Krylov subspace methods for Perron-Frobenius operators in RKHS

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Abstract

- We consider numerical estimations of Perron-Frobenius (P-F) operators in RKHS.
- A P-F operator is a linear operator which describes the time evolution of a dynamical system.
- Recently, using P-F operators for time-series data analysis have been actively researched.
- We investigate theoretical analyses of Krylov subspace methods for estimating P-F operators.

Contents

Dynamical systems with random noise

$(\Omega, \mathcal{F})$: A measurable space,
$(\mathcal{X}, \mathcal{B})$: A Borel measurable and locally compact Hausdorff vector space,
X_t, ξ_t : random variables from Ω to $\mathcal{X}$,
$\{\xi_t\}$: An i.i.d. stochastic process corresponds to the random noise in $\mathcal{X}$ (ξ_t is also independent of X_t),
$h: \mathcal{X} \to \mathcal{X}$ (nonlinear in general)

Dynamical system with random noise

$$X_{t+1} = h(X_t) + \xi_t, \quad (1)$$

P : A probability measure on Ω, X_t

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P : A probability measure on Ω, $\quad X_t \xrightarrow{\text{Transform}} X_{t*}P$,
where $X_{t*}P(B) = P({X_t}^{-1}(B))$ for $B \in \mathcal{B}$: The push forward measure

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$$X_{t+1*}P = \beta_{t*}(X_{t*}P \otimes P), \quad (2)$$

where $\beta_t(x, \omega) = h(x) + \xi_t(\omega)$ linear

RKHS and kernel mean embedding

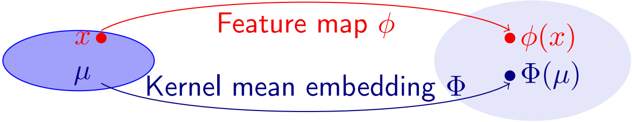
To define an inner product between measures, we employ the theory of RKHSs and kernel mean embeddings.

k : A positive definite kernel, $\phi(x) = k(x, \cdot)$: The feature map

$\mathcal{H}_k = \overline{\{\sum_{t=0}^{m-1} c_t\phi(x_t) \mid m \in \mathbb{N},\ x_t \in \mathcal{X},\ c_t \in \mathbb{C}\}}$: The RKHS

$\mathcal{M}(X)$: The space of all the finite signed Borel measures on $\mathcal{X}$

$\Phi : \mathcal{M}(\mathcal{X}) \to \mathcal{H}_k\ \mu \mapsto \int_{x\in\mathcal{X}} \phi(x)\, d\mu(x)$: The kernel mean embedding



$\mathcal{X}$ (Usually a finite dimensional sp.) $\mathcal{H}_k$ (An infinite dimensional Hilbert sp.)

$\langle\Phi(\mu), \Phi(\nu)\rangle = \int_{y\in\mathcal{X}}\int_{x\in\mathcal{X}} k(x, y)d\mu(x)d\nu(y)$

: The inner product between $\Phi(\mu)$ and $\Phi(\nu)$

Perron-Frobenius operators in RKHSs

Linear relation between ${X_t}_*P$ and ${X_{t+1}}_*P$

$$ {X_{t+1}}_*P = \beta_{t*}({X_t}_*P \otimes P) \quad (2) $$

Definition 1 (Perron Frobenius operator in RKHS)

An operator $K : \Phi(\mathcal{M}(\mathcal{X})) \to \mathcal{H}_k$ is called a *Perron-Frobenius operator* in $\mathcal{H}_k$ if it satisfies

$$ K\Phi(\mu) := \Phi(\beta_{t*}(\mu \otimes P)), \quad (3) $$

for $\mu \in \mathcal{M}(\mathcal{X})$.

It can be shown that:

- K is well-defined with some mild conditions of k.
- K is linear.
- K does not depend on time t.

Construction of a Krylov subspace of the P-F operator

$\{x_0, x_1, \ldots, x_T\} \subseteq \mathcal{X}$: observed time-series data
$\mu_{t,N}^S := 1/N \sum_{i=0}^{N-1} \delta_{x_{t+iS}}$ $(t = 0, \ldots, m)$: empirical measures
(We will drop superscript S for simplicity)
δ_x : Dirc measure of $x \in \mathcal{X}$

Assumptions

1. $\mu_{t,N}$ converge to a finite Borel measure μ_t weakly as $N \to \infty$ for $t = 0, \ldots m$
2. $\lim_{N\to\infty} \frac{1}{N} \sum_{i=0}^{N-1} \int_{\omega\in\Omega} f(h(x_{t+iS}) + \xi_t(\omega))\, dP(\omega)$ (Space average)
   $= \lim_{N\to\infty} \frac{1}{N} \sum_{i=0}^{N-1} f(h(x_{t+iS}) + \xi_{t+iS}(\eta))$ (Time average)
   $a.s.\ \eta \in \Omega$

If K is bounded, $K\Phi(\mu_t) = \Phi(\mu_{t+1})$ $(t = 0, \ldots, m-1)$ (4)

$\mathrm{Span}\{\Phi(\mu_0), \ldots, \Phi(\mu_{m-1})\} = \mathrm{Span}\{\Phi(\mu_0), K\Phi(\mu_0), \ldots, K^{m-1}\Phi(\mu_0)\}$
: Krylov subspace of K and $\Phi(\mu_0)$, denoted as $\mathcal{K}_m(K, \Phi(\mu_0))$

Numerical estimation for the P-F operator[1]

$\mathcal{K}_m(K, \Phi(\mu_0)) = \mathrm{Span}\{\Phi(\mu_0), \ldots, \Phi(\mu_{m-1})\}$

$\cdots$ constructed only with observed data

$[\Phi(\mu_0), \ldots, \Phi(\mu_{m-1})] = Q_m \mathbf{R}_m$: QR decomposition

Proposition 1 (Numerical estimation of K)

Let $\mathbf{K}_m := Q_m^* K Q_m$, the operator projected onto $\mathcal{K}_m(K, \Phi(\mu_0^S))$. Then, $\mathbf{K}_m$ is represented only with observed data as:

$$\mathbf{K}_m = Q^*[\Phi(\mu_0), \ldots, \Phi(\mu_{m-1})]\mathbf{R}_m^{-1} \quad (5)$$

For application, we want to know the time evolution of the dynamical system at some time $t > T$ → Estimate Kv for $v = \phi(x_t)$ Observable at time t
(T : The number of observables in the time-series data)

Arnoldi approximation of Kv

$$Kv \approx Q_T \mathbf{K}_m Q_T^* v \quad (6)$$

[1]Hashimoto et al., arXiv:1909.03634v3, 2019.

Unboundedness of the P-F operator

In fact, the P-F operators can be unbounded[2]. In this case, the Arnoldi approximation $\mathbf{K}_m$ does not converge to K as $m \to \infty$.

K (Unbounded) $\xrightarrow{\text{Transform}}$ $(\gamma I - K)^{-1}$ (Bounded), where $\gamma \notin \Lambda(K)$
$u_{t,N} = \sum_{i=0}^{t} \binom{t}{i} (-1)^i \gamma^{t-i} \Phi(\mu_{i,N})$, $\lim_{N\to\infty} u_{t,N} = u_t$

$$(\gamma I - K)^{-1} u_{t+1} = u_t \tag{7}$$

$\mathcal{K}_m((\gamma I - K)^{-1}, u_m^S) = \mathrm{Span}\{u_1, \ldots, u_m\}$
$[u_1^S, \ldots, u_m^S] = Q_m \mathbf{R}_m$: QR decomposition
$\mathbf{L}_m := Q_T^*(\gamma I - K)^{-1} Q_T = Q_T^*[u_1, \ldots, u_m]\mathbf{R}_m^{-1}$

Shift-invert Arnoldi approximation of Kv

$$Kv \approx Q_T \mathbf{K}_m Q_T^* v, \quad \mathbf{K}_m := \gamma \mathbf{I} - \mathbf{L}_m^{-1} \tag{8}$$

[2] Ikeda, Ishikawa and Sawano, arXiv:1911.11992, 2019.

Difference from classical settings

Our setting with P-F operators is different from classical ones in numerical linear algebra. Although the analyses for classical settings have been actively investigated, those for P-F operators have not been investigated.

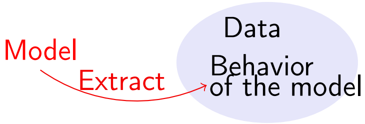
Our setting with a P-F operator K

- *Data* driven approach
- K is *not given*, instead, observed data are given
- Kv for a vector v have to be *estimated by data*

The Classical setting with a linear operator A

(A typical example of A : Laplace operator)

- *Model* driven approach
- Operators are *given*
- Av for a vector v can be computed



New analyses for the Krylov subspace methods for P-F operators are needed

Residual of a Krylov approximation

Krylov approximations for classical settings have a strong connection with their residuals. $\rightarrow$ We also investigate a connection of the Krylov approximations of P-F operators with their residuals.

$Kv \approx u_m \rightarrow \|v - K^{-1}u_m\|$: residual of u_m

The steps of our analysis :

1. Find a minimizer of the residual
2. Derive the relation between the residual of the Arnoldi approximation and that of the minimizer

Theorem 1 (Minimizer of the Residual)

Let $\tilde{u}_m := Q_{m+1}\mathbf{K}_{m+1}Q_{m+1}^* Q_m Q_m^* v$. Then, $\tilde{u}_m$ minimizes the residual in $\mathcal{K}_m(K, \Phi(\mu_1))$, that is:

$$\tilde{u}_m = \operatorname*{arg\,min}_{u \in \mathcal{K}_m(K,\Phi(\mu_1))} \|v - K^{-1}u\|. \tag{9}$$

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Proof. $Q_m Q_m^* v =: p_{m-1}(K)\Phi(\mu_0)$
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Projection onto $\mathcal{K}_m(K, \Phi(\mu_0))$

$$\operatorname*{arg\,min}_{u \in \mathcal{K}_m(K, \Phi(\mu_0))} \|v - u\| = \boxed{Q_m Q_m^* v} \quad (10)$$

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$\Phi(\mu_1) = K\Phi(\mu_0)$: Time evolution of μ_0

$$= p_{m-1}(K)K^{-1}\Phi(\mu_1) = K^{-1}p_{m-1}(K)\Phi(\mu_1). \tag{10}$$

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$$\therefore \quad p_{m-1}(K)\Phi(\mu_1) = \operatorname*{arg\,min}_{u \in \mathcal{K}_m(K,\Phi(\mu_1))} \|v - K^{-1}u\|. \tag{11}$$

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(12)

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Proof

$$\begin{aligned} p_{m-1}(K)\Phi(\mu_1) &\in \mathcal{K}_{m+1}(K, \Phi(\mu_0)) \\ &= Q_{m+1}Q_{m+1}^* p_{m-1}(K)\Phi(\mu_1) \\ &= Q_{m+1}Q_{m+1}^* K p_{m-1}(K)\Phi(\mu_0) \in \mathcal{K}_{m+1}(K, \Phi(\mu_0)) \\ &= Q_{m+1}Q_{m+1}^* K Q_{m+1}Q_{m+1}^* p_{m-1}(K)\Phi(\mu_0) \\ &= Q_{m+1}\mathbf{K}_{m+1}Q_{m+1}^* Q_m Q_m^* v \\ &= \tilde{u}_m. \end{aligned} \tag{12}$$

$\Phi(\mu_1) = K\Phi(\mu_0)$: Time evolution of μ_0

By the def. of $\mathbf{K}_{m+1}$

By the def. of p_{m-1}

Residual of a Krylov approximation

$\tilde{u}_m = \arg\min_{u \in \mathcal{K}_m(K, \Phi(\mu_1))} \|v - K^{-1}u\|$

$\cdots$ A minimizer of the residual

Theorem 2 (Residual of an Arnoldi approximation)

let $u_m := Q_m \mathbf{K}_m Q_m^* v \in \mathcal{K}_m(K, \Phi(\mu_0^S))$ be the Arnoldi approximation of Kv. Then, there exists $C_m > 0$ such that

$$\|v - K^{-1}u_m\| \leq (1 + C_m)\|v - K^{-1}\tilde{u}_{m-1}\|. \tag{13}$$

For $\epsilon > 0$, if m is sufficiently large so that the Krylov subspace $\mathcal{K}_m(K, \Phi(\mu_0^S))$ is sufficiently close to $\mathcal{H}_k$, and if K is bounded, then

$$C_m \leq 1 + \|K^{-1}\|\|K\|\,\epsilon. \tag{14}$$

We have also shown similar theorems about the Shift-invert Arnoldi approximations.

Numerical experiments

Example 1 (Landau equation)

$\mathcal{X} = [0, \infty)$

$$\frac{dr}{dt} = 0.5r - r^3 \tag{15}$$

$\downarrow$ Discretizing and adding random noise

$$X_t = X_{t-1} + \Delta t(0.5X_{t-1} - X_{t-1}^3 + \xi_t) \tag{16}$$

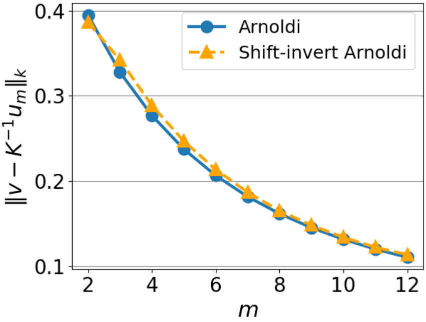

Fig. 1: The dimension of the Krylov subspace m versus the residual

Numerical experiments

Example 2 (Real-world Internet traffic data)

x_t : the amount of Internet traffic (gbps) that passed through a certain node (ID 12) in a network composed of 23 nodes and 227 links at time t.

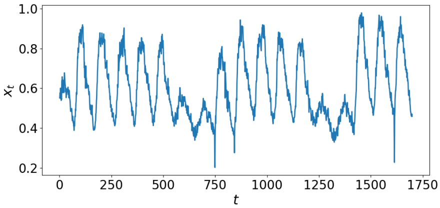

Fig. 2: The amount of Internet traffic at each t

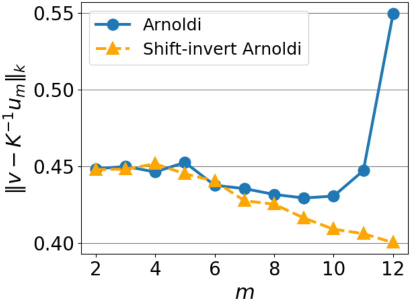

Fig. 3: The dimension of the Krylov subspace m versus the residual

Conclusions

- We considered Krylov subspace methods for P-F operators.
- Since the setting with P-F operators is different from classical settings in numerical linear algebra, new analyses for the Krylov subspace methods for P-F operators are required.
- We have shown connections of the Krylov approximations with their residuals.