v}}.
\]
Therefore, by the standard functional analysis argument, it turns out that there exists an isometry $U: M_k \otimes_{\mathbb{R}} W \rightarrow \mathcal{H}_k^v$ such that $U(\phi(x)c \otimes w) = \phi(x)(cw)$ holds for all $x \in X$, $c \in \mathcal{B}(W)$ and $w \in W$. Since the image of $U$ is closed and dense in $\mathcal{H}_k^v$, $U$ is surjective. Thus $U$ is a unitary map.

4. Kernel mean embedding in RKHM

We generalize KME, which is widely used in analyzing distributions, in RKHSs to RKHMs. By using the framework of RKHM, we can embed $A$-valued measures instead of probability measures (more generally, complex-valued measures). We first review $A$-valued measures and the integral with respect to $A$-valued measures in Subsection 4.1, define a KME in RKHMs in Subsection 4.2 and show its theoretical properties in Subsection 4.3.

To define a KME by using $A$-valued measures and integrals, we first define $c_0$-kernels.

**Definition 4.1 (Function space $C_0(X, A)$)** For a locally compact Hausdorff space $X$, the set of all $A$-valued continuous functions on $X$ vanishing at infinity is denoted as $C_0(X, A)$. Here, an $A$-valued continuous function $u$ is said to vanish at infinity if the set $\{x \in X | \|u(x)\|_A \geq \epsilon\}$ is compact for any $\epsilon > 0$. The space $C_0(X, A)$ is a Banach $A$-module with respect to the sup norm.

Note that if $X$ is compact, any continuous function is contained in $C_0(X, A)$.

**Definition 4.2 ($c_0$-kernel)** Let $X$ be a locally compact Hausdorff space. An $A$-valued positive definite kernel $k : X \times X \rightarrow A$ is referred to as a $c_0$-kernel if $k$ is bounded and $\phi(x) \in C_0(X, A)$ for any $x \in X$.

In this section, we impose the following assumption.

**Assumption 4.3** We assume $X$ is a locally compact Hausdorff space and $k$ is an $A$-valued $c_0$-positive definite kernel in Section 4.

For example, we often consider $X = \mathbb{R}^d$ in practical situations. Also, we provide examples of $c_0$-kernels as follows.

**Example 4.4**
1. Let $A = L^\infty([0,1])$ and $k$ is an $A$-valued positive definite kernel defined such that $k(x,y)(t)$ is a complex-valued $c_0$-positive definite kernel for $t \in [0,1]$ (see Example 3.3.2). If $\|k(x,y)\|_A$ is continuous with respect to $y$ for any $x \in X$, then the inclusion
   $$\{y \in X | \|k(x,y)\|_A \geq \epsilon\} \subseteq \{y \in X | k(x,y)(t_0) \geq \epsilon\},$$
holds for some $t_0 \in [0,1]$ and any $x \in X$ and $\epsilon > 0$. Since $k(\cdot, \cdot)(t_0)$ is a $c_0$-kernel, the set $\{y \in X | k(x,y)(t_0) \geq \epsilon\}$ is compact (see Definition 4.1). Thus, $\{y \in X | \|k(x,y)\|_A \geq \epsilon\}$ is also compact and $k$ is an $A$-valued $c_0$-positive definite kernel. Examples of complex-valued $c_0$-positive definite kernel are Gaussian, Laplacian and $B_{2n+1}$-spline kernels.
2. Let \( \mathcal{W} \) be a separable Hilbert space and let \( \{e_i\}_{i=1}^{\infty} \) be an orthonormal basis of \( \mathcal{W} \). Let \( \mathcal{A} = \mathcal{B}(\mathcal{W}) \) and let \( k : \mathcal{X} \times \mathcal{X} \to \mathcal{A} \) be defined as \( k(x,y)e_i = k_i(x,y)e_i \), where \( k_i : \mathcal{X} \times \mathcal{X} \to \mathbb{C} \) is a complex-valued positive definite kernel for any \( i = 1, 2, \ldots \) (see Example 3.3.3). If \( \|k(x,y)\|_\mathcal{A} \) is continuous with respect to \( y \) for any \( x \in \mathcal{X} \), \( k \) is shown to be an \( \mathcal{A} \)-valued \( c_0 \)-positive definite kernel in the same manner as the above example.

4.1 \( \mathcal{A} \)-valued measure and integral

We introduce \( \mathcal{A} \)-valued measure and integral in preparation for defining a KME in RKHMs. The notions of measures and the Lebesgue integrals are generalized to \( \mathcal{A} \)-valued. The left and right integral of an \( \mathcal{A} \)-valued function \( u \) with respect to an \( \mathcal{A} \)-valued measure \( \mu \) is defined through \( \mathcal{A} \)-valued step functions.

**Definition 4.5 (\( \mathcal{A} \)-valued measure)** Let \( \Sigma \) be a \( \sigma \)-algebra on \( \mathcal{X} \).

1. An \( \mathcal{A} \)-valued map \( \mu : \Sigma \to \mathcal{A} \) is called a (countably additive) \( \mathcal{A} \)-valued measure if \( \mu(\bigcup_{i=1}^{\infty} E_i) = \sum_{i=1}^{\infty} \mu(E_i) \) for all countable collections \( \{E_i\}_{i=1}^{\infty} \) of pairwise disjoint sets in \( \Sigma \).

2. An \( \mathcal{A} \)-valued measure \( \mu \) is said to be finite if \( |\mu| := \sup\{\sum_{i=1}^{n} \|\mu(E_i)\|_\mathcal{A} \mid n \in \mathbb{N}, \{E_i\}_{i=1}^{n} \) is a finite partition of \( E \in \Sigma \} < \infty \). We call \( |\mu| \) the total variation of \( \mu \).

3. An \( \mathcal{A} \)-valued measure \( \mu \) is said to be regular if for all \( E \in \Sigma \) and \( \epsilon > 0 \), there exist a compact set \( K \subseteq E \) and open set \( G \supseteq E \) such that \( \|\mu(F)\|_\mathcal{A} \leq \epsilon \) for any \( F \subseteq G \setminus K \). The regularity corresponds to the continuity of \( \mathcal{A} \)-valued measures.

4. An \( \mathcal{A} \)-valued measure \( \mu \) is called a Borel measure if \( \Sigma = \mathcal{B} \), where \( \mathcal{B} \) is the Borel \( \sigma \)-algebra on \( \mathcal{X} \) (\( \sigma \)-algebra generated by all compact subsets of \( \mathcal{X} \)).

The set of all \( \mathcal{A} \)-valued finite regular Borel measures is denoted as \( \mathcal{D}(\mathcal{X}, \mathcal{A}) \).

**Definition 4.6 (\( \mathcal{A} \)-valued Dirac measure)** For \( x \in \mathcal{X} \), we define \( \delta_x \in \mathcal{D}(\mathcal{X}, \mathcal{A}) \) as \( \delta_x(E) = 1_A \) for \( x \in E \) and \( \delta_x(E) = 0 \) for \( x \notin E \). The measure \( \delta_x \) is referred to as the \( \mathcal{A} \)-valued Dirac measure at \( x \).

Similar to the Lebesgue integrals, an integral of an \( \mathcal{A} \)-valued function with respect to an \( \mathcal{A} \)-valued measure is defined through \( \mathcal{A} \)-valued step functions.

**Definition 4.7 (Step function)** An \( \mathcal{A} \)-valued map \( s : \mathcal{X} \to \mathcal{A} \) is called a step function if \( s(x) = \sum_{i=1}^{n} c_i \chi_{E_i}(x) \) for some \( n \in \mathbb{N} \), \( c_i \in \mathcal{A} \) and finite partition \( \{E_i\}_{i=1}^{n} \) of \( \mathcal{X} \), where \( \chi_E : \mathcal{X} \to \{0,1\} \) is the indicator function for \( E \in \mathcal{B} \). The set of all \( \mathcal{A} \)-valued step functions on \( \mathcal{X} \) is denoted as \( \mathcal{S}(\mathcal{X}, \mathcal{A}) \).

**Definition 4.8 (Integrals of functions in \( \mathcal{S}(\mathcal{X}, \mathcal{A}) \))** For \( s \in \mathcal{S}(\mathcal{X}, \mathcal{A}) \) and \( \mu \in \mathcal{D}(\mathcal{X}, \mathcal{A}) \), the left and right integrals of \( s \) with respect to \( \mu \) are respectively defined as

\[
\int_{x \in \mathcal{X}} s(x) d\mu(x) := \sum_{i=1}^{n} c_i \mu(E_i), \quad \int_{x \in \mathcal{X}} d\mu(x) s(x) := \sum_{i=1}^{n} \mu(E_i) c_i.
\]
As we explain below, the integrals of step functions are extended to those of “integrable functions”. For a real positive finite measure \( \nu \), let \( L^1_\nu(X,A) \) be the set of all \( A \)-valued \( \nu \)-Bochner integrable functions on \( X \), i.e., if \( u \in L^1_\nu(X,A) \), there exists a sequence \( \{ s_i \}_{i=1}^\infty \subseteq S(X,A) \) of step functions such that \( \lim_{i \to \infty} \int_{x \in X} \| u(x) - s_i(x) \|_A d\nu(x) = 0 \) (Diestel, 1984, Chapter IV). Note that \( u \in L^1_\nu(X,A) \) if and only if \( \int_{x \in X} \| u(x) \|_A d\nu(x) < \infty \), and \( L^1_\nu(X,A) \) is a Banach \( A \)-module (i.e., a Banach space equipped with an \( A \)-module structure) with respect to the norm defined as \( \| u \|_{L^1_\nu(X,A)} = \int_{x \in X} \| u(x) \|_A d\nu(x) \).

**Definition 4.9 (Integrals of functions in \( L^1_\nu(X,A) \))** For \( u \in L^1_\nu(X,A) \), the left and right integrals of \( u \) with respect to \( \mu \) is respectively defined as

\[
\lim_{i \to \infty} \int_{x \in X} d\mu(x)s_i(x), \quad \lim_{i \to \infty} \int_{x \in X} s_i(x) d\mu(x),
\]

where \( \{ s_i \}_{i=1}^\infty \subseteq S(X,A) \) is a sequence of step functions whose \( L^1_\nu(X,A) \)-limit is \( u \).

Note that since \( A \) is not commutative in general, the left and right integrals do not always coincide.

There is also a stronger notion for integrability. An \( A \)-valued function \( u \) on \( X \) is said to be totally measurable if it is a uniform limit of a step function, i.e., there exists a sequence \( \{ s_i \}_{i=1}^\infty \subseteq S(X,A) \) of step functions such that \( \lim_{i \to \infty} \sup_{x \in X} \| u(x) - s_i(x) \|_A = 0 \). We denote by \( T(X,A) \) the set of all \( A \)-valued totally measurable functions on \( X \). Note that if \( u \in T(X,A) \), then \( u \in L^1_{|\mu|}(X,A) \) for any \( \mu \in \mathcal{D}(X,A) \). In fact, the continuous functions in \( C_0(X,A) \) is totally measurable (see Definition 4.1 for the definition of \( C_0(X,A) \)).

**Proposition 4.10** The space \( C_0(X,A) \) is contained in \( T(X,A) \). Moreover, for any real positive finite regular measure \( \nu \), it is dense in \( L^1_{|\mu|}(X,A) \) with respect to \( \| \cdot \|_{L^1_{|\mu|}(X,A)} \).

For further details, refer to Dinculeanu (1967, 2000).

### 4.2 Kernel mean embedding of \( C^* \)-algebra-valued measures

We now define a KME in RKHMs.

**Definition 4.11 (KME in RKHMs)** A kernel mean embedding in an RKHM \( \mathcal{M}_k \) is a map \( \Phi : \mathcal{D}(X,A) \to \mathcal{M}_k \) defined by

\[
\Phi(\mu) := \int_{x \in X} \phi(x)d\mu(x).
\]

We emphasize that the well-definedness of \( \Phi \) is not trivial, and von Neumann-algebras are adequate to show it. More precisely, the following theorem derives the well-definedness.

**Theorem 4.12 (Well-definedness for the KME in RKHMs)** Let \( \mu \in \mathcal{D}(X,A) \). Then, \( \Phi(\mu) \in \mathcal{M}_k \). In addition, the following equality holds for any \( v \in \mathcal{M}_k \):

\[
\langle \Phi(\mu), v \rangle_{\mathcal{M}_k} = \int_{x \in X} d\mu^*(x)v(x).
\]

To show Theorem 4.12, we use the Riesz representation theorem for Hilbert \( A \)-module (Skeide, 2000, Theorem 4.16).
Proposition 4.13 (The Riesz representation theorem for Hilbert $\mathcal{A}$-modules) For a bounded $\mathcal{A}$-linear map $L : \mathcal{M} \to \mathcal{A}$ (see Definition 2.19), there exists a unique $u \in \mathcal{M}$ such that $Lv = \langle u, v \rangle_\mathcal{M}$ for all $v \in \mathcal{M}$.

Proof [Proof of Theorem 4.12] Let $L_\mu : \mathcal{M}_k \to \mathcal{A}$ be an $\mathcal{A}$-linear map defined as $L_\mu v := \int_{x \in \mathcal{X}} d\mu^*(x)v(x)$. The following inequalities are derived by the reproducing property and the Cauchy–Schwarz inequality (Lemma 2.16):

$$
\|L_\mu v\|_\mathcal{A} = \int_{x \in \mathcal{X}} \|v\|_\mathcal{M}_k \langle \phi(x), v \rangle_{\mathcal{M}_k} \|d\mu\|_\mathcal{X} = \int_{x \in \mathcal{X}} \|\phi(x)\|_\mathcal{M}_k \|d\mu\|_\mathcal{X} \leq \|v\|_\mathcal{M}_k \sup_{x \in \mathcal{X}} \|\phi(x)\|_\mathcal{M}_k, \quad (6)
$$

where the first inequality is easily checked for a step function $s(x) := \sum_{i=1}^n c_i \chi_{E_i}(x)$ as follows and thus, it holds for any totally measurable functions:

$$
\left\| \int_{x \in \mathcal{X}} d\mu^*(x)s(x) \right\|_\mathcal{A} = \left\| \sum_{i=1}^n \mu(E_i)^* c_i \right\|_\mathcal{A} \leq \sum_{i=1}^n \|\mu(E_i)^*\|_\mathcal{A} |c_i|_\mathcal{A} \leq \sum_{i=1}^n |\mu|(E_i)^* |c_i|_\mathcal{A} = \int_{x \in \mathcal{X}} \|s(x)\|_\mathcal{M}_k \|d\mu\|_\mathcal{X}.
$$

Since both $|\mu|(\mathcal{X})$ and $\sup_{x \in \mathcal{X}} \|\phi(x)\|_\mathcal{M}_k$ are finite, inequality (6) means $L_\mu$ is bounded. Thus, by the Riesz representation theorem for Hilbert $\mathcal{A}$-modules (Proposition 4.13), there exists $u_\mu \in \mathcal{M}_k$ such that $L_\mu v = \langle u_\mu, v \rangle_{\mathcal{M}_k}$. By setting $v = \phi(y)$, we have $u_\mu(y) = L_\mu \phi(y)^* = \int_{x \in \mathcal{X}} k(y, x)d\mu(x)$ for $y \in \mathcal{X}$. Therefore, $\Phi(\mu) = u_\mu \in \mathcal{M}_k$ and $\langle \Phi(\mu), v \rangle_{\mathcal{M}_k} = \int_{x \in \mathcal{X}} d\mu^*(x)v(x)$.

**Corollary 4.14** For $\mu, \nu \in \mathcal{D}(\mathcal{X}, \mathcal{A})$, the inner product between $\Phi(\mu)$ and $\Phi(\nu)$ is given as follows:

$$
\langle \Phi(\mu), \Phi(\nu) \rangle_{\mathcal{M}_k} = \int_{x \in \mathcal{X}} \int_{y \in \mathcal{X}} d\mu^*(x)k(x, y)d\nu(y).
$$

Moreover, many basic properties for the existing KME in RKHS are generalized to the proposed KME as follows.

Proposition 4.15 (Basic properties of the KME $\Phi$) For $\mu, \nu \in \mathcal{D}(\mathcal{X}, \mathcal{A})$ and $c \in \mathcal{A}$, $\Phi(\mu + \nu) = \Phi(\mu) + \Phi(\nu)$ and $\Phi(\mu c) = \Phi(\mu)c$ (i.e., $\Phi$ is $\mathcal{A}$-linear, see Definition 2.19) hold. In addition, for $x \in \mathcal{X}$, $\Phi(\delta_x) = \phi(x)$ (see Definition 4.6 for the definition of the $\mathcal{A}$-valued Dirac measure $\delta_x$).

This is derived from Eqs. (4) and (5). Note that if $\mathcal{A} = \mathbb{C}$, then the proposed KME (4) is equivalent to the existing KME in RKHS considered in Sriperumbudur et al. (2011).

### 4.3 Injectivity and universality

Here, we show the connection between the injectivity of the KME and the universality of RKHM. Proofs of the propositions in this subsection are given in Appendix B.
4.3.1 Injectivity

In practice, the injectivity of \( \Phi \) is important to transform problems in \( D(\mathcal{X}, \mathcal{A}) \) into those in \( \mathcal{M}_k \). This is because if a KME \( \Phi \) in an RKHM is injective, then \( \mathcal{A} \)-valued measures are embedded into \( \mathcal{M}_k \) through \( \Phi \) without loss of information. Note that, for probability measures, the injectivity of the existing KME is also referred to as the “characteristic” property. The injectivity of the existing KME in RKHS has been discussed in, for example, Fukumizu et al. (2008); Sriperumbudur et al. (2010, 2011). These studies give criteria for the injectivity of the KMEs associated with important complex-valued kernels such as transition invariant kernels and radial kernels. Typical examples of these kernels are Gaussian, Laplacian, and inverse multiquadratic kernels. Here, we define the transition invariant kernels and radial kernels for \( \mathcal{A} \)-valued measures, and generalize their criteria to RKHMs associated with \( \mathcal{A} \)-valued kernels.

To characterize transition invariant kernels, we first define a Fourier transform and support of an \( \mathcal{A} \)-valued measure.

**Definition 4.16 (Fourier transform and support of an \( \mathcal{A} \)-valued measure)** For an \( \mathcal{A} \)-valued measure \( \lambda \) on \( \mathbb{R}^d \), the Fourier transform of \( \lambda \), denoted as \( \hat{\lambda} \), is defined as

\[
\hat{\lambda} = \int_{\omega \in \mathbb{R}^d} e^{-\sqrt{-1}x^T\omega} d\lambda(\omega).
\]

In addition, the support of \( \lambda \) is defined as

\[
supp(\lambda) = \{ x \in \mathbb{R}^d \mid \lambda(U) >_{\mathcal{A}} 0 \text{ for any open set } U \text{ such that } x \in U \}.
\]

**Definition 4.17 (Transition invariant kernel and radial kernel)**

1. An \( \mathcal{A} \)-valued positive definite kernel \( k : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathcal{A} \) is called a transition invariant kernel if it is represented as \( k(x, y) = \hat{\lambda}(y - x) \) for a positive \( \mathcal{A} \)-valued measure \( \lambda \).

2. An \( \mathcal{A} \)-valued positive definite kernel \( k : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathcal{A} \) is called a radial kernel if it is represented as \( k(x, y) = \int_{[0, \infty)} e^{-\|x - y\|^2} d\eta(t) \) for a positive \( \mathcal{A} \)-valued measure \( \eta \).

Here, an \( \mathcal{A} \)-valued measure \( \mu \) is said to be positive if \( \mu(E) \geq_{\mathcal{A}} 0 \) for any Borel set \( E \).

We show transition invariant kernels and radial kernels induce injective KMEs.

**Proposition 4.18 (The injectivity for transition invariant kernels)** Let \( \mathcal{A} = \mathbb{C}^{m \times m} \) and \( \mathcal{X} = \mathbb{R}^d \). Assume \( k : \mathcal{X} \times \mathcal{X} \rightarrow \mathcal{A} \) is a transition invariant kernel with a positive \( \mathcal{A} \)-valued measure \( \lambda \) that satisfies \( supp(\lambda) = \mathcal{X} \). Then, KME \( \Phi : D(\mathcal{X}, \mathcal{A}) \rightarrow \mathcal{M}_k \) defined as Eq. (4) is injective.

**Proposition 4.19 (The injectivity for radial kernels)** Let \( \mathcal{A} = \mathbb{C}^{m \times m} \) and \( \mathcal{X} = \mathbb{R}^d \). Assume \( k : \mathcal{X} \times \mathcal{X} \rightarrow \mathcal{A} \) is a radial kernel with a positive definite \( \mathcal{A} \)-valued measure \( \eta \) that satisfies \( supp(\eta) \neq \{0\} \). Then, KME \( \Phi : D(\mathcal{X}, \mathcal{A}) \rightarrow \mathcal{M}_k \) defined as Eq. (4) is injective.

**Example 4.20**

1. If \( k : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{C}^{m \times m} \) is a matrix-valued kernel whose diagonal elements are Gaussian, Laplacian, or \( B_{2n+1} \)-spline and nondiagonal elements are 0, then \( k \) is a \( c_0 \)-kernel (See Example 3.3.1). There exists a matrix-valued measure \( \lambda \) that satisfies \( k(x, y) = \hat{\lambda}(y - x) \) and whose diagonal elements are nonnegative and supported by \( \mathbb{R}^d \) (c.f. Table 2 in Sriperumbudur et al. (2010)) and nondiagonal elements are 0. Thus, by Proposition 4.18, \( \Phi \) is injective.
2. If \( k \) is a matrix-valued kernel whose diagonal elements are inverse multiquadratic and nondiagonal elements are 0, then \( k \) is a \( c_0 \)-kernel. There exists a matrix-valued measure \( \eta \) that satisfies
\[
  k(x, y) = \int_{[0, \infty)} e^{-t\|x-y\|^2} dt, \quad \text{and whose diagonal elements are nonnegative and supp}(\eta) \neq \{0\} \quad \text{and nondiagonal elements are 0} \quad (\text{c.f. Theorem 7.15 in Wendland (2004)}).
\] Thus, by Proposition 4.19, \( \Phi \) is injective.

### 4.3.2 Connection with universality

Another important property for kernel methods is universality, which ensures that kernel-based algorithms approximate each continuous target function arbitrarily well. For RKHS, Sriperumbudur et al. (2011) showed the equivalence of the injectivity of the existing KME in RKHISs and universality of RKHISs. We define a universality of RKHMs as follows.

**Definition 4.21 (Universality)** An RKHM is said to be universal if it is dense in \( C_0(\mathcal{X}, \mathcal{A}) \).

We show the above equivalence holds also for RKHM in the case of \( \mathcal{A} = \mathbb{C}^{m \times m} \).

**Proposition 4.22 (Equivalence of the injectivity and universality for \( \mathcal{A} = \mathbb{C}^{m \times m} \))**

Let \( \mathcal{A} = \mathbb{C}^{m \times m} \). Then, \( \Phi : \mathcal{D}(\mathcal{X}, \mathcal{A}) \rightarrow \mathcal{M}_k \) is injective if and only if \( \mathcal{M}_k \) is dense in \( C_0(\mathcal{X}, \mathcal{A}) \).

By Proposition 4.22, if \( k \) satisfies the condition in Proposition 4.18 or 4.19, then \( \mathcal{M}_k \) is universal.

For the case where \( \mathcal{A} \) is infinite dimensional, the universality of \( \mathcal{M}_k \) in \( C_0(\mathcal{X}, \mathcal{A}) \) is a sufficient condition for the injectivity of the proposed KME.

**Theorem 4.23 (Connection between the injectivity and universality for general \( \mathcal{A} \))**

If \( \mathcal{M}_k \) is dense in \( C_0(\mathcal{X}, \mathcal{A}) \), then \( \Phi : \mathcal{D}(\mathcal{X}, \mathcal{A}) \rightarrow \mathcal{M}_k \) is injective.

However, the equivalence of the injectivity and universality, and the injectivity for transition invariant and radial kernels are open problems. This is because their proofs strongly depend on the Hahn–Banach theorem and Riesz–Markov representation theorem, and generalizations of these theorems to \( \mathcal{A} \)-valued functions and measures are challenging problems due to the situation peculiar to the infinite dimensional spaces. Further details of the proofs of propositions in this section are given in Appendix B.

### 5. Applications

We apply the framework of RKHM described in Sections 3 and 4 to problems in data analysis. We propose kernel PCA in RKHMs in Subsection 5.1, and analyze interaction effects in finite or infinite dimensional data with the proposed KME in RKHMs in Subsection 5.2. Then, we discuss further applications in Subsection 5.3.

#### 5.1 PCA in RKHMs

Principal component analysis (PCA) is a fundamental tool for describing data in a low dimensional space. Its implementation in RKHSs have also been proposed (c.f. Schölkopf and Smola (2001)). It enables us to deal with the nonlinearity of data by virtue of the high
expressive power of RKHSs. Here, we generalize them to capture more information in data, such as multivariate data and functional data, by using the framework of RKHM.

Let \( x_1, \ldots, x_n \in \mathcal{X} \) be given samples. Let \( k : \mathcal{X} \times \mathcal{X} \to \mathcal{A} \) be an \( \mathcal{A} \)-valued positive definite kernel on \( \mathcal{X} \) and let \( \mathcal{M}_k \) be the RKHM associated with \( k \). We explore a useful set of axes \( p_1, \ldots, p_r \) in \( \mathcal{M}_k \), which are referred to as principal axes, to describe the feature of given samples \( x_1, \ldots, x_n \). The corresponding \( \mathcal{A} \)-valued coordinate \( \langle p_j, \phi(x_i) \rangle \) are referred to as principal components. We emphasize our proposed PCA in RKHM provides principal components contained in \( \mathcal{A} \), not in complex numbers. This is a remarkable difference between our method and existing PCAs. When samples have some structures such as among variables or in functional data, \( \mathcal{A} \)-valued principal components provide us richer information than complex-valued ones. For example, if \( \mathcal{X} \) is the space of functions of multivariables and if we set \( \mathcal{A} \) as \( L^\infty([0,1]) \), then we can reduce multi-variable functional data to \( L^\infty([0,1]) \)-valued principal components, i.e., functions of single variable (as illustrated in Section 5.1.3).

To obtain \( \mathcal{A} \)-valued principal components, we consider the following minimization problem regarding the following reconstruction error:

\[
\inf_{\{p_j\}_{j=1}^r \subseteq \mathcal{M}_k} \text{ONS} \sum_{i=1}^n \left| \phi(x_i) - \sum_{j=1}^r p_j \langle p_j, \phi(x_i) \rangle_{\mathcal{M}_k} \right|^2_{\mathcal{M}_k}, \tag{7}
\]

where the infimum is taken with respect to a (pre) order in \( \mathcal{A} \) (see Definition 2.9). Since the identity \( \phi(x_i) - \sum_{j=1}^r p_j \langle p_j, \phi(x_i) \rangle_{\mathcal{M}_k}^2 = k(x_i, x_i) - \sum_{j=1}^r \langle \phi(x_i), p_j \rangle_{\mathcal{M}_k} \langle p_j, \phi(x_i) \rangle_{\mathcal{M}_k} \) holds and \( \langle \phi(x_i), p_j \rangle_{\mathcal{M}_k} \) is represented as \( p_j(x_i) \) by the reproducing property, the problem (7) can be reduced to the minimization problem

\[
\inf_{\{p_j\}_{j=1}^r \subseteq \mathcal{M}_k} \text{ONS} \sum_{i=1}^n \sum_{j=1}^r -p_j(x_i)p_j(x_i)^*. \tag{8}
\]

In the case of RKHS, i.e., \( \mathcal{A} = \mathbb{C} \), the solution of the problem (8) is obtained by computing eigenvalues and eigenvectors of Gram matrices (see, for example, Schölkopf and Smola (2001)). Unfortunately, we cannot extend their procedure to RKHM straightforwardly. Therefore, we develop two methods to obtain approximate solutions of the problem (8): by gradient descents on Hilbert \( C^* \)-modules, and by the minimization of the trace of the \( \mathcal{A} \)-valued objective function.

### 5.1.1 Gradient Descent on Hilbert \( C^* \)-modules

We propose a gradient decent method on Hilbert \( \mathcal{A} \)-module for the case where \( \mathcal{A} \) is commutative. An important example of commutative von Neumann-algebra is \( L^\infty([0,1]) \). The gradient descent for a real-valued function on a Hilbert space has been proposed (Smyrlis and Zisis, 2004). However, in our situation, the objective function of the problem (8) is an \( \mathcal{A} \)-valued function in a Hilbert \( C^* \)-module \( \mathcal{A}^\ast \). Thus, the existing gradient descent is not applicable to our situation. Therefore, we generalize the existing gradient descent algorithm to \( \mathcal{A} \)-valued functions on Hilbert \( C^* \)-modules.

Let \( \mathcal{A} \) be a commutative von Neumann-algebra. Assume the positive definite kernel \( k \) takes its values in \( \mathcal{A}_r := \{ c - d \in \mathcal{A} \mid c, d \in \mathcal{A}_+ \} \). For example, for \( \mathcal{A} = L^\infty([0,1]) \),
\( A_r \) is shown to be equivalent to the space of real-valued \( L^\infty \) functions on \([0, 1]\). By the
representer theorem (Theorem 3.8), if there is a solution of the problem (8), it is represented
as \( p_j = \sum_{i=1}^{n} \phi(x_i)c_{j,i} \) for some \( c_{j,i} \in A \). Moreover, since \( A \) is commutative, \( p_j(x)\star p_j(x)^* \)
is equal to \( p_j(x_i)\star p_j(x_i) \). Therefore, the problem (7) on \( M_k \) is equivalent to the following
problem on the Hilbert \( A \)-module \( A^n \) (see Example 2.15 about \( A^n \)):

\[
\inf_{c_j \in A^n, \{\sqrt{Gc_j}\}} \sum_{j=1}^{r} c_j^*G^2c_j,
\]

where \( G \) is the \( A \)-valued Gram matrix defined as \( G_{i,j} = k(x_i, x_j) \). For simplicity, we assume
\( r = 1 \), i.e., the number of principal axes is 1. We rearrange the problem (9) to the following
problem by adding a penalty term:

\[
\inf_{c \in A^n} (-c^*G^2c + \lambda|c^*Ga - 1|^2_A),
\]

where \( \lambda \) is a real positive weight for the penalty term. For \( r > 1 \), let \( c_1 \) be a solution of
the problem (9). Then, we solve the same problem in the orthogonal complement of the
module spanned by \( \{c_1\} \) and set the solution of this problem as \( c_2 \). Then, we solve the same
problem in the orthogonal complement of the module spanned by \( \{c_1, c_2\} \) and repeat
this procedure to obtain solutions \( c_1, \ldots, c_r \). The problem (10) is the minimization
problem of an \( A \)-valued function defined on the Hilbert \( A \)-module \( A^n \). We search a solution of
the problem (10) along the steepest descent directions. To calculate the steepest descent
directions, we first introduce the Gâteaux derivative of an \( A \)-valued function on a Hilbert
\( C^* \)-module.

**Definition 5.1 (Gâteaux derivative)** Let \( M \) be a Hilbert \( C^* \)-module. Let \( f : M \to A \) be
an \( A \)-valued function defined on \( M \). The function \( f \) is referred to as (Gâteaux) differentiable
at a point \( c \in M \) if there exists a limit

\[
Df_c(u) := \lim_{t \to 0} \frac{f(c + tu) - f(c)}{t} = \frac{d}{dt} f(c + tu) |_{t=0},
\]

for any \( u \in M \). In addition, the operator \( Df_c \) is a \( \mathbb{R} \)-linear operator on \( M \) and referred to
as a Gâteaux derivative of \( f \) at \( c \). Similarly, \( f \) is referred to as \( i \)-times Gâteaux differentiable
at a point \( c \in M \) if there exists

\[
D^i f_c(u) := \frac{d^i}{dt^i} f(c + tu) |_{t=0},
\]

for any \( u \in M \).

The following Taylor’s theorem for the Gâteaux derivative is derived (c.f. Blanchard and
Brüning (2015)).

**Proposition 5.2 (Taylor’s theorem for the Gâteaux derivative)** Let \( c \in M \). Assume
\( f \) is \( m \)-times differentiable and its \( m \)-th derivative is continuous. Then, for \( u \in M \), we have

\[
f(c + u) = \sum_{i=0}^{m} \frac{1}{i!} D^i f_c(u) + R_m(c, u),
\]

where \( R_m(c, u) = 1/(m - 1)! \int_0^1 (1 - t)^{m-1} (D^m f_{c+tu}(u) - D^m f_c(u)) dt \) and thus it satisfies
\( \lim_{u \to 0} \|R_m(c, u)\|_A \|u\|_M = 0 \).
The following gives the derivative of the objective function in problem (10).

**Proposition 5.3 (Derivative of the objective function)** Let $f : \mathcal{A}^n \to \mathcal{A}$ be defined as

$$f(c) = -c^*G^2c + \lambda|c^*Gc - 1_A|^2_A. \tag{11}$$

Then, $f$ is infinitely differentiable and the first derivative of $f$ is calculated as

$$Df_c(u) = -2c^*G^2u - 2\lambda c^*Gu + 4\lambda c^*Gcc^*Gu.$$  

Moreover, for each $c \in \mathcal{A}^n$, there exists a unique $d \in \mathcal{A}^n$ such that $\langle d, u \rangle_{\mathcal{A}^n} = Df_c(u)$ for any $u \in \mathcal{A}^n$. The vector $d$ is calculated as

$$d = -2G^2c - 2\lambda Gc + 4\lambda Gcc^*Gc.$$  

**Proof** The derivative of $f$ is calculated by the definition and the assumption that $\mathcal{A}$ is commutative. Since $Df_c$ is a bounded $\mathcal{A}$-linear operator, by the Riesz representation theorem (Proposition 4.13), there exists a unique $d \in \mathcal{A}^n$ such that $\langle d, u \rangle_{\mathcal{A}^n} = Df_c(u)$.

**Definition 5.4 (Gradient of $\mathcal{A}$-valued functions on Hlibert $C^*$-modules)** Let $f : \mathcal{M} \to \mathcal{A}$ be a differentiable function. Assume for each $c \in \mathcal{M}$, there exists a unique $d \in \mathcal{M}$ such that $\langle d, u \rangle_{\mathcal{A}^n} = Df_c(u)$ for any $u \in \mathcal{M}$. In this case, we denote $d$ by $\nabla f_c$ and call it the gradient of $f$ at $c$.

We now develop an $\mathcal{A}$-valued gradient descent scheme.

**Theorem 5.5** Assume $f : \mathcal{M} \to \mathcal{A}$ is twice differentiable and its second derivative is continuous. Moreover, assume there exists $\nabla f_c$ for any $c \in \mathcal{M}$. Let $\eta_t > 0$. Let $c_0 \in \mathcal{M}$ and

$$c_{t+1} = c_t - \eta_t \nabla f_{c_t}, \tag{12}$$

for $t = 0, 1, \ldots$. Then, we have

$$f(c_{t+1}) = f(c_t) - \eta_t |\nabla f_{c_t}|_{\mathcal{M}}^2 + S(c_t, \eta_t), \tag{13}$$

where $S(c, \eta) = 1/2D^2f_c(-\eta\nabla f_c) + R_2(c, -\eta\nabla f_c)$ and thus satisfies $\lim_{\eta \to 0} \|S(c, \eta)\|_{\mathcal{A}}/\eta^2 = 0$.

The statement is immediately derived by Taylor’s theorem (Proposition 5.2). The following examples show the scheme (12) is valid to solve the problem (10).

**Example 5.6** Let $\mathcal{A} = L^\infty([0,1])$, let $a_t = |\nabla f_{c_t}|_{\mathcal{A}^n} \in \mathcal{A}$ and let $b_{t, \eta} = S(c_t, \eta) \in \mathcal{A}$. If $a_t \geq_{\mathcal{A}} \delta 1_A$ for some positive real value $\delta$, then the function $a_t$ on $[0,1]$ satisfies $a_t(s) > 0$ for almost everywhere $s \in [0,1]$. On the other hand, since $b_{t, \eta}$ satisfies $\lim_{\eta \to 0} \|b_{t, \eta}\|_{\mathcal{A}}/\eta^2 = 0$, there exists sufficiently small positive real value $\eta_{t, 0}$ such that for almost everywhere $s \in [0,1]$, $b_{t, \eta_{t, 0}}(s) \leq \|b_{t, \eta_{t, 0}}\|_{\mathcal{A}} \leq \eta_{t, 0}^2 \delta \leq \eta_{t, 0}(1 - \xi_1) \delta$ holds for some positive real value $\xi_1$. As a result, $-\eta_{t, 0}|\nabla f_{c_t}|_{\mathcal{A}^n}^2 + S(c_t, \eta_{t, 0}) \leq_{\mathcal{A}} -\eta_{t, 0} \xi_1 |\nabla f_{c_t}|_{\mathcal{A}^n}^2$ holds and by the Eq. (13), we have

$$f(c_{t+1}) \leq_{\mathcal{A}} f(c_t), \tag{14}$$
for $t = 0, 1, \ldots$. As we mentioned in Example 2.8, the inequality (14) means the function $f(c_{t+1}) \in L^\infty([0, 1])$ is smaller than the function $f(c_t) \in L^\infty([0, 1])$ at almost every points on $[0, 1]$, i.e.,

$$f(c_{t+1})(s) < f(c_t)(s),$$

for almost every $s \in [0, 1]$.

**Example 5.7** Assume $A$ is a finite dimensional space. If $|\nabla f_{c_t}|^2_A \geq_A \delta_1 A$ for some positive real value $\delta$, the inequality $f(c_{t+1}) \leq_A f(c_t) - \eta_1 |\nabla f_{c_t}|^2_A$ holds for $t = 0, 1, \ldots$ and some $\eta_1$ in the same manner as Example 5.6. Moreover, the function $f$ defined as Eq. (11) is bounded below and $\nabla f_{c_t}$ is Lipschitz continuous on the set $\{c \in A^n \mid f(c) \leq_A f(c_0)\}$. In this case, if there exists a positive real value $\xi_2$ such that $|\nabla f_{c_{t+1}} - \nabla f_{c_t}|_A^2 \leq \xi_2 \nabla f_{c_t}|_A^2$, then we have

$$\xi_2 |\nabla f_{c_t}|_A^2 \leq L |c_{t+1} - c_t|_A^2 \leq L \eta_k \|\nabla f_{c_t}|_A^2,$$

where $L$ is a Lipschitz constant of $\nabla f_{c_t}$. As a result, we have

$$f(c_{t+1}) \leq_A f(c_t) - \eta_1 |\nabla f_{c_t}|^2_A \leq_A f(c_t) - \frac{\xi_1 \xi_2}{L} \|\nabla f_{c_t}|^2_A,$$

which implies $\sum_{t=1}^{T} |\nabla f_{c_t}|_A^2 \leq_A L/(\xi_1 \xi_2) (f(c_1) - f(c_{T+1})).$ Since $f$ is bounded below, the sum $\sum_{t=1}^{\infty} |\nabla f_{c_t}|_A^2$ converges. Therefore, $|\nabla f_{c_t}|_A^2 \to 0$ as $t \to \infty$, i.e., the gradient $\nabla f_{c_t}$ in Eq. (12) converges to 0.

### 5.1.2 Minimization of the Trace

In the case of $A = B(W)$, $p_j(x_i)$ and $p_j(x_i)^*$ in the problem (8) do not always commute. Therefore, we rearrange the problem (8) to the following problem:

$$\inf_{\{p_j\}_{j=1}^n \subseteq \mathcal{F}_k: \text{ONS}} \mathrm{tr} \left( \sum_{i=1}^{n} \sum_{j=1}^{r} -p_j(x_i)p_j(x_i)^* \right),$$

where $\mathcal{F}_k = \{v \in \mathcal{M}_k \mid v(x) \text{ is a rank } N \text{ operator for any } x \in X\}$. This can be reduced to

$$\inf_{c_j \in F, \{\sqrt{G}c_j\}_{j=1}^r: \text{ONS}} -\tr \left( \sum_{j=1}^{r} c_j^* G^2 c_j \right),$$

where $F = \{c \in A^n \mid c_i \text{ is a rank } N \text{ operator for } i = 1, \ldots, n\}$. If $A = \mathbb{C}^{m \times m}$, i.e., $W$ is a finite dimensional space, then we solve the problem (16) by regarding $G$ as an $mn \times mn$ matrix and computing the eigenvalues and eigenvectors of $G$.

**Proposition 5.8** Let $A = \mathbb{C}^{m \times m}$ and $N = 1$. Let $\lambda_1, \ldots, \lambda_r \in \mathbb{C}$ and $v_1, \ldots, v_r \in \mathbb{C}^m$ be the largest $r$ eigenvalues and the corresponding orthonormal eigenvectors of $G \in \mathbb{C}^{mn \times mn}$. Then, $c_j = [v_j, 0, \ldots, 0] \lambda_j^{-1/2}$ is a solution of the problem (16).

**Proof** Since the identity $\sum_{j=1}^{r} c_j^* G^2 c_j = \sum_{j=1}^{r} (\sqrt{G}c_j)^* G (\sqrt{G}c_j)$ holds, any solution $c_j$ of the problem (16) satisfies $\sqrt{G}c_j = v_j u^*$ for a normalized vector $u \in \mathbb{C}^m$. Thus, $p_j = \sum_{i=1}^{n} \phi(x_i) c_{i,j}$ where $c_{j} = \lambda_j^{-1/2}[v_j, 0, \ldots, 0]$ is a solution of the problem. \[\square\]
If \( \mathcal{W} \) is an infinite dimensional space, we regard \( \mathbf{G} \) as a linear operator on the Hilbert space \( \mathcal{W}^n \). The following theorem shows we can reduce the problem in \( \mathcal{A}^n \) to a problem in \( \mathcal{W}^n \). Then, we can apply the standard gradient decent method in Hilbert spaces to the problem in \( \mathcal{W}^n \) (Smyrlis and Zisis, 2004).

**Proposition 5.9** Assume \( \mathcal{W} \) is a separable Hilbert space and \( \{ e_j \}_{j=1}^\infty \) is an orthonormal basis of \( \mathcal{W} \). Let \( [d_1,1, \ldots, d_{n,1}]^T = d_1, \ldots, [d_{1,N}, \ldots, d_{n,N}]^T = d_N \in \mathcal{W}^n \) and let 

\[
[c_1, \ldots, c_n]^T = \mathbf{c} \in \mathcal{B}(\mathcal{W})^n \text{ be a vector in the Hilbert } C^*\text{-module } \mathcal{B}(\mathcal{W})^n \text{ such that } c_i \in \mathcal{B}(\mathcal{W}) \text{ is a rank } N \text{ operator satisfying } c_i e_j = d_i,j \text{ for } i = 1, \ldots, n \text{ and } j = 1, \ldots, N, \text{ and } c_i e_j = 0 \text{ for } i = 1, \ldots, n \text{ and } j \geq N + 1. \]

Then, we have

\[
\sum_{j=1}^N \langle d_j, \mathbf{G}^2 d_j \rangle_{\mathcal{W}^n} = \text{tr}(\mathbf{c}^* \mathbf{G}^2 \mathbf{c}),
\]

and if \( \{ \sqrt{G} d_j \}_{j=1}^N \) is an orthonormal system in \( \mathcal{W}^n \), then \( \sqrt{G} \mathbf{c} \) is a normalized vector in \( \mathcal{B}(\mathcal{W})^n \).

**Proof** Let \( g_{i,l} \in \mathcal{B}(\mathcal{W}) \) be the \((i,l)\)-element of \( \mathbf{G} \). By the definition of \( \mathbf{c} \), we have

\[
\text{tr}(\mathbf{c}^* \mathbf{G}^2 \mathbf{c}) = \sum_{j=1}^\infty \sum_{i,j=1}^n c_i^* g_{i,j} c_e e_j \mathcal{W} = \sum_{j=1}^N \sum_{i,j=1}^n \langle c_i e_j, g_{i,l} c_e e_j \rangle_{\mathcal{W}}
\]

\[
= \sum_{j=1}^N \sum_{i,j=1}^n \langle d_{i,j}, g_{i,l} d_{i,j} \rangle_{\mathcal{W}} = \sum_{j=1}^N \langle d_j, \mathbf{G}^2 d_j \rangle_{\mathcal{W}^n}.
\]

In addition, \( \langle \mathbf{c}, \mathbf{G} \mathbf{c} \rangle_{\mathcal{B}(\mathcal{W})^n} \) is a rank \( N \) operator all of whose nonzero eigenvalues are 1, which implies \( \sqrt{G} \mathbf{c} \) is a normalized vector in \( \mathcal{B}(\mathcal{W})^n \).

Therefore, we consider the problem

\[
\inf_{d_j \in \mathcal{W}^n, \{ \sqrt{G} d_j \}_{j=1}^N: \text{ONS}} - \sum_{j=1}^N d_j^* \mathbf{G}^2 d_j, \tag{17}
\]

instead of the problem (16). Since the problem (17) is defined on the Hilbert space \( \mathcal{W}^n \), we solve it by the gradient descent method in Hilbert spaces (Smyrlis and Zisis, 2004). Then, we put \( [c_{1,l}, \ldots, c_{n,l}]^T = \mathbf{c}_l \in \mathcal{B}(\mathcal{W})^n \) such that \( c_{i,l} e_j = d_{i,(l-1)s+j} \) for \( l = 1, \ldots, r \), \( j = 1, \ldots, N \), and \( i = 1, \ldots, n \).

### 5.1.3 Numerical examples

We applied the above PCA with \( \mathcal{A} = L^\infty([0,1]) \) to functional data. We randomly generated three kinds of sample-sets from the following functions of two variables:

\[
y_1(s,t) = e^{10(s-t)}, \quad y_2(s,t) = 10st, \quad y_3(s,t) = \cos(10(s-t)).
\]

Each sample-set \( i \) is composed of 20 samples obtained by discretizing \( y_i \) at 11 equally spaced points in \([0,1]\) and adding noise. The noise was randomly drawn from the Gaussian
distribution with mean 0 and standard deviation 0.3. Since $L^\infty([0,1])$ is commutative, we applied the gradient descent proposed in Subsection 5.1.1 to solve the problem (7). The parameters were set as $\lambda = 0.1$ and $\eta_t = 0.01$. We set the $L^\infty([0,1])$-valued positive definite kernel $k$ as
\[
(k(x_1, x_2))(t) = \int_0^1 \int_0^1 (t - x_1(s_1, s_2))(t - x_2(s_1, s_2)) ds_1 ds_2
\]
(see Example 3.3.1). Moreover, we set $c_0$ as the constant function $[1, \ldots, 1]^T \in A^n$ and computed $c_1, c_2, \ldots$ according to Eq. (12). For comparison, we also vectorized the samples and applied the standard kernel PCA in the RKHS associated with the Laplacian kernel on $R^{121}$. The results are illustrated in Figure 1. Since the samples are contaminated by the noise, the PCA in the RKHS cannot separate three sample-sets. On the other hand, the $L^\infty([0,1])$-valued principal components obtained by the proposed PCA in the RKHM reduce the information of the samples as functions. As a result, it clearly separates three sample-sets.

Figure 2 shows the convergence of the proposed gradient descent. In this example, we only compute the first principal components, hence $r$ is set as 1. For the objective function $f$ defined as $f(c) = -c^*G^2c + \lambda cGcc^*Gc + \lambda c^*Gc$, functions $f(c_t) \in L^\infty([0,1])$ for $t = 0, \ldots, 9$ are illustrated. We can see $f(c_{t+1}) < f(c_t)$ and $f(c_t)$ gradually approaches to a certain function as $t$ grows.

5.2 Analysis of interaction effects

Polynomial regression is a classical problem in statistics (Hastie et al., 2009) and analyzing interacting effects by the polynomial regression has been investigated (for its recent improvements, see, for example, Suzumura et al. (2017)). Most of the existing methods focus on the case of finite dimensional (discrete) data. However, in practice, we often encounter situations where we cannot fix the dimension of data. For example, observations are obtained at multiple locations and the locations are not fixed. It may be changed depending on time. Therefore, analysing interaction effects of infinite dimensional (continuous) data is essential. We show the framework of RKHM provides us a method for the analysis of infinite dimensional data by setting $A$ as a infinite dimensional space such as $B(W)$. Moreover, the proposed method does not need the assumption that interaction effects are described.
by a polynomial. We first develop the analysis in RKHMs for the case of finite dimensional data in Subsection 5.2.1. Then, we show the analysis is naturally generalized to the infinite dimensional data in Subsection 5.2.2.

5.2.1 The case of finite dimensional data

In this subsection, we assume $A = \mathbb{C}^{m \times m}$. Let $\mathcal{X}$ be a locally compact Hausdorff space and let $x_1, \ldots, x_n \in \mathcal{X}^{m \times m}$ and $y_1, \ldots, y_n \in A$ be given samples. We assume there exists functions $f_{j,l} : \mathcal{X} \to A$ such that

$$y_i = \sum_{j,l=1}^{m} f_{j,l}(x_{i,j,l}),$$

for $i = 1, \ldots, n$. For example, the $(j,l)$-element of each $x_i$ describes an interaction between the $j$-th element and $l$-th element of $x_i$ and $f_{j,l}$ is a nonlinear function describing an impact of the interaction between the $j$-th element and $l$-th element to the value $y_i$. If the given samples $y_i$ are real or complex-valued, we can regard them as $y_i, 1_A$ to meet the above setting. Let $\mu_x \in D(\mathcal{X}, \mathbb{C}^{m \times m})$ be a $\mathbb{C}^{m \times m}$-valued measure defined as $(\mu_x)_{j,l} = \delta_{x_{j,l}}$, where $\delta_x$ for $x \in \mathcal{X}$ is the standard (complex-valued) Dirac measure centered at $x$. Note that the $(j,l)$-element of $\mu_x$ describes a measure regarding the element $x_{j,l}$. Let $k$ be an $A$-valued $c_0$-kernel (see Definition 4.2), let $M_k$ be the RKHM associated with $k$, and let $\Phi$ be the KME defined in Section 4.2. In addition, let $\mathcal{V}$ be the submodule of $M_k$ spanned by $\{\Phi(\mu_{x_1}), \ldots, \Phi(\mu_{x_n})\}$, and let $P_f : \mathcal{V} \to \mathbb{C}^{m \times m}$ be a $\mathbb{C}^{m \times m}$-linear map (see Definition 2.19) which satisfies

$$P_f \Phi(\mu_{x_i}) = \sum_{j,l=1}^{m} f_{j,l}(x_{i,j,l}),$$

for $i = 1, \ldots, n$. Here, we assume the vectors $\Phi(\mu_{x_1}), \ldots, \Phi(\mu_{x_n})$ are $\mathbb{C}^{m \times m}$-linearly independent (see Definition 2.20).
5.2.2 Generalization to the continuous case

We generalize the setting mentioned in Subsection 5.2.1 to the case of functional data. We set \( \mathcal{A} \) as \( \mathcal{B}(L^2([0, 1])) \) instead of \( \mathbb{C}^{m \times m} \) in this subsection. Let \( x_1, \ldots, x_n \in C([0, 1] \times [0, 1], \mathcal{X}) \) and \( y_1, \ldots, y_n \in \mathcal{A} \) be given samples. We assume there exists a integrable function \( f : [0, 1] \times [0, 1] \times \mathcal{X} \rightarrow \mathcal{A} \) such that

\[
y_i = \int_0^1 \int_0^1 f(s, t, x_i(s, t)) ds dt,
\]

for \( i = 1, \ldots, n \). We consider an \( \mathcal{A} \)-valued positive definite kernel \( k \) on \( \mathcal{X} \), the RKHM \( \mathcal{M}_k \) associated with \( k \), and the KME \( \Phi \) in \( \mathcal{M}_k \). Let \( \mu_x \in \mathcal{D}(\mathcal{X}, \mathcal{B}(L^2([0, 1]))) \) be a \( \mathcal{B}(L^2([0, 1])) \)-valued measure defined as \( \mu_x(E) = \langle \chi_E(x(s, \cdot)), v \rangle_{L^2([0, 1])} \) for a Borel set \( E \) on \( \mathcal{X} \). Here, \( \chi_E : \mathcal{X} \rightarrow \{0, 1\} \) is the indicator function for \( E \). Note that the linear operator \( \mu_x(E) \) can be extended to the space of complex-valued finite regular Borel measures on \([0, 1]\) through a map \( \nu \rightarrow \int_0^1 \chi_E(x(s, t)) d\nu(t) \). In addition, the complex-valued measure \( \int_0^1 \mu_x \delta d\delta_x \) describes a measure regarding the point \( x(s, t) \). Let \( \mathcal{V} \) be the submodule of \( \mathcal{M}_k \) spanned by \( \{ \Phi(\mu_{x_1}), \ldots, \Phi(\mu_{x_n}) \} \), and let \( P_f : \mathcal{V} \rightarrow \mathcal{B}(L^2([0, 1])) \) be a \( \mathcal{B}(L^2([0, 1])) \)-linear map (see Definition 2.19) which satisfies

\[
P_f \Phi(\mu_{x_i}) = \int_0^1 \int_0^1 f(s, t, x_i(s, t)) ds dt,
\]

for \( i = 1, \ldots, n \). Here, we assume the vectors \( \Phi(\mu_{x_1}), \ldots, \Phi(\mu_{x_n}) \) are \( \mathcal{B}(L^2([0, 1])) \)-linearly independent (see Definition 2.20).

We estimate \( P_f \) by restricting it to a submodule of \( \mathcal{V} \). For this purpose, we apply the PCA in RKHM proposed in Section 5.1 and obtain principal axes \( p_1, \ldots, p_r \) to construct the submodule. We replace \( \phi(x_i) \) in the problem (7) with \( \Phi(\mu_{x_i}) \) and consider the problem

\[
\inf_{\{p_j\}_{j=1}^{r} \subseteq \mathcal{M}_k} \mathrm{ONS} \sum_{i=1}^{n} \left| \Phi(\mu_{x_i}) - \sum_{j=1}^{r} p_j \langle p_j, \Phi(\mu_{x_i}) \rangle_{\mathcal{M}_k} \right|^2_{\mathcal{M}_k}.
\]

The projection operator onto the submodule spanned by \( p_1, \ldots, p_r \) is represented as \( QQ^* \), where \( Q = [p_1, \ldots, p_r] \). Therefore, we estimate \( P_f \) by \( P_f QQ^* \). We can compute \( P_f QQ^* \) as follows.

**Proposition 5.10** The solution of the problem (18) is represented as \( p_j = \sum_{i=1}^{n} \Phi(\mu_{x_i}) c_{i,j} \) for some \( c_{i,j} \in \mathcal{A} \). Let \( C = [c_{i,j}]_{i,j} \). Then, the estimation \( P_f QQ^* \) is computed as

\[
P_f QQ^* = [y_1, \ldots, y_n]CQ^*.
\]

The following proposition shows we can obtain a vector which attains the largest transformation by \( P_f \).

**Proposition 5.11** Let \( u \in \mathcal{M}_k \) be a unique vector satisfying \( \langle u, v \rangle_{\mathcal{M}_k} = P_f QQ^* v \) for any \( v \in \mathcal{M}_k \). For \( \epsilon > 0 \), let \( b_\epsilon = (|u|_{\mathcal{M}_k} + \epsilon 1_{\mathcal{A}})^{-1} \) and let \( v_\epsilon = ub_\epsilon \). Then, \( P_f QQ^* v_\epsilon \) converges to

\[
\sup_{v \in \mathcal{M}_k, \|v\|_{\mathcal{M}_k} \leq 1} P_f QQ^* v,
\]

(19)
as $\epsilon \to 0$, where the supremum is taken with respect to a (pre) order in $A$ (see Definition 2.9). If $A = \mathbb{C}^{m \times m}$, then the supremum is replaced with the maximum. In this case, let $|u|^2_{M_k} = a^*d a$ be the eigenvalue decomposition of the positive semi-definite matrix $|u|^2_{M_k}$ and let $b = a^*d^+ a$, where the $i$-th diagonal element of $d^+$ is $d_{i,i}^{-1/2}$ if $d_{i,i} \neq 0$ and 0 if $d_{i,i} = 0$. Then, $ub$ is the solution of the maximization problem.

**Proof** By the Riesz representation theorem (Proposition 4.13), there exists a unique $u \in M_k$ satisfying $\langle u, v \rangle_{M_k} = P_f Q Q^* v$ for any $v \in M_k$. Then, for $v \in M_k$ which satisfies $\|v\|_{M_k} = 1$, by the Cauchy–Schwarz inequality (Lemma 2.16), we have

$$P_f Q Q^* v = \langle u, v \rangle_{M_k} \leq_A |u|_{M_k} \|v\|_{M_k} \leq_A |u|_{M_k}. \quad (20)$$

The vector $v_\epsilon$ satisfies $\|v_\epsilon\|_{M_k} \leq 1$. In addition, we have

$$(|u|_{M_k} + \epsilon 1_A)|u|^2_{M_k} - (|u|^2_{M_k} - \epsilon^2 1_A)(|u|_{M_k} + \epsilon 1_A) = \epsilon^2 (|u|_{M_k} + \epsilon 1_A) \geq_A 0.$$ 

By multiplying $(|u|_{M_k} + \epsilon 1_A)^{-1}$ on the both sides, we have $\|u\|_{M_k} - \langle u, v_\epsilon \rangle_{M_k} \leq \epsilon$, and $\lim_{\epsilon \to 0} P_f Q Q^* v_\epsilon = \lim_{\epsilon \to 0} \langle u, v_\epsilon \rangle_{M_k} = |u|_{M_k}$. Since $\langle u, v_\epsilon \rangle_{M_k} \leq_A d$ for any upper bound $d$ of $\{ |\langle u, v \rangle_{M_k} | \|v\|_{M_k} \leq 1 \}$, $|u|_{M_k} \leq_A d$ holds. As a result, $|u|_{M_k}$ is the supremum of $P_f Q Q^* v$. In the case of $A = \mathbb{C}^{m \times m}$, the inequality (20) is replaced with the equality by setting $v = ub$.

The vector $ub_\epsilon$ is represented as $ub_\epsilon = QC^*[y_1, \ldots, y_n]^T b_\epsilon = \sum_{i=1}^n \Phi(\mu_{x_i})d_i$, where $d_i \in A$ is the $i$-th element of $CC^*[y_1, \ldots, y_n]^T b_\epsilon \in A^0$, and $\Phi$ is $A$-linear (see Proposition 4.15). Therefore, the vector $ub_\epsilon$ corresponds to the $A$-valued measure $\sum_{i=1}^n \mu_{x_i}d_i$, and if $\Phi$ is injective (see Example 4.20), the corresponding measure is unique. This means that if we transform the samples $x_i$ according to the measure $\sum_{i=1}^n \mu_{x_i}d_i$, then the transformation makes a large impact to $y_i$.

### 5.2.3 Numerical examples

We applied our method to functional data $x_1, \ldots, x_n \in C([0, 1] \times [0, 1], [0, 1])$, where $n = 30$, $x_i(s, t) = e^{\omega_1 1_s t} e^{\omega_2 1_t}$, and $\omega_1, \omega_2, \omega_3, \omega_4, \omega_5, \omega_6, \omega_7, \omega_8$ were randomly and independently drawn from the uniform distribution on $[-1, 0]$. Then, we set $y_i$ as

$$y_i = \int_0^1 \int_0^1 x_i(s, t)^2 - 5|s - t| ds dt.$$ 

We set $A = B(L^2([0, 1]))$ and $k(x_1, x_2) = \tilde{k}(x_1, x_2)1_A$, where $\tilde{k}$ is a complex-valued positive definite kernel on $[0, 1]$ defined as $\tilde{k}(x_1, x_2) = (x_1^2 + x_2^2 + 1)(x_1^2 + x_2^2 + 1)$. We applied the PCA proposed in Subsection 5.1.2 with $N = 1$ and $r = 3$, and then computed $\lim_{\epsilon \to 0} ub_\epsilon \in M_k$ in Proposition 5.10, which can be represented as $\Phi(\sum_{i=1}^n \mu_{x_i}d_i)$. The parameter $\lambda$ in the objective function of the PCA was set as 0.1. For the computed $B(L^2([0, 1]))$-valued measure $\sum_{i=1}^n \mu_{x_i}d_i$, Figure 3 shows the density function of the complex-valued measure $\int_0^1 \mu_x \tilde{d} \tilde{d}s$ for $s = 0.1$ and $t = 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8$. Recall that the complex-valued measure $\int_0^1 \mu_x \tilde{d} \tilde{d}s$ describes a measure regarding the point $x(s, t)$. Thus, if we transform the samples $x_i(s, t)$ according to the measure $\int_0^1 \mu_x \tilde{d} \tilde{d}s$, then the transformation makes a large impact to corresponds to $y_i$. In fact, for $s = 0.1$ and $t = 0.2$, $y_i$ becomes larger as $x_i(s, t)$ becomes
larger since the exponent $2 - 5|s - t|$ is larger than 0. On the other hand, for $s = 0.1$ and $t = 0.8$, $y_i$ becomes larger as $x_i(s, t)$ becomes smaller since the exponent $2 - 5|s - t|$ is smaller than 0. This property is extracted through the $\mathcal{A}$-valued measure.

5.3 Other applications

5.3.1 Maximum mean discrepancy with kernel mean embedding

Maximum mean discrepancy (MMD) is a metric of measures according to the largest difference in means over a certain subset of a function space. It is also known as integral probability metric (IPM). For a set $\mathcal{U}$ of real-valued bounded measurable functions on $\mathcal{X}$ and two real-valued probability measures $\mu$ and $\nu$, MMD $\gamma(\mu, \nu, \mathcal{U})$ is defined as follows (Müller, 1997; Gretton et al., 2012):

$$\sup_{u \in \mathcal{U}} \left| \int_{x \in \mathcal{X}} u(x) d\mu(x) - \int_{x \in \mathcal{X}} u(x) d\nu(x) \right|.$$

For example, if $\mathcal{U}$ is the unit ball of an RKHS, denoted as $\mathcal{U}_{\text{RKHS}}$, the MMD can be represented using the KME $\tilde{\Phi}$ in the RKHS as $\gamma(\mu, \nu, \mathcal{U}_{\text{RKHS}}) = \| \tilde{\Phi}(\mu) - \tilde{\Phi}(\nu) \|_{\mathcal{H}_K}$. In addition, let $\mathcal{U}_K = \{ u \mid \| u \|_L \leq 1 \}$ and let $\mathcal{U}_D = \{ u \mid \| u \|_{\infty} + \| u \|_L \leq 1 \}$, where, $\| u \|_L := \sup_{x \neq y} |u(x) - u(y)|/|x - y|$, and $\| u \|_{\infty}$ is the sup norm of $u$. The MMDs with $\mathcal{U}_K$ and $\mathcal{U}_D$ are also discussed in Rachev (1985); Dudley (2002); Sriperumbudur et al. (2012).

Let $\mathcal{X}$ be a locally compact Hausdorff space, let $\mathcal{U}_A$ be a set of $\mathcal{A}$-valued bounded and measurable functions, and let $\mu, \nu \in \mathcal{D}(\mathcal{X}, \mathcal{A})$. We generalize the MMD to that for $\mathcal{A}$-valued measures as follows:

$$\gamma_{\mathcal{A}}(\mu, \nu, \mathcal{U}_A) := \sup_{u \in \mathcal{U}_A} \left| \int_{x \in \mathcal{X}} u(x) d\mu(x) - \int_{x \in \mathcal{X}} u(x) d\nu(x) \right|_{\mathcal{A}},$$

where the supremum is taken with respect to a (pre) order in $\mathcal{A}$ (see Definition 2.9). Let $k$ be an $\mathcal{A}$-valued $c_0$-kernel (see Definition 4.2), let $\mathcal{M}_k$ be the RKHM associated with $k$, and let $\Phi$ be the KME defined in Section 4.2. The following theorem shows that similar to the
case of RKHS, if $A$ is the unit ball of an RKHM, the generalized MMD $\gamma_A(\mu, \nu, U_A)$ can also be represented using the proposed KME in the RKHM.

**Proposition 5.12** Let $U_{\text{RKHM}} := \{ u \in \mathcal{M}_k \mid \| u \|_{\mathcal{M}_k} \leq 1 \}$. Then, for $\mu, \nu \in \mathcal{D}(X, A)$, we have

$$\gamma_A(\mu, \nu, U_{\text{RKHM}}) = |\Phi(\mu) - \Phi(\nu)|_{\mathcal{M}_k}.$$  

**Proof** By the Cauchy–Schwarz inequality (Lemma 2.16), we have

$$\left| \int_{x \in X} d\mu^* u(x) - \int_{x \in X} d\nu^* u(x) \right|_A \leq_A \| u \|_{\mathcal{M}_k} |\Phi(\mu - \nu)|_{\mathcal{M}_k} \leq_A |\Phi(\mu - \nu)|_{\mathcal{M}_k},$$

for any $u \in \mathcal{M}_k$ such that $\| u \|_{\mathcal{M}_k} \leq 1$. Let $\epsilon > 0$. We put $v = \Phi(\mu - \nu)$ and $u_\epsilon = v(|v|_{\mathcal{M}_k} + \epsilon A)^{-1}$. In the same manner as Proposition 5.11, $|\Phi(\mu - \nu)|_{\mathcal{M}_k}$ is shown to be the supremum of $|\Phi(\mu - \nu)|_{\mathcal{M}_k}$. $\square$

Various methods with the existing MMD of real-valued probability measures are generalized to $A$-valued measures by applying our MMD. Using our MMD of $A$-valued measures instead of the existing MMD allows us to evaluate discrepancies between measures regarding each point of structured data such as multivariate data and functional data. For example, the following existing methods can be generalized:

**Two-sample test:** In two-sample test, samples from two distributions (measures) are compared by computing the MMD of these measures (Gretton et al., 2012).

**Kernel mean matching for generative models:** In generative models, MMD is used in finding points whose distribution is as close as to that of input points (Jitkrittum et al., 2019).

**Domain adaptation:** In domain adaptation, MMD is used in describing the difference between the distribution of target domain data and that of source domain data (Li et al., 2019).

### 5.3.2 Time-series data analysis

Recently, random dynamical systems, which are (nonlinear) dynamical systems with random effects, have been extensively researched. Analyses of them by using the existing KME in RKHSs have been proposed (Klus et al., 2020; Hashimoto et al., 2019). Our framework can generalize these results by replacing the existing KME with our KME of $A$-valued measures. If we set $A$ as $B(L^2([0, 1]))$ and consider a positive definite kernel on $C([0, 1], X)$, then we can describe the time evolution of functional data in $C([0, 1], X)$.

### 6. Connection with existing methods

In this section, we discuss connections between the proposed methods and existing methods. We show the connection with the PCA in vv RKHSs in Subsection 6.1 and an existing notion in quantum mechanics.
6.1 Connection with PCA in vv RKHSs

We show that PCA in vv RKHSs is a special case of the proposed PCA in RKHMs. Let \( W \) be a Hilbert space and we set \( \mathcal{A} = \mathcal{B}(W) \). Let \( k : X \times X \to \mathcal{B}(W) \) be a \( \mathcal{B}(W) \)-valued positive definite kernel. In addition, let \( x_1, \ldots, x_n \in X \) be given data and \( w_{1,1}, \ldots, w_{1,N}, \ldots, w_{n,1}, \ldots, w_{n,N} \in W \) be fixed vectors in \( W \). The following proposition shows that we can reconstruct principal components of PCA in vv RKHSs by using the proposed PCA in RKHMs.

**Proposition 6.1** Let \( W_j : X \to W \) be a map satisfying \( W_j(x_i) = w_{i,j} \) for \( j = 1, \ldots, N \) and \( W = [W_1, \ldots, W_N] \), and let \( \hat{k} : X \times X \to \mathbb{C}^{r \times r} \) be defined as \( \hat{k}(x,y) = W(x)^*k(x,y)W(y) \). Let \( \{q_1, \ldots, q_r\} \subseteq \mathcal{M}_k \) be a solution of the minimization problem

\[
\min_{\{q_j\}_{j=1}^r \subseteq \mathcal{M}_k}: \text{ONS} \sum_{i=1}^n \text{tr} \left( (\phi(x_i) - q \langle \phi(x_i) \rangle_{\mathcal{F}_k})^2 \right), \tag{21}
\]

where \( \mathcal{F}_k = \{v \in \mathcal{M}_k \mid v(x) \text{ is a rank 1 operator for any } x \in X\} \). In addition, let \( p_1, \ldots, p_r \in H_k^r \) be the solution of the minimization problem

\[
\min_{\{p_j\}_{j=1}^r \subseteq H_k^r}: \text{ONS} \sum_{i=1}^n \sum_{l=1}^n \left| \phi(x_i)w_{i,l} - \sum_{j=1}^r p_j \langle \phi(x_i)w_{i,l} \rangle_{H_k^r} \right|^2. \tag{22}
\]

Then, \( \| (\langle q_j, \hat{\phi}(x_i) \rangle_{\mathcal{M}_k}) \|_{CN} = \langle p_j, \phi(x_i)w_{i,l} \rangle_{H_k^r} \) for \( i = 1, \ldots, n \), \( j = 1, \ldots, r \), and \( l = 1, \ldots, N \). Here, \( (\langle q_j, \hat{\phi}(x_i) \rangle_{\mathcal{M}_k}) \) is the \( l \)-th column of the matrix \( (q_j, \hat{\phi}(x_i))_{\mathcal{M}_k} \in \mathbb{C}^{N \times N} \).

**Proof** Let \( G \in (\mathbb{C}^{N \times N})^{n \times n} \) be defined as \( G_{i,j} = \hat{k}(x_i, x_j) \). By Proposition 5.8, any solution of the problem (21) is represented as \( q_j = \sum_{i=1}^n c_i \hat{k}(x_i) w_{i,l} \hat{k}(x_i) \) for \( i = 1, \ldots, r \) and \( c_{1,j}, \ldots, c_{n,j} \) are the largest \( r \) eigenvalues and \( v_j \) are the corresponding orthonormal eigenvectors of the matrix \( G \). Therefore, by the definition of \( k \), the principal components are calculated as

\[
\langle q_j, \hat{\phi}(x_i) \rangle_{\mathcal{M}_k}^* W(x_i)^* k(x_i, x_1) W(x_1), \ldots, k(x_i, x_n) W(x_n) ] v_j u^*. \tag{23}
\]

On the other hand, in the same manner as Proposition 5.8, the solution of the problem (22) is shown to be represented as \( p_j = \sum_{i=1}^n c_i \hat{k}(x_i) w_{i,l} \alpha_{i_l} \) for \( j = 1, \ldots, r \) and \( c_{1,j}, \ldots, c_{n,j} \) are the corresponding orthonormal eigenvectors of the matrix \( G \). Therefore, the principal components are calculated as

\[
\langle p_j, \hat{\phi}(x_i) w_{i,l} \rangle_{H_k^r}^* W(x_i)^* k(x_i, x_1) W(x_1), \ldots, k(x_i, x_n) W(x_n) ] v_j, \tag{24}
\]

which completes the proof of the proposition.

6.2 Connection with quantum mechanics

Positive operator-valued measures play an important role in quantum mechanics. A positive operator-valued measure is defined as an \( \mathcal{A} \)-valued measure \( \mu \) such that \( \mu(X) = I \) and \( \mu(E) \)
is positive for any Borel set $E$. It enables us to extract information of the probabilities of outcomes from a state \cite{Peres and Terno 2004, Holevo 2011}. We show that the existing inner product considered for quantum states \cite{Balkir 2014, Deb 2016} is generalized with our KME of positive operator-valued measures.

Let $\mathcal{X} = \mathbb{C}^m$ and $\mathcal{A} = \mathbb{C}^{m \times m}$. Let $\rho \in \mathcal{A}$ be a positive semi-definite matrix with unit trace, called a density matrix. A density matrix describes the states of a quantum system, and information about outcomes is described as measure $\mu \rho \in \mathcal{D}(\mathcal{X}, \mathcal{A})$. We have the following proposition. Here, we use the bra-ket notation, i.e., $|\alpha\rangle \in \mathcal{X}$ represents a (column) vector in $\mathcal{X}$, and $\langle \alpha |$ is defined as $|\alpha\rangle^\ast$:

**Proposition 6.2** Assume $\mathcal{X} = \mathbb{C}^m$, $\mathcal{A} = \mathbb{C}^{m \times m}$, and $k : \mathcal{X} \times \mathcal{X} \to \mathcal{A}$ is a positive definite kernel defined as $k(|\alpha\rangle, |\beta\rangle) = |\alpha\rangle \langle \alpha | \beta \rangle \langle \beta |$. If $\mu$ is represented as $\mu = \sum_{i=1}^m \delta_{|\psi_i\rangle}|\psi_i\rangle \langle \psi_i|$ for an orthonormal basis $\{|\psi_1\rangle, \ldots, |\psi_m\rangle\}$ of $\mathcal{X}$, then $\text{tr}(\langle \Phi(\mu \rho_1), \Phi(\mu \rho_2) \rangle_{\mathcal{M}_k}) = \langle \rho_1, \rho_2 \rangle_{\text{HS}}$ holds. Here, $\langle \cdot, \cdot \rangle_{\text{HS}}$ is the Hilbert–Schmidt inner product.

**Proof** Let $M_i = |\psi_i\rangle \langle \psi_i|$ for $i = 1, \ldots, m$. The inner product between $\Phi(\mu \rho_1)$ and $\Phi(\mu \rho_2)$ is calculated as follows:

$$\langle \Phi(\mu \rho_1), \Phi(\mu \rho_2) \rangle_{\mathcal{M}_k} = \int_{x \in \mathcal{X}} \int_{y \in \mathcal{X}} \rho_1^* k(x, y) \rho_2(y) = \sum_{i,j=1}^m \rho_1^* M_i k(|\psi_i\rangle, |\psi_j\rangle) M_j \rho_2.$$

Since the identity $k(|\psi_i\rangle, |\psi_j\rangle) = M_i M_j^\ast$ holds and $\{|\psi_1\rangle, \ldots, |\psi_m\rangle\}$ is orthonormal, we have $\langle \Phi(\mu \rho_1), \Phi(\mu \rho_2) \rangle_{\mathcal{M}_k} = \sum_{i=1}^m \rho_1^* M_i \rho_2$. By using the identity $\sum_{i=1}^m M_i = I$, we have

$$\text{tr}(\sum_{i=1}^m \rho_1^* M_i \rho_2) = \text{tr}(\sum_{i=1}^m M_i \rho_2 \rho_1^*) = \text{tr}(\rho_2 \rho_1^*),$$

which completes the proof of the proposition.

In previous studies \cite{Balkir 2014, Deb 2016}, the Hilbert–Schmidt inner product between density matrices was considered to represent similarities between two quantum states. Liu and Rebetrost \cite{Liu and Rebetrost 2018} considered the Hilbert–Schmidt inner product between square roots of density matrices. Theorem 6.2 shows that these inner products are represented via our KME in RKHMs.

### 7. Conclusions and future works

In this paper, we proposed a new data analysis framework with RKHM and developed a KME in RKHMs for analyzing distributions. We showed the theoretical validity for applying those to data analysis. Then, we applied it to kernel PCA and analysis of interaction effects in finite or infinite dimensional data. RKHM is a generalization of RKHS in terms of $C^*$-algebra, and we can extract rich information about structures in data such as multivariate data and functional data by using $C^*$-algebras. For example, we can reduce multi-variable functional data to functions of single variable by considering the space of functions of single variables as a $C^*$-algebra and then by applying the proposed PCA in RKHMs. Moreover, we can extract information of interaction effects in continuously distributed spatio data by considering the space of bounded linear operators on a function space as a $C^*$-algebra.
As future works, we will address $C^*$-algebra-valued supervised problems on the basis of the representer theorem (Theorem 3.8) and apply the proposed KME in RKHMs to quantum mechanics.

**Appendix A. Proofs of the lemmas and propositions in Section 3.1**

**Proof of Lemma 3.4**

Let $k$ be an $\mathcal{A}$-valued positive definite kernel defined in Definition 3.2. Let $w \in \mathcal{W}$. For $n \in \mathbb{N}$, $w_1, \ldots, w_n \in \mathcal{W}$, let $c_i \in \mathcal{B}(\mathcal{W})$ be defined as $c_i h := \langle w, h \rangle_{\mathcal{W}} / \langle w, w \rangle_{\mathcal{W}}$ for $h \in \mathcal{W}$. Since $w_i = c_i w$ holds, the following equalities are derived for $x_1, \ldots, x_n \in \mathcal{X}$:

$$
\sum_{i,j=1}^{n} \langle w_i, k(x_i, x_j)w_j \rangle_{\mathcal{W}} = \sum_{i,j=1}^{n} \langle c_i w, k(x_i, x_j)c_j w \rangle_{\mathcal{W}} = \left\langle w, \sum_{i,j=1}^{n} c_i^* k(x_i, x_j) c_i w \right\rangle_{\mathcal{W}}.
$$

By the positivity of $\sum_{i,j=1}^{n} c_i^* k(x_i, x_j) c_j$, $\langle w, \sum_{i,j=1}^{n} c_i^* k(x_i, x_j) c_j w \rangle_{\mathcal{W}} \geq 0$ holds, which implies $k$ is an operator valued positive definite kernel defined in Definition 2.2.

On the other hand, let $k$ be an operator valued positive definite kernel defined in Definition 2.2. Let $v \in \mathcal{W}$. For $n \in \mathbb{N}$, $c_1, \ldots, c_n \in \mathcal{A}$ and $x_1, \ldots, x_n \in \mathcal{X}$, the following equality is derived:

$$
\left\langle w, \sum_{i,j=1}^{n} c_i^* k(x_i, x_j) c_j w \right\rangle_{\mathcal{W}} = \sum_{i,j=1}^{n} \langle c_i w, k(x_i, x_j)c_j w \rangle_{\mathcal{W}}.
$$

By Definition 2.2, $\sum_{i,j=1}^{n} \langle c_i w, k(x_i, x_j)c_j w \rangle_{\mathcal{W}} \geq 0$ holds, which implies $k$ is an $\mathcal{A}$-valued positive definite kernel defined in Definition 3.2.

**Proof of Proposition 3.5**

(Existence) For $u, v \in \mathcal{M}_k$, there exist $u_i, v_i \in \mathcal{M}_{k,0}$ ($i = 1, 2, \ldots$) such that $v = \lim_{i \to \infty} v_i$ and $w = \lim_{i \to \infty} w_i$. By the Cauchy-Schwarz inequality (Lemma 2.16), the following inequalities hold:

$$
\| \langle u_i, v_i \rangle_{\mathcal{M}_k} - \langle u_j, v_j \rangle_{\mathcal{M}_k} \|_{\mathcal{A}} \leq \| \langle u_i, v_i - v_j \rangle_{\mathcal{M}_k} \|_{\mathcal{A}} + \| \langle u_i - u_j, v_j \rangle_{\mathcal{M}_k} \|_{\mathcal{A}}
$$

$$
\leq \| u_i \|_{\mathcal{M}_k} \| v_i - v_j \|_{\mathcal{M}_k} + \| u_i - u_j \|_{\mathcal{M}_k} \| v_j \|_{\mathcal{M}_k}
$$

$$
\to 0 \ (i, j \to \infty),
$$

which implies $\{ \langle u_i, v_i \rangle_{\mathcal{M}_k} \}_{i=1}^{\infty}$ is a Cauchy sequence in $\mathcal{A}$. By the completeness of $\mathcal{A}$, there exists a limit $\lim_{i \to \infty} \langle u_i, v_i \rangle_{\mathcal{M}_k}$.

(Well-definedness) Assume there exist $u_i', v_i' \in \mathcal{M}_{k,0}$ ($i = 1, 2, \ldots$) such that $u = \lim_{i \to \infty} u_i = \lim_{i \to \infty} u_i'$ and $v = \lim_{i \to \infty} v_i = \lim_{i \to \infty} v_i'$. By the Cauchy-Schwarz inequality (Lemma 2.16), we have

$$
\| \langle u_i, v_i \rangle_{\mathcal{M}_k} - \langle u_i', v_i' \rangle_{\mathcal{M}_k} \|_{\mathcal{A}} \leq \| u_i \|_{\mathcal{M}_k} \| v_i - v_i' \|_{\mathcal{M}_k} + \| u_i - u_i' \|_{\mathcal{M}_k} \| v_i' \|_{\mathcal{M}_k} \to 0 \ (i \to \infty),
$$

which implies $\lim_{i \to \infty} \langle u_i, v_i \rangle_{\mathcal{M}_k} = \lim_{i \to \infty} \langle u_i', v_i' \rangle_{\mathcal{M}_k}$.
(Injectivity) For \( u, v \in \mathcal{M}_k \), we assume \( \langle \phi(x), u \rangle_{\mathcal{M}_k} = \langle \phi(x), v \rangle_{\mathcal{M}_k} \) for \( x \in \mathcal{X} \). By the linearity of \( \langle \cdot, \cdot \rangle_{\mathcal{M}_k} \), \( \langle p, u \rangle_{\mathcal{M}_k} = \langle p, v \rangle_{\mathcal{M}_k} \) holds for \( p \in \mathcal{M}_{k,0} \). For \( p \in \mathcal{M}_k \), there exist \( p_i \in \mathcal{M}_{k,0} \) (\( i = 1, 2, \ldots \)) such that \( p = \lim_{i \to \infty} p_i \). Therefore, \( \langle p, u - v \rangle_{\mathcal{M}_k} = \lim_{i \to \infty} \langle p_i, u - v \rangle_{\mathcal{M}_k} = 0 \). As a result, \( \langle u - v, u - v \rangle_{\mathcal{M}_k} = 0 \) holds by setting \( p = u - v \), which implies \( u = v \).

**Proof of Proposition 3.6**

We define \( \Psi : \mathcal{M}_{k,0} \to \mathcal{M} \) as an \( \mathcal{A} \)-linear map that satisfies \( \Psi(\phi(x)) = \psi(x) \). We show \( \Psi \) can be extended to a unique \( \mathcal{A} \)-linear bijection map on \( \mathcal{M}_k \), which preserves the inner product.

(Injectivity) For \( u, v \in \mathcal{M}_k \), we have

\[
\langle \Psi(\phi(x)), \Psi(\phi(y)) \rangle_{\mathcal{M}_k} = \langle \psi(x), \psi(y) \rangle_{\mathcal{M}} = k(x, y) = \langle \phi(x), \phi(y) \rangle_{\mathcal{M}_k}.
\]

Since \( \Psi \) is \( \mathcal{A} \)-linear, \( \Psi \) preserves the inner products between arbitrary \( u, v \in \mathcal{M}_{k,0} \).

(Well-definedness) Since \( \Phi \) preserves the inner product, if \( \{v_i\}_{i=1}^{\infty} \subseteq \mathcal{M}_k \) is a Cauchy sequence, \( \{\Phi(v_i)\}_{i=1}^{\infty} \subseteq \mathcal{M} \) is also a Cauchy sequence. Therefore, by the completeness of \( \mathcal{M} \), \( \Psi \) also preserves the inner product in \( \mathcal{M}_k \), and for \( v \in \mathcal{M}_k \), \( \|\Psi(v)\|_{\mathcal{M}} = \|v\|_{\mathcal{M}_k} \) holds. As a result, for \( v \in \mathcal{M}_k \), if \( v = 0 \), \( \|\Psi(v)\|_{\mathcal{M}} = \|v\|_{\mathcal{M}_k} = 0 \) holds. This implies \( \Psi(v) = 0 \).

(Surjectivity) It follows directly by the condition \( \{\sum_{i=0}^{n} \psi(x_i) c_i \mid x_i \in \mathcal{Y}, c_i \in \mathcal{A}\} = \mathcal{M} \).

**Appendix B. Proofs of the propositions and theorem in Section 4.3**

Before proving the propositions and theorem, we introduce some definitions and show fundamental properties which are related to the propositions and theorem.

**Definition B.1 (\( \mathcal{A} \)-dual)** For a Banach \( \mathcal{A} \)-module \( \mathcal{M} \), the \( \mathcal{A} \)-dual of \( \mathcal{M} \) is defined as \( \mathcal{M}' := \{f : \mathcal{M} \to \mathcal{A} \mid f \text{ is bounded and } \mathcal{A} \text{-linear}\} \).

Note that for a right Banach \( \mathcal{A} \)-module \( \mathcal{M} \), \( \mathcal{M}' \) is a left Banach \( \mathcal{A} \)-module.

**Definition B.2 (Orthogonal complement)** For an \( \mathcal{A} \)-submodule \( \mathcal{M}_0 \) of a Banach \( \mathcal{A} \)-module \( \mathcal{M} \), the orthogonal complement of \( \mathcal{M}_0 \) is defined as a closed submodule \( \mathcal{M}_0^\perp := \bigcap_{u \in \mathcal{M}_0} \{f \in \mathcal{M}' \mid f(u) = 0\} \) of \( \mathcal{M}' \). In addition, for an \( \mathcal{A} \)-submodule \( \mathcal{N}_0 \) of \( \mathcal{M}' \), the orthogonal complement of \( \mathcal{N}_0 \) is defined as a closed submodule \( \mathcal{N}_0^\perp := \bigcap_{f \in \mathcal{N}_0} \{u \in \mathcal{M} \mid f(u) = 0\} \) of \( \mathcal{M} \).

Note that for a von Neumann-algebra \( \mathcal{A} \) and Hilbert \( \mathcal{A} \)-module \( \mathcal{M} \), by Proposition 4.13, \( \mathcal{M}' \) and \( \mathcal{M} \) are isomorphic. The following lemma shows a connection between an orthogonal complement and the density property.

**Lemma B.3** For a Banach \( \mathcal{A} \)-module \( \mathcal{M} \) and its submodule \( \mathcal{M}_0 \), \( \mathcal{M}_0^\perp = \{0\} \) if \( \mathcal{M}_0 \) is dense in \( \mathcal{M} \).
Proof We first show $\overline{M_0} \subseteq (M_0^+)^\perp$. Let $u \in M_0$. By the definition of orthogonal complements, $u \in (M_0^+)^\perp$. Since $(M_0^+)^\perp$ is closed, $\overline{M_0} \subseteq (M_0^+)^\perp$. If $M_0$ is dense in $M$, $\overline{M_0} \subseteq (M_0^+)^\perp$ holds, which means $M_0^+ = \{0\}$. \hfill \Box

Moreover, in the case of $A = \mathbb{C}^{m \times m}$, a generalization of the Riesz–Markov representation theorem for $\mathcal{D}(\mathcal{X}, A)$ holds.

**Proposition B.4 (Riesz–Markov representation theorem for $\mathbb{C}^{m \times m}$-valued measures)** Let $A = \mathbb{C}^{m \times m}$. There exists an isomorphism between $\mathcal{D}(\mathcal{X}, A)$ and $C_0(\mathcal{X}, A)'$.

**Proof** For $f \in C_0(\mathcal{X}, A)'$, let $f_{i,j} \in C_0(\mathcal{X}, \mathbb{C})'$ be defined as $f_{i,j}(u) = (f(u_{1,A}))_{i,j}$ for $u \in C_0(\mathcal{X}, \mathbb{C})$. Then, by the Riesz–Markov representation theorem for complex-valued measure, there exists a unique finite complex-valued regular measure $\mu_{i,j}$ such that $f_{i,j}(u) = \int_{x \in Y} u(x) d\mu_{i,j}(x)$. Let $\mu(E) := [\mu_{i,j}(E)]_{i,j}$ for $E \in \mathcal{B}$. Then, $\mu \in \mathcal{D}(\mathcal{X}, A)$, and we have

$$f(u) = f \left( \sum_{l,l'}^{m} u_{l,l'} e_{l,l'} \right) = \sum_{l,l'}^{m} \left[ f_{i,j}(u_{l,l'}) \right]_{i,j} e_{l,l'} = \sum_{l,l'}^{m} \int_{x \in Y} u_{l,l'}(x) d\mu_{i,j}(x) e_{l,l'} = \int_{x \in Y} d\mu(x) u(x),$$

where $e_{i,j}$ is an $m \times m$ matrix whose $(i,j)$-element is 1 and all the other elements are 0. Therefore, if we define $h' : C_0(\mathcal{X}, A)' \to \mathcal{D}(\mathcal{X}, A)$ as $f \mapsto \mu$, $h'$ is the inverse of $h$, which completes the proof of the proposition. \hfill \Box

### B.1 Proofs of Propositions 4.18 and 4.19

To show Propositions 4.18 and 4.19, the following lemma is used.

**Lemma B.5** $\Phi : \mathcal{D}(\mathcal{X}, A) \to \mathcal{M}_k$ is injective if and only if $(\Phi(\mu), \Phi(\mu))_{\mathcal{M}_k} \neq 0$ for any nonzero $\mu \in \mathcal{D}(\mathcal{X}, A)$.

**Proof** ($\Rightarrow$) Suppose there exists a nonzero $\mu \in \mathcal{D}(\mathcal{X}, A)$ such that $(\Phi(\mu), \Phi(\mu))_{\mathcal{M}_k} = 0$. Then, $\Phi(\mu) = \Phi(0) = 0$ holds, and thus, $\Phi$ is not injective.

($\Leftarrow$) Suppose $\Phi$ is not injective. Then, there exist $\mu, \nu \in \mathcal{D}(\mathcal{X}, A)$ such that $\Phi(\mu) = \Phi(\nu)$ and $\mu \neq \nu$, which implies $\Phi(\mu - \nu) = 0$ and $\mu - \nu \neq 0$.

We now show Propositions 4.18 and 4.19.

**Proof** [Proof of Theorem 4.18] Let $\mu \in \mathcal{D}(\mathcal{X}, A)$, $\mu \neq 0$. We have

$$\langle \Phi(\mu), \Phi(\mu) \rangle = \int_{x \in \mathbb{R}^d} \int_{y \in \mathbb{R}^d} d\mu^*(x) k(x, y) d\mu(y)$$

$$= \int_{x \in \mathbb{R}^d} \int_{y \in \mathbb{R}^d} d\mu^*(x) \int_{\omega \in \mathbb{R}^d} e^{-\sqrt{-1}(y-x)^T \omega} d\lambda(\omega) d\mu(y)$$

$$= \int_{\omega \in \mathbb{R}^d} \int_{y \in \mathbb{R}^d} e^{-\sqrt{-1}x^T \omega} d\mu^*(x) d\lambda(\omega) \int_{y \in \mathbb{R}^d} e^{-\sqrt{-1}y^T \omega} d\mu(y)$$

$$= \int_{\omega \in \mathbb{R}^d} \hat{\mu}(\omega)^* d\lambda(\omega) \hat{\mu}(\omega).$$
Assume \( \hat{\mu} = 0 \). Then, \( \int_{x \in \mathcal{X}} u(x) d\hat{\mu}(x) = 0 \) for any \( u \in C_0(\mathcal{X}, \mathcal{A}) \) holds, which implies \( \mu \in C_0(\mathcal{X}, \mathcal{A})^\perp = \{0\} \) by Proposition B.4 and Lemma B.3. Thus, \( \hat{\mu} = 0 \). In addition, by the assumption, \( \text{supp}(\lambda) = \mathbb{R}^d \) holds. As a result, \( \int_{\omega \in \mathbb{R}^d} \hat{\mu}(\omega)^* d\lambda(\omega) \hat{\mu}(\omega) \neq 0 \) holds. By Lemma B.5, \( \Phi \) is injective.

**Proof** [Proof of Theorem 4.19] Let \( \mu \in \mathcal{D}(\mathcal{X}, \mathcal{A}), \mu \neq 0 \). We have

\[
\langle \Phi(\mu), \Phi(\mu) \rangle = \int_{x \in \mathbb{R}^d} \int_{y \in \mathbb{R}^d} d\mu^*(x)k(x, y)d\mu(y)
\]

\[
= \int_{x \in \mathbb{R}^d} \int_{y \in \mathbb{R}^d} d\mu^*(x) \int_{t \in [0, \infty)} e^{-\|x-y\|^2/4t} d\eta(t)d\mu(y)
\]

\[
= \int_{x \in \mathbb{R}^d} \int_{y \in \mathbb{R}^d} d\mu^*(x) \int_{t \in [0, \infty)} \frac{1}{(2t)^{d/2}} \int_{\omega \in \mathbb{R}^d} e^{-\sqrt{-1}(y-x)^T \omega - \|\omega\|^2/4t} d\omega d\eta(t)d\mu(y)
\]

\[
= \int_{\omega \in \mathbb{R}^d} \hat{\mu}(\omega)^* \int_{t \in [0, \infty)} \frac{1}{(2t)^{d/2}} e^{-\|\omega\|^2/4t} d\eta(t)\hat{\mu}(\omega)d\omega,
\]

(23)

where we applied a formula \( e^{-\|x-y\|^2/2} \int_{\omega \in \mathbb{R}^d} e^{-\sqrt{-1}x^T \omega - \|\omega\|^2/(4t)} d\omega \) in the third equality. In the same manner as the proof of Theorem 4.18, \( \hat{\mu} \neq 0 \) holds. In addition, since \( \text{supp}(\eta) \neq \{0\} \) holds, \( \int_{t \in [0, \infty)} (2t)^{-d/2} e^{-\|\omega\|^2/(4t)} d\eta(t) \) is positive definite. As a result, the last formula in Eq. (23) is nonzero. By Lemma B.5, \( \Phi \) is injective.

**B.2 Proofs of Proposition 4.22 and Theorem 4.23**

Let \( \mathcal{R}_+(\mathcal{X}) \) be the set of all real positive-valued regular measures, and \( \mathcal{D}_\nu(\mathcal{X}, \mathcal{A}) \) the set of all finite regular \( \mathcal{A} \)-valued measures \( \mu \) whose total variations are dominated by \( \nu \in \mathcal{R}_+(\mathcal{X}) \) (i.e., \( |\mu| \leq \nu \)). We apply the following representation theorem to derive Theorem 4.23.

**Proposition B.6** For \( \nu \in \mathcal{R}_+(\mathcal{X}) \), there exists an isomorphism between \( \mathcal{D}_\nu(\mathcal{X}, \mathcal{A}) \) and \( L^1(\mathcal{X}, \mathcal{A})' \).

**Proof** For \( \mu \in \mathcal{D}_\nu(\mathcal{X}, \mathcal{A}) \) and \( u \in L^1(\mathcal{X}, \mathcal{A}) \), we have

\[
\left\| \int_{x \in \mathcal{Y}} d\mu(x)u(x) \right\|_{\mathcal{A}} \leq \int_{x \in \mathcal{Y}} \|u(x)\|_\mathcal{A} d\|\mu|(x) \leq \int_{x \in \mathcal{Y}} \|u(x)\|_\mathcal{A} d\nu(x).
\]

Thus, we define \( h : \mathcal{D}_\nu(\mathcal{X}, \mathcal{A}) \rightarrow L^1(\mathcal{X}, \mathcal{A})' \) as \( \mu \mapsto (u \mapsto \int_{x \in \mathcal{Y}} d\mu(x)u(x)) \).

Meanwhile, for \( f \in L^1(\mathcal{X}, \mathcal{A})' \) and \( E \in \mathcal{B} \), we have

\[
\|f(\chi_E 1_A)\|_\mathcal{A} \leq C \int_{x \in \mathcal{X}} \|\chi_E 1_A\|_\mathcal{A} d\nu(x) = C\nu(E),
\]

for some \( C > 0 \) since \( f \) is bounded. Here, \( \chi_E \) is an indicator function for a Borel set \( E \). Thus, we define \( h' : L^1(\mathcal{X}, \mathcal{A})' \rightarrow \mathcal{D}_\nu(\mathcal{X}, \mathcal{A}) \) as \( f \mapsto (E \mapsto f(\chi_E 1_A)) \).

By the definitions of \( h \) and \( h' \), \( h(h'(f))(s) = f(s) \) holds for \( s \in \mathcal{S}(\mathcal{X}, \mathcal{A}) \). Since \( \mathcal{S}(\mathcal{X}, \mathcal{A}) \) is dense in \( L^1(\mathcal{X}, \mathcal{A}) \), \( h(h'(f))(u) = f(u) \) holds for \( u \in L^1(\mathcal{X}, \mathcal{A}) \). Moreover,
h'(h(\mu))(E) = \mu(E) \text{ holds for } E \in \mathcal{B}. \text{ Therefore, } \mathcal{D}_C(\mathcal{X}, \mathcal{A}) \text{ and } L^1_\nu(\mathcal{X}, \mathcal{A})' \text{ are isomorphic.}

**Proof** [Proof of Theorem 4.23] Assume \( \mathcal{M}_k \) is dense in \( C_0(\mathcal{X}, \mathcal{A}) \). Since \( C_0(\mathcal{X}, \mathcal{A}) \) is dense in \( L^1_\nu(\mathcal{X}, \mathcal{A}) \) for any \( \nu \in \mathcal{R}_+(\mathcal{X}) \), \( \mathcal{M}_k \) is dense in \( L^1_\nu(\mathcal{X}, \mathcal{A}) \) for any \( \nu \in \mathcal{R}_+(\mathcal{X}) \). By Proposition B.3, \( \mathcal{M}_k = \{0\} \) holds. Let \( \mu \in \mathcal{D}(\mathcal{X}, \mathcal{A}) \). There exists \( \nu \in \mathcal{R}_+(\mathcal{X}) \) such that \( \mu \in \mathcal{D}_\nu(\mathcal{X}, \mathcal{A}) \). By Proposition B.6, if \( \int_{\mathcal{X}} \nu d\mu(x)(x) = 0 \) for any \( u \in \mathcal{M}_k, \mu = 0 \). Since \( \int_{\mathcal{X}} \nu d\mu(x)(x) = \langle u, \Phi(\mu) \rangle_{\mathcal{M}_k}, \int_{\mathcal{X}} \nu d\mu(x)(x) = 0 \) means \( \Phi(\mu) = 0 \). Therefore, by Lemma B.5. \( \Phi \) is injective.

For the case of \( \mathcal{A} = \mathbb{C}^{m \times m} \), we apply the following extension theorem to derive the converse of Theorem 4.23.

**Proposition B.7 (c.f. Theorem in Helemskii (1994))** Let \( \mathcal{A} = \mathbb{C}^{m \times m} \). Let \( \mathcal{M} \) be a Banach \( \mathcal{A} \)-module, \( \mathcal{M}_0 \) be a closed submodule of \( \mathcal{M} \), and \( f_0: \mathcal{M}_0 \to \mathcal{A} \) be a bounded \( \mathcal{A} \)-linear map. Then, there exists a bounded \( \mathcal{A} \)-linear map \( f: \mathcal{M} \to \mathcal{A} \) that extends \( f_0 \) (i.e., \( f(u) = f_0(u) \) for \( u \in \mathcal{M}_0 \)).

**Proof** Von Neumann-algebra \( \mathcal{A} \) itself is regarded as an \( \mathcal{A} \)-module and is normal. Also, \( \mathbb{C}^{m \times m} \) is a Banach \( \mathcal{A} \)-module. By Theorem in Helemskii (1994), \( \mathcal{A} \) is an injective object in the category of Banach \( \mathcal{A} \)-modules. The statement is derived by the definition of injective objects in category theory.

We derive the following lemma and proposition by Proposition B.7

**Lemma B.8** Let \( \mathcal{A} = \mathbb{C}^{m \times m} \). Let \( \mathcal{M} \) be a Banach \( \mathcal{A} \)-module and \( \mathcal{M}_0 \) be a closed submodule of \( \mathcal{M} \). For \( u_1 \in \mathcal{M} \setminus \mathcal{M}_0 \), there exists a bounded \( \mathcal{A} \)-linear map \( f: \mathcal{M} \to \mathcal{A} \) such that \( f(u_0) = 0 \) for \( u_0 \in \mathcal{M}_0 \) and \( f(u_1) \neq 0 \).

**Proof** Let \( q: \mathcal{M} \to \mathcal{M}/\mathcal{M}_0 \) be the quotient map to \( \mathcal{M}/\mathcal{M}_0 \), and \( \mathcal{U}_1 := \{q(u_1)c \mid c \in \mathcal{A}\} \). Note that \( \mathcal{M}/\mathcal{M}_0 \) is a Banach \( \mathcal{A} \)-module and \( \mathcal{U}_1 \) is its closed submodule. Let \( \mathcal{V} := \{c \in \mathcal{A} \mid q(u_1)c = 0\} \), which is a closed subspace of \( \mathcal{A} \). Since \( \mathcal{V} \) is orthogonally complemented (Manuilov and Troitsky, 2000, Proposition 2.5.4), \( \mathcal{A} \) is decomposed into \( \mathcal{A} = \mathcal{V} + \mathcal{V}^\perp \). Let \( p: \mathcal{A} \to \mathcal{V}^\perp \) be the projection onto \( \mathcal{V}^\perp \) and \( f_0: \mathcal{U}_1 \to \mathcal{A} \) defined as \( q(u_1)c \mapsto p(c) \). Since \( p \) is \( \mathcal{A} \)-linear, \( f_0 \) is also \( \mathcal{A} \)-linear. Also, for \( c \in \mathcal{A} \), we have

\[
\|q(u_1)c\|_{\mathcal{M}/\mathcal{M}_0} = \|q(u_1)(c_1 + c_2)\|_{\mathcal{M}/\mathcal{M}_0} = \|q(u_1)c_1\|_{\mathcal{M}/\mathcal{M}_0} \geq \inf_{d \in \mathcal{V}^\perp, \|d\|_{\mathcal{A}} = 1} \|q(u_1)d\|_{\mathcal{M}/\mathcal{M}_0} \|c_1\|_{\mathcal{A}} = \inf_{d \in \mathcal{V}^\perp, \|d\|_{\mathcal{A}} = 1} \|q(u_1)d\|_{\mathcal{M}/\mathcal{M}_0} \|p(c)\|_{\mathcal{A}},
\]

where \( c_1 = p(c) \) and \( c_2 = c_1 - p(c) \). Since \( \inf_{d \in \mathcal{V}^\perp, \|d\|_{\mathcal{A}} = 1} \|q(u_1)d\|_{\mathcal{M}/\mathcal{M}_0} \|p(c)\|_{\mathcal{A}} > 0 \), \( f_0 \) is bounded. By Proposition B.7, \( f_0 \) is extended to a bounded \( \mathcal{A} \)-linear map \( f_1: \mathcal{M}/\mathcal{M}_0 \to \mathcal{A} \). Setting \( f := f_1 \circ q \) completes the proof of the lemma.

Then we prove the converse of Lemma B.3.

**Proposition B.9** Let \( \mathcal{A} = \mathbb{C}^{m \times m} \). For a Banach \( \mathcal{A} \)-module \( \mathcal{M} \) and its submodule \( \mathcal{M}_0 \), \( \mathcal{M}_0 \) is dense in \( \mathcal{M} \) if \( \mathcal{M}_0^\perp = \{0\} \).
Proof Assume \( u \notin M_0 \). We show \( M_0 \supseteq (M_0^\perp)^\perp \) By Lemma B.8, there exists \( f \in M' \) such that \( f(u) \neq 0 \) and \( f(u_0) = 0 \) for any \( u_0 \in M_0 \). Thus, \( u \notin (M_0^\perp)^\perp \). As a result, \( M_0 \supseteq (M_0^\perp)^\perp \). Therefore, if \( M_0^\perp = \{0\} \), then \( M_0 \) is dense in \( M \).

As a result, we derive Proposition 4.22 as follows.

Proof [Proof of Proposition 4.22] Let \( \mu \in D(\mathcal{X}, \mathcal{A}) \). Then, \( \Phi(\mu) = 0 \) is equivalent to \( \int_{x \in \mathcal{Y}} d\mu(x)u(x) = \langle \Phi(\mu), u \rangle_{M_k} = 0 \) for any \( u \in M_k \). Thus, by Proposition B.4, \( \Phi(\mu) = 0 \Rightarrow \mu = 0 \) is equivalent to \( f \in C_0(\mathcal{X}, \mathcal{A})', f(u) = 0 \) for any \( u \in M_k \Rightarrow f = 0 \).

By the definition of \( M_k^\perp \) and Proposition B.9, \( M_k \) is dense in \( C_0(\mathcal{X}, \mathcal{A}) \).

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