Continuity of Koopman operators on reproducing kernel Hilbert spaces with analytic positive definite function

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Mathematical foundations of Machine Learning

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Brief Self-Introduction

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Major: Partial Differential Equations (Functional Analysis, Real Analysis)

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Aim of this presentation

To introduce

Boundedness of composition (Koopman) operators on reproducing kernel Hilbert spaces with analytic positive definite functions, J. Math. Anal. Appl. (2022).

This is a joint work with

- Isao Ishikawa (Ehime Univ.) → Number theory, Machine learning
- Yoshihiro Sawano (Chuo Univ.) → Theory of function spaces

Motivation(roughly)

Want to give a theoretical guarantee to a method of data analysis

- Operator Theoretic Approach ⟷ Koopman operator
- Kernel Method ⟷ Reproducing kernel

Koopman (composition) operator

- E, E' : (non-empty)sets • $f : E \to E'$: map
- V (resp. W) : function space on E (resp. E')
- $C_f : V \to W$: Koopman operator $C_f(h) := h \circ f$

- Advantage of the usage of KO

||

Even if f is **nonlinear**, C_f is **linear** → **Techniques** of **functional analysis**

$$C_f(a_1 h_1 + a_2 h_2) = a_1 C_f(h_1) + a_2 C_f(h_2)$$

- Typical example = (Nonlinear) dynamical system

$$x_{t+1} = f(x_t),\ t \in \{0,1,\cdots,\}$$

→ h lifting

$$h(x_t) = h(f(x_{t-1})) = C_f(h)(x_{t-1})$$

$$= C_f C_f(h(x_{t-2})) = \cdots = C_f^t(h(x_0))$$

Time behavior of x_t

Continuity (Boundedness)

Problem Is the Koopman operator C_f

well-defined ? | continuous ? | compact ? | decomposable ?

↕ Most fundamental

↕ Today's main object

↕ Information of spectrum

↕ Time behavior of C_f^t

Assume V (resp.W) is endowed with a norm $\|\cdot\|_V$ (resp.$\|\cdot\|_W$).

An operator $C : V \to W$ is **continuous (bounded)**

$$\overset{\text{def}}{\iff} \quad \exists A > 0 \text{ s.t. } \|C(h)\|_X \leq A\|h\|_Y, \ \forall h \in Y.$$

Continuity

is often assumed to verify a convergence of the finite-dimensional approximation of C_f to itself.

Reproducing kernel Hilbert space (RKHS)

Definition

$\mathscr{M}$: set

$k : \mathscr{M} \times \mathscr{M} \to \mathbb{C}$: **positive definite kernel** on $\mathscr{M}$ **iff**

for any $n > 0$ and $x_1, \ldots, x_n \in \mathscr{M}$, the matrix

$$\left(k(x_i, x_j)\right)_{i,j=1,\ldots,n}$$

is a **positive semi-definite Hermitian matrix**

Theorem(Moore-Aronszajn)

k: positive definite kernel on $\mathscr{M}$, $k_a : \mathscr{M} \to \mathbb{C}; x \mapsto k(x, a)$

$\exists! H_k$: Hilbert space (**RKHS**) $\subset \mathbb{C}^{\mathscr{M}}$ *s.t.*

(i) $\forall a \in \mathscr{M}, \quad k_a \in H_k$

(ii) $\forall a \in \mathscr{M}, \forall h \in H_k, \quad \langle k_a, h \rangle_{H_k} = h(a)$

Positive definite functions

Definition

$u\colon \mathbb{R}^d \to \mathbb{C}$: **positive definite function iff**

$k(x, y) := u(x - y)$: positive definite kernel

Theorem(Bochner)

u: continuous positive definite function **iff**

$\exists \mu$: finite Borel measure on $\mathbb{R}^d$ *s.t.* $u(x) = \widehat{\mu}(x) := \int_{\mathbb{R}^d} e^{2\pi x^\top \xi} \, d\mu(\xi)$

Example

(i) $u(x) = e^{-|x|^2}$

(ii) $u(x) = \dfrac{\sin(x)}{x}$

Examples of RKHS

$\{z \in \mathbb{C} : |z| < 1\}$

(i) (Hardy space) $\mathscr{M} = \mathbb{D}$, $k(z, w) := (1 - z\overline{w})^{-1}$

$$H_k = \left\{ h\text{: regular on } \mathbb{D} : \sup_{0<r<1} \int_{|z|=r} |h(z)|^2 \, dz < \infty \right\}$$

(ii) (Fock space) $\mathscr{M} = \mathbb{C}^d$, $k(z, w) := e^{\overline{z}^\top w}$

$$H_k = \left\{ h\text{: regular on } \mathbb{C}^d : \int_{\mathbb{R}^d \times \mathbb{R}^d} |h(x + iy)|^2 \, e^{-|x|^2 - |y|^2} dxdy < \infty \right\}$$

(iii) $\mathscr{M} = \mathbb{R}^d$, $k(x, y) := u(x - y)$ ($u \in C^0 \cap L^2$ and $\hat{u} \in L^1$)

$$H_k = \left\{ h \in C^0 \cap L^2 \; : \; \int_{\mathbb{R}^d} |\,\hat{h}(\xi)|^2 \, \hat{u}(\xi)^{-1} \, d\xi < \infty \right\}$$

Continuity of Koopman operator

Which $f : \mathscr{X} \to \mathscr{Y}$ induces a continuous Koopman operator C_f ?

Theorem(Littlewood's subordinate theorem)

$\mathscr{X} = \mathscr{Y} = \mathbb{D}$, $k(z, w) := (1 - z\overline{w})^{-1}$,

$C_f : H_k \to H_k$: continuous **iff** f : holomorphic

Theorem(Carswell-MacCluer-Schuster)

$\mathscr{X} = \mathscr{Y} = \mathbb{C}^d$, $k(z, w) := e^{\overline{z}^\top w}$,

$C_f : H_k \to H_k$: continuous **iff** $f(z) = Az + b$,

where, $A \in \mathrm{M}_d(\mathbb{C})$, $b \in \mathbb{C}^d$ *s.t.*

$$\|A\| \leq 1$$

$\overline{b}^\top \zeta = 0$ for $\forall \zeta$ satisfying $|A\zeta| = |\zeta|$

Main result

How about $k(x, y) := u(x-y)$ ($u \in C^0 \cap L^2$ and $\hat{u} \in L^1$) case?

Main result(rough)

We determine which $f : U \to \mathbb{R}^d$ induces a continuous Koopman operator $C_f : H_k \to H_{k|_{U^2}}$ for a wide class of positive definite functions u, where $U \subset \mathbb{R}^d$ is an open subset and $k(x, y) = u(x-y)$

Notation

$$L^2(\hat{u}) := \left\{ h\text{: mesurable on } \mathbb{R}^d : \int_{\mathbb{R}^d} |h(\xi)|^2 \hat{u}(\xi)\, d\xi < \infty \right\}$$

$$m_z : L^2(\hat{u}) \to L^2(\hat{u}); h(\xi) \mapsto e^{z^\top \xi} h(\xi) \quad \left(z \in \mathbb{C}^d \right)$$

$$P_n := \left\{ p \in \mathbb{C}[\xi_1, \ldots, \xi_d] : \text{total degree of } p \leq n \right\}$$

$$\mathcal{G}(u) := \left\{ A \in \mathrm{GL}_d(\mathbb{R}) : \lambda_A \hat{u}(A^\top \xi) \geq \hat{u}(\xi) \text{ for some } \lambda_A > 0 \right\}$$

Main result

Main theorem(Ikeda-Ishikawa-Sawano)

$u \in C^0 \cap L^2$: positive definite function

Suppose

(I) $\forall a > 0, \ \exists C > 0$ *s.t.* $|\hat{u}(\xi)| < Ce^{-a|\xi|}$

(II) $\sup_{z \in \mathbb{C}} \left(\limsup_{n \to \infty} \| m_z|_{P_n} \|^{1/n} \right) < \infty$

We regard $P_n \subset L^2(\hat{u})$

(III) $\pm Q \in \mathcal{G}(u)$ for some $Q \in \mathrm{GL}_d(\mathbb{R})$

(IV) $\langle \mathcal{G}(u) \rangle_{\mathbb{R}} = \mathrm{M}_d(\mathbb{R})$

For $U \subset \mathbb{R}^d$: open and $f : U \to \mathbb{R}^d$: any map,

$$C_f : H_k \to H_{k|_{U^2}} : \text{ continuous } \textbf{iff } f(x) = Ax + b,$$

where, $A \in \mathcal{G}(u)$, $b \in \mathbb{R}^d$

Main result

Remark

- The condition (I) is almost the same as entireness of u (Paley-Winer theorem)
- The condition (II) always holds if $\mathrm{supp}(\hat{u})$ is compact or $u(x) = e^{-|x|^2}$
- The condition (III) always holds if u is $\mathbb{R}$-valued (take $Q = 1$)
- The condition (IV) always holds if $d = 1$, $\mathrm{supp}(\hat{u})$ is compact containing open ball at 0, or $u(x) = e^{-|x|^2}$
- Characterization of f via properties of C_f considerably depends on the choice of k
- We also prove C_f **cannot** be compact
- The same results are proved by Chacon-Chacon-Gimenez(2007) in the case $d = 1$ and $u(x) = \sin(x)/x$ in terms of other method

2. Sketch of the proof

Rough strategy

We only consider $U = \mathbb{R}^d$ case here

A) "if" part is easy

B) "Only if" part is hard

1. Affine-ness for special f:

   prove if $\exists \tilde{f} : \mathbb{C}^d \to \mathbb{C}^d$: holomorphic *s.t.* $\tilde{f}|_{\mathbb{R}^d} = f$,

   then Main theorem holds

2. Analytic continuation of general f:

   prove $\exists \tilde{f} : \mathbb{C}^d \to \mathbb{C}^d$: holomorphic *s.t.* $\tilde{f}|_{\mathbb{R}^d} = f$

Proof of "if" part

Let $f(x) = Ax + b$ $\left(A \in \mathcal{G}(u),\ b \in \mathbb{R}^d \right)$

For $h \in H_k$, we have

$$\| C_f h \|_{H_k}^2 = \int_{\mathbb{R}^d} | \widehat{C_f h}(\xi) |^2 \, \hat{u}(\xi)^{-1} \, d\xi$$

$$= | A |^{-1} \int_{\mathbb{R}^d} | \hat{h}(\xi) |^2 \, \hat{u}(A^\top \xi)^{-1} \, d\xi$$

$$\leq \lambda_A | A |^{-1} \cdot \| h \|_{H_k}^2$$

□

Affine-ness: Statement

Theorem A(Ikeda-I.-Sawano)

$u \in C^0 \cap L^2$: positive definite function

Suppose

(I) $\forall a > 0, \ \exists C > 0$ *s.t.* $|\hat{u}(\xi)| < Ce^{-a|\xi|}$

(II) $\sup_{z \in \mathbb{C}} \left(\limsup_{n \geq 0} \| m_z|_{P_n} \|^{1/n} \right) < \infty$

(III) $\langle \mathcal{G}(u) \rangle_{\mathbb{R}} = \mathrm{M}_d(\mathbb{R})$

For $f : \mathbb{R}^d \to \mathbb{R}^d$ *s.t.* $\exists \tilde{f} : \mathbb{C}^d \to \mathbb{C}^d$: holomorphic with $\tilde{f}|_{\mathbb{R}^d} = f$,

if $C_f : H_k \to H_k$: bounded, then $f(x) = Ax + b$,

where, $A \in \mathcal{G}(u)$, $b \in \mathbb{R}^d$

Affine-ness: Sketch of the proof

Notation

$\phi : \mathbb{C}^d \to L^2(\hat{u});\ z \mapsto e^{2\pi i z^\top \xi}$

$S : L^2(\hat{u}) \to H_k;\ h \mapsto \left(h\hat{u}\right)^\vee$ Note: S is an isomorphism

$K_f := S^{-1}C_f^* S : L^2(\hat{u}) \to L^2(\hat{u})$ Note: $K_f\phi(z) = \phi(\tilde{f}(z))$ $(z \in \mathbb{C}^d)$

Lemma

Assume (I) in Theorem A. For $n > 0$ and $z \in \mathbb{C}$,

$$K_f\left(m_z(P_n)\right) \subset m_{\tilde{f}(z)}(P_n)$$

Moreover, for homogeneous polynomial $q(\xi_1, \ldots, \xi_d)$, we have

$$K_f m_z q(\xi_1, \ldots, \xi_d) = m_{\tilde{f}(z)} q\left(J_{\tilde{f}}(z) \cdot (\xi_i)_i\right) + \text{(poly. of degree} < \deg(q))$$

where $J_{\tilde{f}}(z)$ is the Jacobian of $\tilde{f}$ at z

By considering K_f's action on polynomials, we can extract information of of $J_{\tilde{f}}$

Affine-ness: Sketch of the proof

Corollary

Assume (I) in Theorem A. We have the commutative diagram

$$P_n/P_{n-1} \xrightarrow{\overline{m}_z} m_z P_n / m_z P_{n-1} \xrightarrow{\overline{K}_f} m_{\tilde{f}(z)} P_n / m_{\tilde{f}(z)} P_{n-1} \xrightarrow{\overline{m}_{-\tilde{f}(z)}} P_n/P_{n-1}$$

$$\begin{array}{ccc} \wr\| & & \wr\| \\ \mathbb{C}[\xi_1, \dots, \xi_d]_n & \xrightarrow{\mathcal{S}^n J_{\tilde{f}}(z)} & \mathbb{C}[\xi_1, \dots, \xi_d]_n \end{array}$$

$\mathbb{C}[\xi_1, \dots, \xi_d]_n$: space of homogeneous polynomials of degree n

$\mathcal{S}^n J_f(z)$: natural linear map determined by $\xi_i \mapsto \sum_{r=1}^{d} \frac{\partial \tilde{f}_r}{\partial x_i}(z) \xi_r$

Proposition

Assume (I) and (II) in Theorem A. If C_f is bounded, $z \mapsto \mathrm{tr} J_{\tilde{f}}(z)$ is constant.

For any $A \in \mathcal{G}(u)$, $C_{A \circ f}$ is also bounded, thus $\mathrm{tr} J_{A \circ \tilde{f}}(z) = \mathrm{tr} A J_{\tilde{f}}(z)$ is also constant.
Therefore, (III) deduces $J_{\tilde{f}}(z)$ is constant

Analytic continuation: Statement

Theorem B(Ikeda-I.-Sawano)

$u \in C^0 \cap L^2$: positive definite function

Suppose

(I) $\forall a > 0, \ \exists C > 0$ s.t. $|\hat{u}(\xi)| < Ce^{-a|\xi|}$

(II) $\pm Q \in \mathcal{G}(u)$ for some $Q \in \mathrm{GL}_d(\mathbb{R})$

For $f : \mathbb{R}^d \to \mathbb{R}^d$: any map,

if $C_f : H_k \to H_k$: bounded, then $\exists \tilde{f} : \mathbb{C}^d \to \mathbb{C}^d$: holomorphic with $\tilde{f}|_{\mathbb{R}^d} = f$

Analytic continuation: Idea of the proof

$K_f\phi(z)$ must be $\phi(\tilde{f}(z))$ for some holomorphic $\tilde{f} : \mathbb{C}^d \to \mathbb{C}^d$

Lemma

Under (I) in Theorem B, we have

(i) ϕ is an injective $L^2(\hat{u})$-valued holomorphic map

(ii) $\phi^{-1} : \phi(\mathbb{C}^d) \to \mathbb{C}^d$ is continuous

Steps of the proof

Step 1. show f is continuous ($\because f = \phi^{-1} K_f \phi$)

Step 2. show f is analytic on $\mathbb{R}^d$

Step 3. Construct $\tilde{f}$ in terms of $K_{Q \circ f}\phi(z)$ and $K_{-Q \circ f}\phi(z)$

3. Conclusion & Future works

Conclusion & Future works

Conclusion

- Continuity of Koopman operators strongly confines the shape of the maps
- We prove $f : U \to \mathbb{R}^d$ is an affine map if $C_f : H_k \to H_{k|_{U^2}}$ is continuous by means of the polynomial structures in $L^2(\hat{u})$, and complex analysis, where $U \subset \mathbb{R}^d$ is open, and $k(x, y) = u(x - y)$ for suitable positive definite function u

Future works

$$\sup_{z\in\mathbb{C}} \left(\limsup_{n\geq 0} \| m_z|_{P_n} \|^{1/n} \right) < \infty$$

- Remove the condition (II) in Main theorem

$\forall a > 0,\ \exists C > 0$ s.t. $|\hat{u}(\xi)| < Ce^{-a|\xi|}$

- Weaken the condition (I) in Main theorem (consider $\hat{u}$ decaying more slowly)
- generalize $\mathbb{R}^d$ to general locally compact abelian groups or Lie groups