Reproducing kernel Hilbert C^*-module for data analysis[*1] [*2]

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$*1$ JMLR, 22(267):1–56 (updated version : arXiv:2101.11410v2)

$*2$ Joint work with Isao Ishikawa, Masahiro Ikeda, Fuyuta Komura, Takeshi Katsura, and Yoshinobu Kawahara

Introduction

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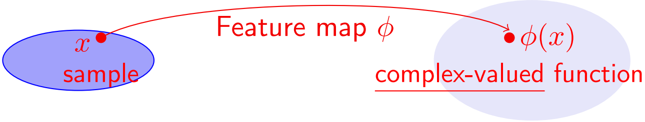
- 2018 Received Master's degree from Keio University
- 2018- NTT Network Service Systems Laboratories
- 2022 Received Ph.D. from Keio University

Backgrounds / Interests

- Operator theoretic data analysis
- Kernel methods
- Numerical linear algebra

Contents

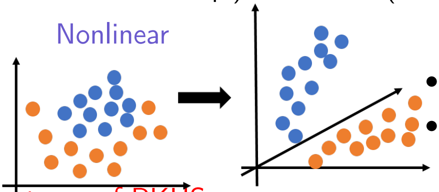
Kernel methods



$\mathcal{X}$
(Finite dimensional sp.)

RKHS[1]
(Infinite dimensional Hilbert sp.)

Nonlinear



Linear

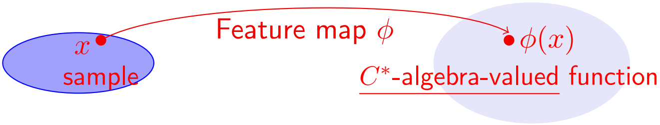
- Kernel PCA, Kernel SVM
- Learning complex-valued functions

Advantages of RKHS

- Nonlinearity in the original space is transformed into a linear one.
- We can compute inner products in RKHS exactly by computers.

[1] Schölkopf and Smola, MIT Press, Cambridge, 2001

Goal: Generalization of data analysis in RKHS to RKHM



$\mathcal{X}$
(Structured data sp.)

Nonlinear

RKHM
(Infinite dimensional Hilbert C^*-module)

Linear + C^*-algebra-valued inner product

Data analysis in RKHM

Advantages of RKHM:

- C^*-algebra-valued inner products extract information of structures.

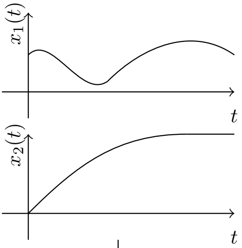
We constructed a framework of data analysis with RKHM.

- We can reconstruct existing RKHSs by using RKHMs.
- We have shown fundamental properties for data analysis in RKHMs, similar to RKHSs (e.g. orthogonal projection, representer theorem).

Advantages of RKHM

Algorithms in RKHS

x_1,x_2 : Functional data
$x_1, x_2 \in \mathcal{H}$

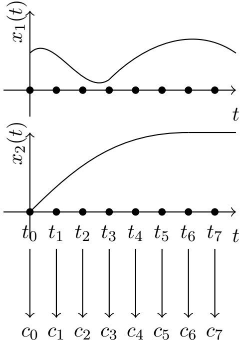


Compute the inner product

$\langle x_1, x_2 \rangle_{\mathcal{H}} \in \mathbb{C}$

Degenerates information along t

$x_1(t), x_2(t) \in \mathcal{X}$

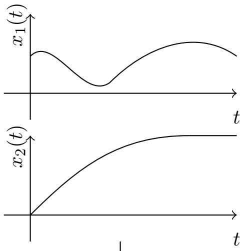


$c_i = \langle x_1(t_i), x_2(t_i) \rangle_{\mathcal{X}} \in \mathbb{C}$

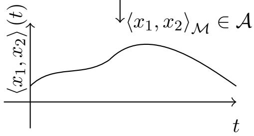
Fails to capture continuous behavior (derivatives, total variation, frequency components,...)

Algorithms in RKHM

$x_1, x_2 \in \mathcal{M}$



$\langle x_1, x_2 \rangle_{\mathcal{M}} \in \mathcal{A}$



Capture and control continuous behavior

Review: Reproducing kernel Hilbert space (RKHS)

Let $\mathcal{X}$ be a set. A map $k : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ is called a positive definite kernel if it satisfies:

1. $k(x, y) = \overline{k(y, x)}$ for $x, y \in \mathcal{X}$ and
2. $\sum_{t,s=1}^{n} \overline{c_t} k(x_t, x_s) c_s \geq 0$ for $n \in \mathbb{N}$, $c_1, \ldots, c_n \in \mathbb{C}$, $x_1, \ldots, x_n \in \mathcal{X}$.

$\phi(x) := k(\cdot, x)$ ($\phi : \mathcal{X} \to \mathbb{C}^{\mathcal{X}}$: feature map associated with k),

$$\mathcal{H}_{k,0} := \left\{ \sum_{t=1}^{n} \phi(x_t) c_t \,\middle|\, n \in \mathbb{N},\ c_t \in \mathbb{C},\ x_t \in \mathcal{X} \right\}. \tag{1}$$

We can define an inner product $\langle \cdot, \cdot \rangle_k : \mathcal{H}_{k,0} \times \mathcal{H}_{k,0} \to \mathbb{C}$ as

$$\left\langle \sum_{s=1}^{n} \phi(x_s) c_s, \sum_{t=1}^{l} \phi(y_t) d_t \right\rangle_k := \sum_{s=1}^{n} \sum_{t=1}^{l} c_s^* k(x_s, y_t) d_t. \tag{2}$$

RKHS $\mathcal{H}_k$: completion of $\mathcal{H}_{k,0}$

Review: Hilbert C^*-module

$\mathcal{A}$: C^*-algebra, e.g., $\mathcal{A} = \mathcal{B}(\mathcal{W})$, $L^\infty([0,1])$
(Banach space equipped with a product structure and an involution * + α)
$\mathcal{M}$: right $\mathcal{A}$-module ($u \in \mathcal{M}$, $c \in \mathcal{A} \to uc \in \mathcal{M}$)

Definition 1 $\mathcal{A}$-valued inner product

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

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 if $\langle u, u \rangle = 0$ then $u = 0$.

$\to$ *$\mathcal{A}$-valued absolute value* $|u| := \langle u, u \rangle^{1/2}$ $\quad\to$ Norm $\|u\| := \| \langle u, u \rangle \|_{\mathcal{A}}^{1/2}$

Hilbert C^*-module $\mathcal{M}$[2]: complete $\mathcal{A}$-module equipped with an $\mathcal{A}$-valued inner-product

[2]Lance, Cambridge University Press, 1995.

Short review of reproducing kernel Hilbert C^*-module

$\mathcal{A}$: C^*-algebra

We can generalize complex-valued notions to operator ($\mathcal{B}(\mathcal{W})$) and function ($L^\infty([0,1])$)-valued ones. (e.g. eigenvalues, principal components)

RKHS ($\mathcal{H}_k$):

- $\mathbb{C}$-valued positive definite kernel k
- $\mathbb{C}$-valued functions
- $\mathbb{C}$-valued inner product

RKHM over $\mathcal{A}$ ($\mathcal{M}_k$):

- $\mathcal{A}$-valued positive definite kernel k
- $\mathcal{A}$-valued functions
- $\mathcal{A}$-valued inner product

Orthonormality in Hilbert C^*-modules

To project a vector onto a finitely generated submodule, we introduce orthonormality[3]

Definition 2 Orthonormal

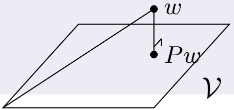
Let $\mathcal{M}$ be a Hilbert C^*-module.

1. A vector $q \in \mathcal{M}$ is said to be normalized if $0 \neq \langle q, q \rangle = \langle q, q \rangle^2$.
2. Two vectors $p, q \in \mathcal{M}$ are said to be orthogonal if $\langle p, q \rangle = 0$.

Theorem 1 Minimization property

Let $\mathcal{A}$ be a unital C^*-algebra and let $\mathcal{T}$ be a finite index set. Let $\mathcal{V}$ be the module spanned by an orthonormal system $\{q_t\}_{t \in \mathcal{T}}$ and let $P : \mathcal{M} \to \mathcal{V}$ be the projection operator. For $w \in \mathcal{M}$,

$$Pw = \underset{v \in \mathcal{V}}{\arg\min} \, |w - v|^2 \qquad (3)$$



[3] Bakić and Guljăs, Journal of Operator Theory, 2001.

Representer theorem in RKHMs

To generalize complex-valued supervised problems to $\mathcal{A}$-valued ones, we show a representer theorem.

$\mathcal{M}_k$: RKHM over $\mathcal{A}$

Theorem 2 Representer theorem in RKHMs

Let $\mathcal{A}$ be a unital C^*-algebra, $x_1, \ldots, x_n \in \mathcal{X}$ and $a_1, \ldots, a_n \in \mathcal{A}$. Let $h : \mathcal{X} \times \mathcal{A}^2 \to \mathcal{A}_+$ be an error function and $g : \mathcal{A}_+ \to \mathcal{A}_+$ satisfy $g(c) < g(d)$ for $c < d$. If $\mathrm{Span}_{\mathcal{A}}\{\phi(x_i)\}_{i=1}^n$ is closed, any $u \in \mathcal{M}_k$ minimizing $\sum_{i=1}^n h(x_i, a_i, u(x_i)) + g(|u|_k)$ admits a representation of the form $\sum_{i=1}^n \phi(x_i) c_i$ for some $c_1, \ldots, c_n \in \mathcal{A}$.

Key point of the proofs:
For a Hilbert C^*-module $\mathcal{M}$ over a unital C^*-algebra $\mathcal{A}$ and any finitely generated closed submodule $\mathcal{V}$ of $\mathcal{M}$, $u \in \mathcal{M}$ is decomposed into $u = u_1 + u_2$ where $u_1 \in \mathcal{V}$ and $u_2 \in \mathcal{V}^\perp$.

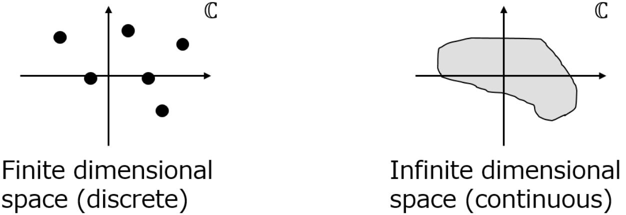
Conclusion

- RKHM is a natural generalization of RKHS.
- RKHM enables us to extract continuous behaviors of functional data.
- We showed fundamental properties of RKHM for data analysis.

Ongoing work related to Hilbert C^*-modules and dynamical systems*

$*$ Joint work with Isao Ishikawa, Masahiro Ikeda, Suddhasattwa Das, Joanna Slawinska, and Dimitrios Giannakis

- Koopman operators (composition operators with respect to dynamical systems) are defined on infinite-dimensional Hilbert spaces.
- Koopman operators have continuous spectra.
- Continuous spectrum is not described by operators in finite dimensional spaces.



Goal and approach

Goal:
Generalize the discrete decomposition in finite-dimensional spaces to that in infinite-dimensional space.

Approach:

1. Extend the Koopman operator on a Hilbert space to a Hilbert C^*-module.
2. Construct vectors in a Hilbert C^*-module using cocycles.
3. Decompose the operator on the Hilbert C^*-module using the above vectors.