Analysis of Interacting Dynamical Systems with Reproducing Kernel Hilbert C^*-module

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1 Introduction

The problem of analyzing dynamical systems from observed data by Perron-Frobenius operators and their adjoints (called Koopman operators), which are linear operators expressing the time evolution of dynamical systems, has recently attracted attention in various fields [2, 3, 10, 14, 16, 17]. And, several methods for this problem using RKHSs (reproducing kernel Hilbert spaces) or vv-RKHSs (vector-valued RKHSs) have also been proposed [4, 5, 7, 9, 11], In these methods, sequential data is supposed to be generated from dynamical systems and is analyzed through those corresponding representations with Perron-Frobenius operators.

In this paper, we propose a generalized method with RKHMs (reproducing kernel Hilbert C^*-modules) for the analysis with Perron-Frobenius operators for cases where multiple dynamical systems interact, which often occurs in various dynamic phenomena around us. RKHM is a generalization of RKHS in terms of C^*-algebra [6, 8, 15]. A C^*-algebra is a generalization of the space of complex values. An important example of C^*-algebra is the space of bounded linear operators on a Hilbert space (the space of matrices if the Hilbert space is finite dimensional). We introduce RKHM in Section 2. Then, we define the Perron-Frobenius operators in RKHMs in Section 3 and show their applications in Section 4.

2 Background

2.1 C^*-algebra and C^*-module

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

A C^*-algebra is defined as a Banach space equipped with a product structure and an involution $(\cdot)^* : \mathscr{A} \to \mathscr{A}$.

Definition 2.1 (C^*-algebra) *A set $\mathscr{A}$ is called a* C^*-algebra *if it satisfies the following conditions:*

1. *$\mathscr{A}$ is an algebra over $\mathbb{C}$, and there exists a bijection $(\cdot)^* : \mathscr{A} \to \mathscr{A}$ that satisfies the following conditions for $\lambda, \mu \in \mathbb{C}$ and $c, d \in \mathscr{A}$:*
   • $(\lambda c + \mu d)^* = \overline{\lambda} c^* + \overline{\mu} d^*$, • $(cd)^* = d^* c^*$, • $(c^*)^* = c$
2. *$\mathscr{A}$ is a norm space with $\|\cdot\|_{\mathscr{A}}$, and for $c, d \in \mathscr{A}$, $\|cd\|_{\mathscr{A}} \le \|c\|_{\mathscr{A}} \|d\|_{\mathscr{A}}$ holds. In addition, $\mathscr{A}$ is complete with respect to $\|\cdot\|_{\mathscr{A}}$.*
3. *For $c \in \mathscr{A}$, $\|c^* c\|_{\mathscr{A}} = \|c\|_{\mathscr{A}}^2$ holds.*

A main example of C^*-algebras is $\mathscr{B}(\mathscr{H})$, the set of all bounded linear operators on a Hilbert space $\mathscr{H}$. In particular, if $\mathscr{H}$ is finite dimensional, it is equal to the space of matrices. In this case, the product structure is the usual product of operators, the involution is the Hermitian conjugate, and the norm $\|\cdot\|_{\mathscr{A}}$ is the operator norm.

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

Definition 2.2 (Positive) *$c \in \mathscr{A}$ is called* positive *if there exists $d \in \mathscr{A}$ such that $c = d^*d$ holds. For a positive element $c \in \mathscr{A}$, we denote $c \geq 0$.*

In the case of $\mathscr{A} = \mathscr{B}(\mathscr{H})$, the positiveness corresponds to positive semi-definiteness of operators. The notion of positiveness provides us the (pre) order in $\mathscr{A}$, and thus, enables us to consider optimization problems in $\mathscr{A}$.

A *C^*-module $\mathscr{M}$* over $\mathscr{A}$ is a linear space $\mathscr{M}$ equipped with a *right $\mathscr{A}$-multiplication*.

Definition 2.3 ((Right) multiplication) *Let $\mathscr{M}$ be an abelian group with operation $+$. For $c,d \in \mathscr{A}$ and $u,v \in \mathscr{M}$, if an operation $\cdot : \mathscr{M} \times \mathscr{A} \to \mathscr{M}$ satisfies*

1. $(u+v) \cdot c = u \cdot c + v \cdot c$,
2. $u \cdot (c+d) = u \cdot c + u \cdot d$,
3. $u \cdot (cd) = (u \cdot d) \cdot c$, *and*
4. $u \cdot 1_{\mathscr{A}} = u$,

*where $1_{\mathscr{A}}$ is the multiplicative identity of $\mathscr{A}$, then, $\cdot$ is called (right) $\mathscr{A}$-*multiplication*. The multiplication $u \cdot c$ is usually denoted as uc.*

Definition 2.4 (C^*-module) *Let $\mathscr{M}$ be an abelian group with operation $+$. If $\mathscr{M}$ has the structure of a (right) $\mathscr{A}$-multiplication, $\mathscr{M}$ is called a (right) C^*-*module *over $\mathscr{A}$.*

2.2 C^*-algebra-valued inner product and RKHM

We consider an $\mathscr{A}$-valued inner product in a C^*-module $\mathscr{M}$, which is a straightforward generalization of a complex-valued one.

Definition 2.5 ($\mathscr{A}$-valued inner product) *A map $\langle \cdot, \cdot \rangle : \mathscr{M} \times \mathscr{M} \to \mathscr{A}$ is called an $\mathscr{A}$-valued* inner product *if it satisfies the following properties for $u,v,w \in \mathscr{M}$ and $c,d \in \mathscr{A}$:*

1. $\langle u, vc + wd \rangle = \langle u, v \rangle c + \langle u, w \rangle d$,
2. $\langle v, u \rangle = \langle u, v \rangle^*$,
3. $\langle u, u \rangle \geq 0$, *and*
4. *If* $\langle u, u \rangle = 0$ *then* $u = 0$.

For $u \in \mathscr{M}$, we define the *$\mathscr{A}$-valued absolute value* $|u|$ on $\mathscr{M}$ by the positive element $|u|$ of $\mathscr{A}$ such that $|u|^2 = \langle u, u \rangle$. Since $|\cdot|$ takes values in more structured space $\mathscr{A}$, it behaves more complicatedly, but provides us with more information. The $\mathscr{A}$-valued absolute value $|\cdot|$ defines a norm $\|\cdot\|$ on $\mathscr{M}$ by $\|u\| := \big\||u|\big\|_{\mathscr{A}}$. We call $\mathscr{M}$ equipped with $\langle \cdot, \cdot \rangle$ a *Hilbert C^*-module* if $\mathscr{M}$ is complete with respect to the norm $\|\cdot\|$.

We now summarize the theory of RKHMs. Similar to the case of RKHSs, we begin with an $\mathscr{A}$-valued positive definite kernel on a non-empty set $\mathscr{Y}$.

Definition 2.6 ($\mathscr{A}$-valued positive definite kernel) *An $\mathscr{A}$-valued map $k : \mathscr{Y} \times \mathscr{Y} \to \mathscr{A}$ is called a* positive definite kernel *if it satisfies the following conditions:*

1. $k(x,y) = k(y,x)^*$ *for* $x,y \in \mathscr{Y}$,
2. $\sum_{t,s=1}^{n} c_t^* k(x_t, x_s) c_s \geq 0$ *for* $n \in \mathbb{N}$, $c_i \in \mathscr{A}$, $x_i \in \mathscr{Y}$.

Let $\phi : \mathcal{Y} \to \mathcal{A}^{\mathcal{Y}}$ be the *feature map* associated with k, which is defined as $\phi(x) = k(\cdot, x)$ for $x \in \mathcal{Y}$. Similar to the case of RKHSs, we construct C^*-module composed of $\mathcal{A}$-valued functions by means of ϕ as $\mathcal{M}_{k,0} := \left\{ \sum_{t=1}^n \phi(x_t)c_t \,\middle|\, n \in \mathbb{N},\ c_t \in \mathcal{A},\ x_t \in \mathcal{Y} \right\}$. An $\mathcal{A}$-valued map $\langle \cdot, \cdot \rangle_k : \mathcal{M}_{k,0} \times \mathcal{M}_{k,0} \to \mathcal{A}$ is defined as

$$\left\langle \sum_{s=1}^n \phi(x_s)c_s,\ \sum_{t=1}^l \phi(y_t)d_t \right\rangle_k := \sum_{s=1}^n \sum_{t=1}^l c_s^* k(x_s, y_t) d_t.$$

By Definition 2.6 of k, $\langle \cdot, \cdot \rangle_k$ is well-defined and has the reproducing property. Also, it satisfies the properties in Definition 2.5. Thus, $\langle \cdot, \cdot \rangle_k$ is an $\mathcal{A}$-valued inner product.

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

We denote by $\mathcal{M}_k$ the RKHM associated with k. We also denote by $|\cdot|_k$ and $\|\cdot\|_k$ the absolute value and norm on $\mathcal{M}_k$, respectively.

2.3 Orthonormality with C^*-algebra-valued inner products

Orthonormality plays an important role in data analysis because an orthonormal basis constructs orthogonal projections and an orthogonally projected vector minimizes the deviation from its original vector in the projected space. We refer to, for example, Definition 1.2 in [1].

Definition 2.7 (Normalized) *A vector $q \in \mathcal{M}$ is* normalized *if $0 \neq \langle q, q \rangle = \langle q, q \rangle^2$.*

Note that in the case of a general C^*-valued-inner product, for a normalized vector q , $\langle q, q \rangle$ is not always equal to the identity of $\mathcal{A}$ in contrast to the case of a complex-valued inner product.

Definition 2.8 (Orthonormal system and basis) *Let $\mathcal{T}$ be an index set. A set $\mathcal{S} = \{q_t\}_{t \in \mathcal{T}} \subseteq \mathcal{M}$ is called an* orthonormal system (ONS) *of $\mathcal{M}$ if q_t is normalized for any $t \in \mathcal{T}$ and $\langle q_s, q_t \rangle = 0$ for $s \neq t$. We call $\mathcal{S}$ an* orthonormal basis (ONB) *if $\mathcal{S}$ is an ONS and dense in $\mathcal{M}$.*

Unlike Hilbert spaces, Hilbert C^*-modules do not always have an ONB for general $\mathcal{A}$ [12, 13]. However, the following proposition shows the validity of considering ONBs in RKHMs over $\mathcal{B}(\mathcal{H})$.

Proposition 2.9 *Any Hilbert C^*-module over $\mathcal{B}(\mathcal{H})$ has an orthonormal basis.*

We now consider a practical approach for orthonormalization with matrix-valued inner products.

Proposition 2.10 (Normalization) *Let $\mathcal{A} = \mathbb{C}^{m \times m}$. Let $\varepsilon \geq 0$ and let $\hat{q} \in \mathcal{M}$ satisfy $\|\hat{q}\| > \varepsilon$. Then, there exists $\hat{b} \in \mathbb{C}^{m \times m}$ such that $\|\hat{b}\|_{\mathbb{C}^{m \times m}} < 1/\varepsilon$ and $q := \hat{q}\hat{b}$ is normalized. In addition, there exists $b \in \mathbb{C}^{m \times m}$ such that $\|\hat{q} - qb\| \leq \varepsilon$.*

Sketch of the proof : Let $\lambda_1 \geq \ldots \geq \lambda_m \geq 0$ be the eigenvelues of $\langle \hat{q}, \hat{q} \rangle$. Since $\langle \hat{q}, \hat{q} \rangle$ is positive, there exists an unitary matrix c such that $\langle \hat{q}, \hat{q} \rangle = c^* \operatorname{diag}\{\lambda_1, \ldots, \lambda_m\} c$. Let $m' := \max\{j \mid \lambda_j > \varepsilon^2\}$ and let $\hat{b} := c^* \operatorname{diag}\{1/\sqrt{\lambda_1}, \ldots, 1/\sqrt{\lambda_{m'}}, 0, \ldots, 0\} c$. The existance of m' follows by the inequality $\|\hat{q}\| > \varepsilon$. Then, it can be shown that $q := \hat{q}\hat{b}$ is normalized. In addition, let $b := c^* \operatorname{diag}\{\sqrt{\lambda_1}, \ldots, \sqrt{\lambda_{m'}}, 0, \ldots, 0\} c$. Then, it can be shown that $\|\hat{q} - qb\| \leq \varepsilon$ holds. □

Proposition 2.10 and its proof provide a concrete procedure to obtain normalized vectors in $\mathcal{M}$ in practical situations. This enables us to compute an ONB practically by applying Gram-Schmidt orthonormalization with respect to matrix-valued inner product.

Proposition 2.11 (Gram-Schmidt orthonormalization) *Let $\{w_t\}_{t=1}^{\infty}$ be a sequence in $\mathscr{M}$. Consider the following scheme for $t=1,2,\ldots$ and $\varepsilon \geq 0$:*

$$\hat{q}_t = w_t - \sum_{s=1}^{t-1} q_s \langle q_s, w_t \rangle, \quad q_t = \hat{q}_t \hat{b}_t \quad \text{if } \|\hat{q}_t\| > \varepsilon, \quad q_t = 0 \quad \text{o.w.}, \tag{1}$$

where $\hat{b}_t$ is defined as $\hat{b}$ in Proposition 2.10 by setting $\hat{q} = \hat{q}_t$. Then, $\{q_t\}_{t=1}^{\infty}$ is an ONS in $\mathscr{M}$ such that any w_t is contained in the ε-neighborhood of the space spanned by $\{q_t\}_{t=1}^{\infty}$.

Corollary 2.12 *If $\varepsilon = 0$, and the space spanned by $\{w_t\}_{t=1}^{\infty}$ is dense in $\mathscr{M}$, then $\{q_t\}_{t=1}^{\infty}$ is an ONB of $\mathscr{M}$.*

In practical computations, scheme (1) should be represented with matrices. For this purpose, we derive the following about QR decomposition from Proposition 2.11.

Corollary 2.13 (QR decomposition) *For $n \in \mathbb{N}$, let $W := [w_1, \ldots, w_n]$ and $Q := [q_1, \ldots, q_n]$. Let $\varepsilon \geq 0$. Then, there exist $\mathbf{R}, \mathbf{R}_{\mathrm{inv}} \in \mathbb{C}^{mn \times mn}$ that satisfies*

$$Q = W\mathbf{R}_{\mathrm{inv}}, \quad \|W - Q\mathbf{R}\| \leq \varepsilon. \tag{2}$$

Decompositions (2) are called QR decompositions. By applying QR decomposition, we only have to compute $\mathbf{R}_{\mathrm{inv}}$ and $\mathbf{R}$ although we are treating vectors in an infinite dimensional space $\mathscr{M}$.

The following proposition shows the orthogonally projected vector onto a subspace $\mathscr{V}$ of $\mathscr{M}$ uniquely minimizes the deviation from an original vector in $\mathscr{V}$. Thus, with an orthonormalization approach proposed above, we can generalize methods related to orthogonal projections in RKHSs to RKHMs.

Proposition 2.14 *Let $\mathscr{A} = \mathscr{B}(\mathscr{H})$, $\{q_t\}_{t\in\mathscr{T}}$ be an ONS of $\mathscr{M}$, and $\mathscr{V}$ be the completion of the space spanned by $\{q_t\}_{t\in\mathscr{T}}$. For $w \in \mathscr{M}_k$, let $P : \mathscr{M} \to \mathscr{V}$ be the projection operator defined as $Pw := \sum_{t\in\mathscr{T}} q_t \langle q_t, w\rangle$. Then Pw is the unique solution of the following minimization problem:*

$$\min_{v\in\mathscr{V}} |w - v|^2.$$

3 Perron-Frobenius operators in RKHMs

We define Perron-Frobenius operators in RKHMs. First, let $\mathscr{X}$ be a topological space, $\mathscr{Y} := \{x_0, x_1, \ldots\} \subseteq \mathscr{X}^m$ be observed data, where $x_t = [x_{t,1}, \ldots, x_{t,m}]$, and $f_i : \mathscr{X}^m \to \mathscr{X}$ be a (possibly, nonlinear) map. And, consider the following interacting dynamical system:

$$x_{t+1,i} = f_i(x_{t,1}, \ldots, x_{t,m}) \quad (i = 1, \ldots, m).$$

Let $\mathscr{M}_{k,0}(\mathscr{Y}) := \{\sum_{t=0}^{n} \phi(x_t)c_t \mid n \in \mathbb{N},\ x_t \in \mathscr{Y},\ c_t \in \mathbb{C}^{m\times m}\}$. In an RKHM $\mathscr{M}_k$, we define the Perron-Frobenius operator $K : \mathscr{M}_{k,0}(\mathscr{Y}) \to \mathscr{M}_k$ that describs the time evolution of the system as follows:

$$K\phi(x) := \phi([f_1(x), \ldots, f_m(x)]) \quad x \in \mathscr{Y}.$$

We now estimate K with finite observables $x_0, \ldots, x_T$ through the following minimization problem:

$$\min_{\hat{K}\in\mathscr{L}(\mathscr{W}_T)} \sum_{t=0}^{T-1} \left|\hat{K}\phi(x_t) - \phi(x_{t+1})\right|_k^2, \tag{3}$$

whose solution $\hat{K}$ well approximates K. Here, $\mathscr{W}_T$ is the space spanned by $\{\phi(x_t)\}_{t=0}^{T-1}$ and $\mathscr{L}(\mathscr{W}_T)$ is the space of all $\mathbb{C}^{m\times m}$-linear maps L (i.e., $L(uc) = (Lu)c$ for $u \in \mathscr{M}_k$ and $c \in \mathbb{C}^{m\times m}$) on $\mathscr{W}_T$. Existence of a solution of problem (3) follows from Proposition 2.14. Thus, we apply the Gram-Schmidt orthonormalization to obtain Q_T and $\mathbf{R}_{\mathrm{inv},T}$ such that $Q_T = [\phi(x_0), \ldots, \phi(x_{T-1})]\mathbf{R}_{\mathrm{inv},T}$ (see Corollary 2.13). Then, the solution of problem (3) is explicitly represented as follows:

Theorem 3.1 *If $\varepsilon = 0$ and $\{\phi(x_t)\}_{t=0}^{T-1}$ is linearly independent, $Q_T Q_T^* K Q_T Q_T^*$ is the unique solution of problem (3). Also, $Q_T^* K Q_T = Q_T^*[\phi(x_1), \ldots, \phi(x_T)]\mathbf{R}_{\mathrm{inv},T}$ holds.*

Remark 3.2 *Let $\mathbf{K}_T = Q_T^* K Q_T$. Then, $\mathbf{K}_T$ is regarded as a matrix representation of $Q_T Q_T^* K Q_T Q_T^*$ with respect to the ONB $\{q_t\}_{t=0}^{T-1}$. Since $\mathbf{K}_T = Q_T^*[\phi(x_1), \ldots, \phi(x_T)]\mathbf{R}_{\mathrm{inv},T}$ holds, $\mathbf{K}_T$ can be computed only with finite observables.*

4 Application to modal decomposition

We introduce a notion of $\mathbb{C}^{m\times m}$-valued eigenpairs of the estimated operator $\mathbf{K}_T$ and give a method for extracting relations invariant with respect to time. This method is applicable to, for example, causal estimation of time-series data. A $\mathbb{C}^{m\times m}$-valued eigenpair of $\mathbf{K}_T$ is a pair (a,v) that satisfies $\mathbf{K}_T v = va$. In practical situations, it is easy to find them as follows: Let $\lambda_1,\ldots,\lambda_{mT} \in \mathbb{C}$ be the eigenvalues of $\mathbf{K}_T$ and $\mathrm{v}_1,\ldots,\mathrm{v}_{mT} \in \mathbb{C}^{mT}$ be the eigenvectors of $\mathbf{K}_T$ with respect to $\lambda_1,\ldots,\lambda_{mT}$. We set $\mathbf{v}_t := [\mathrm{v}_t,0,\ldots,0] \in (\mathbb{C}^{m\times m})^T$ and $a_t := \mathrm{diag}\{\lambda_t,0,\ldots,0\} \in \mathbb{C}^{m\times m}$. Then, we can see, for $t=1,\ldots,mT$, the pair $(a_t,\mathbf{v}_t)$ is a $\mathbb{C}^{m\times m}$-valued eigenpair. Since the relation $\phi(x_s) = K^s\phi(x_0)$ holds for time s, we approximate $\phi(x_s)$ as $Q_T\mathbf{K}_T^s Q_T^*\phi(x_0)$, and apply the above eigenpairs for extracting time-invariant relations.

Proposition 4.1 *Assume* $[\mathrm{v}_1,\ldots,\mathrm{v}_{mT}] \in \mathbb{C}^{mT\times mT}$ *is invertible. Let* $c_t \in \mathbb{C}^{m\times m}$ *satisfy* $Q_T^*\phi(x_0) = \sum_{t=1}^{mT}\mathbf{v}_t c_t$ *and* $\mathscr{T} := \{t \mid |\lambda_t| = 1\}$. *Then,* $|Q_T\mathbf{K}_T^s Q_T^*\phi(x_0)|_k^2$ *is decomposed into* $\sum_{t,l=1}^{mT} c_t^*(a_t^*)^s\langle\mathbf{v}_t,\mathbf{v}_l\rangle a_l^s c_l$. *And, the following value is invariant with respect to s:*

$$c_{\mathrm{inv}} := \sum_{t\in\mathscr{T}} c_t^*(a_t^*)^s\langle\mathbf{v}_t,\mathbf{v}_t\rangle a_t^s c_t,$$

For example, we consider the following matrix-valued positive definite kernel: Let $\tilde{k} : \mathscr{X}\times\mathscr{X}\to\mathbb{C}$ be a complex-valued positive definite kernel and $\mathscr{H}_{\tilde{k}}$ be the RKHS associated with $\tilde{k}$.

Lemma 4.2 *Let* $k : \mathscr{X}^m\times\mathscr{X}^m \to \mathbb{C}^{m\times m}$ *be a matrix valued map where the* (i,j)*-elements of* $k(x_1,x_2)$ *are defined as* $\tilde{k}(x_{1,i},x_{2,j})$ *for* $x_t = [x_{t,1},\ldots,x_{t,m}] \in \mathscr{X}^m$ *for* $t=1,2$. *Then, k is a* $\mathbb{C}^{m\times m}$*-valued positive definite kernel.*

The (i,j)-element of $k(x_1,x_2) = \langle\phi(x_1),\phi(x_2)\rangle_k$ for $x_1,x_2 \in \mathscr{X}^m$ equals $\tilde{k}(x_{1,i},x_{2,j})$, which represents the similarities between $x_{1,i}$ and $x_{2,j}$ in $\mathscr{H}_{\tilde{k}}$. Thus, the inner product between $\phi(x_1)$ and $\phi(x_2)$ describes the similarities of all combinations of pairs of elements of x_1 and x_2. If the (i,j) element of c_{inv} is large, the i-th and j-th elements of x_s are similar for any s. This is because the (i,j) element of $|\phi(x_s)|_k^2 = k(x_s,x_s)$ represents the similarity between the i-th and j-th elements of x_s. As a result, we can extract the similarities that are invariant with respect to time.

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