

# Stochastic system consideration for EDMD

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## 1 Notation introduction

A list of all the notation and relevant definition:

1. (Autonomous) SDE in the dynamical system  $(\Omega, \mu)$ :

$$dX_t = b(X_t)dt + \sigma(X_t)dW_t$$

2.  $\Phi^t$ : Transformation map/flow
3.  $m$ : Number of (i.i.d.) data points
4.  $n, t = \frac{1}{n}$ : sampling frequency and time step between two data snapshots
5.  $N$ : Dictionary size
6.  $\Psi = \{\psi_i\}_{i=1}^N$ : Dictionary or set of basis functions
7.  $\mathcal{F} := L^2(\Omega, \mu)$ ,  $\mathcal{F}_N := \text{span}\{\psi_1, \dots, \psi_N\} \subset \mathcal{F}$
8.  $\mathcal{P}_N$ : Projection onto the subspace  $\mathcal{F}_N$
9. Data(i.i.d.) snapshots:

$$X = \begin{bmatrix} | & & | \\ x_1 & \cdots & x_m \\ | & & | \end{bmatrix}, \quad Y = \begin{bmatrix} | & & | \\ y_1 & \cdots & y_m \\ | & & | \end{bmatrix}$$

10. (Row)Vector of basis functions:

$$\Psi_N(x) := [\psi_1(x), \dots, \psi_N(x)]$$

11. Matrices of dictionary  $\{\psi_j\}_{j=1}^N$  evaluated on data  $\{x_i, y_i\}_{i=1}^m$ :

$$\Psi_X = \begin{bmatrix} \text{---} & \Psi_N(x_1) & \text{---} \\ & \vdots & \\ \text{---} & \Psi_N(x_m) & \text{---} \end{bmatrix} = \begin{bmatrix} \psi_1(x_1) & \cdots & \psi_N(x_1) \\ \vdots & \ddots & \vdots \\ \psi_1(x_m) & \cdots & \psi_N(x_m) \end{bmatrix}$$

$$\Psi_Y = \begin{bmatrix} \text{---} & \Psi_N(y_1) & \text{---} \\ & \vdots & \\ \text{---} & \Psi_N(y_m) & \text{---} \end{bmatrix} = \begin{bmatrix} \psi_1(y_1) & \cdots & \psi_N(y_1) \\ \vdots & \ddots & \vdots \\ \psi_1(y_m) & \cdots & \psi_N(y_m) \end{bmatrix}$$

12. Definition of Koopman operator in deterministic system:

$$\mathcal{K}f = f \circ \Phi$$

Definition of stochastic Koopman operator (semigroup):

$$\mathcal{K}^t f = \mathbb{E}[f \circ \Phi^t]$$

Remark: In the deterministic system, we can still use  $\mathcal{K}^t, \Phi^t$  where  $t$  is the (fixed) time interval between two sampling snapshots.

13. Definition of Koopman generator:

$$\begin{aligned} \mathcal{L}f(x) &:= \lim_{t \rightarrow 0} \frac{[\mathcal{K}^t f(x)] - f(x)}{t} \\ &= \lim_{t \rightarrow 0} \frac{\mathbb{E}[f \circ \Phi^t(x)] - f(x)}{t} \end{aligned} \tag{1}$$

## EDMD framework review

Let  $f(x) = \Psi_N(x)a$ . Then

$$\mathcal{K}f(x) = f(y) = \Psi_N(y)a = \Psi_N(x)Ka + r(x)$$

where  $r(x)$  is the residual. Notice that the span of  $\{\psi_1, \dots, \psi_N\}$  is not necessarily invariant under  $\mathcal{K}$ .

In the EDMD framework, given a dataset  $\{(x_i, y_i)\}_{i=1}^M$ , we want to minimize the residual over the finite data set:

$$J := \sum_{i=1}^M |r(x_i)|^2 = \sum_{i=1}^M |(\Psi_N(y_i) - \Psi_N(x_i)K)a|^2,$$

so, this is equivalent to  $\min_K \|\Psi_Y - \Psi_X K\|_F$  and the minimal  $K$  is

$$K = \Psi_X^\dagger \Psi_Y = (\Psi_X^T \Psi_X)^\dagger (\Psi_X^T \Psi_Y) = G^\dagger A$$

where  $\dagger$  is the pseudoinverse and  $G = \frac{1}{m} \Psi_X^T \Psi_X$ ,  $A = \frac{1}{m} \Psi_X^T \Psi_Y$ .

**Remark.** *Regularization through truncated SVD or by adding a small perturbation is typically applied.*

## S-EDMD framework

First, we can expand the Koopman operator (semigroup)  $\mathcal{K}(t)$  similar as in EDMD:

$$\begin{aligned}\mathcal{K}(t)f(x) &= \mathbb{E}[f(y)] \\ &= \Psi_N(x)K(t)\mathbf{a} + r(x)\end{aligned}\quad (2)$$

Alternatively, we approximate the Koopman operator(semigroup)  $\mathcal{K}(t)$  analogous to Taylor expansion using the definition of generator(1):

$$\begin{aligned}\mathcal{K}(t)f(x) &= \mathbb{E}[f(y)] \\ &= \mathbb{E}[\Psi_N(y)]\mathbf{a} \\ &= [\Psi_N(x) + t \cdot \mathcal{L}\Psi_N(x) + O(t^2)]\mathbf{a}\end{aligned}\quad (3)$$

where  $\mathcal{L}\Psi_N(x) = [\mathcal{L}\psi_1(x), \dots, \mathcal{L}\psi_N(x)]$  and

$$\mathcal{L}\psi_j(x) = b(x) \cdot \nabla \psi_j(x) + \frac{1}{2}\sigma^2(x) : \nabla^2 \psi_j(x) \quad (4)$$

**Remark.** We can get explicit higher order term  $O(t^2)$  in (3) by applying Itô's formula recursively. See A for more details. Or we can simply apply Taylor expansion here to obtain  $O(t^2)$ .

**Remark.** In order to obtain (4), we can use Itô's formula. From Itô's formula, we know that given  $f \in C_b^2(\Omega)$  and  $X_0 = x$ ,

$$df(X_t) = \left( b(X_t) \cdot \nabla f(X_t) + \frac{1}{2}\sigma^2(x) : \nabla^2 f(X_t) \right) dt + \sigma(X_t) \cdot \nabla f(X_t) dW_t$$

Taking expectation on its integral form, we have:

$$\mathbb{E}[f(X_t)|X_0 = x] - f(x) = \int_0^t \left( b(X_s) \cdot \nabla f(X_s) + \frac{1}{2}\sigma^2(X_s) : \nabla^2 f(X_s) \right) ds$$

Let  $t \rightarrow 0$ , we have

$$\begin{aligned}\frac{d}{dt}f &= \mathcal{L}f(x) := \lim_{t \rightarrow 0} \frac{\mathbb{E}[f(X_t) - f(x)|X_0 = x]}{t} \\ &= b(X_t) \cdot \nabla f(X_t) + \frac{1}{2}\sigma^2(x) : \nabla^2 f(X_t)\end{aligned}$$

In our case, combining (3) and (2), we can minimize the following:

$$J := \sum_{i=1}^m |r(x_i)|^2 = \sum_{i=1}^m \left| [\Psi_N(x_i) + t \cdot \mathcal{L}\Psi_N(x_i) + O(t^2) - \Psi_N(x_i)K]\mathbf{a} \right|^2$$

which is equivalent to minimize

$$J = \min_K \|\Psi_X + t \cdot \mathcal{L}\Psi_X + O(t^2) - \Psi_X K\|_F^2 \quad (5)$$

and the minimal  $K(t)$  is

$$K(t) = \Psi_X^\dagger (\Psi_X + t \cdot \mathcal{L}\Psi_X + O(t^2)) \quad (6)$$

where the generator(time differential) matrix approximation  $[\mathcal{L}\Psi_X]_{ij} = \mathcal{L}\psi_j(x_i)$ .

**Remark.**  $O(t^2)$  in (7), (3) and (5) are different. They are scalar, vector and matrix respectively. For example, each element of  $O(t^2)$  in (3) and (5) is a scalar  $O(t^2)$  in (7).

Empirically, if  $t$  is very small, we update the Koopman matrix approximation in the following way with  $O(t^2)$  omitted:

$$\widehat{K}(t) = \widehat{\Psi}_X^\dagger (\widehat{\Psi}_X + t \cdot \widehat{\mathcal{L}}\widehat{\Psi}_X)$$

**Remark.** For the case of trained basis by NN, we replace  $\Psi_X + t \cdot \mathcal{L}\Psi_X + O(t^2)$  by  $\Psi_Y$  in (5),

Now, we will show that the computed  $K_{N,n,m}$  by our S-EDMD method converges not only in large data  $m$  and large dictionary size  $N$ , but also in zero-limit of sampling time  $t = 1/n$ .

## 2 Convergence in the limit of large data

(1) i.i.d. data:

$$\begin{aligned}
& P\left(\|\widehat{K}_{N,n,m} - K_{N,n,m}\|_F > \epsilon\right) \\
&= P\left(\|\widehat{\Psi}_X^\dagger(\widehat{\Psi}_X + t\widehat{\mathcal{L}\Psi}_X) - \Psi_X^\dagger(\Psi_X + t\mathcal{L}\Psi_X + O(t^2))\|_F > \epsilon\right) \\
&= P\left(\|t\widehat{\Psi}_X^\dagger\widehat{\mathcal{L}\Psi}_X - t\Psi_X^\dagger\mathcal{L}\Psi_X + O(t^2)\|_F > \epsilon\right) \\
&\leq P\left(t\|\widehat{\Psi}_X^\dagger\widehat{\mathcal{L}\Psi}_X - \Psi_X^\dagger\mathcal{L}\Psi_X\|_F + O(t^2) > \epsilon\right) \\
&= P\left(t\|\widehat{G}^{-1}\widehat{A} - G^{-1}A\|_F + O(t^2) > \epsilon\right)
\end{aligned}$$

where  $G = \frac{1}{m}\Psi_X^*\Psi_X$  and  $A = \frac{1}{m}\Psi_X^*\mathcal{L}\Psi_X$ .

(From Wiki) A function  $f : \mathcal{X}_1 \times \mathcal{X}_2 \times \dots \times \mathcal{X}_n \rightarrow \mathbb{R}$  satisfies the *bounded differences property* if substituting the value of the  $i$ th coordinate  $x_i$  changes the value of  $f$  by at most  $c_i$ . More formally, if there are constants  $c_1, c_2, \dots, c_n$  such that for all  $i \in [n]$ , and all  $x_1 \in \mathcal{X}_1, x_2 \in \mathcal{X}_2, \dots, x_n \in \mathcal{X}_n$ ,

$$\sup_{x'_i \in \mathcal{X}_i} |f(x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_n) - f(x_1, \dots, x_{i-1}, x'_i, x_{i+1}, \dots, x_n)| \leq c_i.$$

**Lemma 1** (McDiarmid's Inequality). *Let  $f : \mathcal{X}_1 \times \mathcal{X}_2 \times \dots \times \mathcal{X}_n \rightarrow \mathbb{R}$  satisfy the bounded differences property with bounds  $c_1, c_2, \dots, c_n$ . Consider independent random variables  $X_1, X_2, \dots, X_n$  where  $X_i \in \mathcal{X}_i$  for all  $i$ . Then, for any  $\epsilon > 0$ ,*

$$\mathbb{P}(|f(X_1, X_2, \dots, X_n) - \mathbb{E}[f(X_1, X_2, \dots, X_n)]| \geq \epsilon) \leq 2 \exp\left(-\frac{2\epsilon^2}{\sum_{i=1}^n c_i^2}\right).$$

*Proof.* Omitted.  $\square$

**Lemma 2** (Hoeffding's Inequality). *Assume  $X_i \in [a_i, b_i]$ . Then, for any  $\epsilon > 0$ ,*

$$\mathbb{P}\left(\sum_{i=1}^n X_i - \mathbb{E}\left[\sum_{i=1}^n X_i\right] \geq \epsilon\right) \leq e^{-\frac{2\epsilon^2}{\sum_{i=1}^n (b_i - a_i)^2}}$$

and

$$\mathbb{P}\left(\left|\sum_{i=1}^n X_i - \mathbb{E}\left[\sum_{i=1}^n X_i\right]\right| \geq \epsilon\right) \leq 2e^{-\frac{2\epsilon^2}{\sum_{i=1}^n (b_i - a_i)^2}}$$

*Proof.* The McDiarmid's Inequality(1) directly implies Hoeffding's inequality by taking  $f(X_1, \dots, X_n) = \sum_{i=1}^n X_i$ .  $\square$

**Theorem 3.** *Let  $|\psi_i(X_k)| \leq C$   $\mathbb{P}$ -a.e. for all  $1 \leq i \leq N$  and  $1 \leq k \leq m$ . Suppose  $\|\mathcal{L}_{N,n,m}\| \leq L$ . Then, for any  $\epsilon > 0$ ,*

$$\begin{aligned}
\mathbb{P}\left(\|\widehat{G} - G\|_F \geq \epsilon\right) &\leq 2N^2 \exp\left(-\frac{m\epsilon^2}{8N^2C^4}\right), \\
\mathbb{P}\left(\|\widehat{A} - A\|_F \geq \epsilon\right) &\leq 2N^2 \exp\left(-\frac{m\epsilon^2}{8N^2C^4L^2}\right).
\end{aligned}$$

*Proof.* Define the random matrix  $\eta(X) := \Psi(X)^T \Psi(X) \in \mathbb{R}^{N \times N}$ , i.e.,  $\eta_{ij}(X) = \psi_i(X)\psi_j(X)$ . Let  $G = \mathbb{E}[\eta(X_1)]$ ,  $\widehat{G} = \frac{1}{m} \sum_{k=1}^m \eta(X_k)$ . Then,

$$\begin{aligned} \|\widehat{G} - G\|_F^2 &= \sum_{i=1}^N \sum_{j=1}^N \left| \widehat{G}_{ij} - G_{ij} \right|^2 \\ &= \sum_{i=1}^N \sum_{j=1}^N \left| \frac{1}{m} \sum_{k=1}^m \eta_{ij}(X_k) - \mathbb{E}[\eta_{ij}(X_k)] \right|^2 \end{aligned}$$

where  $\tilde{\eta}(X) := \eta(X) - \mathbb{E}[\eta(X_1)]$  and thus  $|\tilde{\eta}_{ij}(X)| \leq 2C^2$  for all  $1 \leq i, j \leq N$ . Next, applying Hoeffding's inequality (2) and union bound, we have

$$\begin{aligned} \mathbb{P}\left(\|\widehat{G} - G\|_F \geq \epsilon\right) &= \mathbb{P}\left(\|\widehat{G} - G\|_F^2 \geq \epsilon^2\right) \\ &\leq \mathbb{P}\left(\sum_{i=1}^N \sum_{j=1}^N \left| \frac{1}{m} \sum_{k=1}^m \tilde{\eta}_{ij}(X_k) \right|^2 \geq \epsilon^2\right) \\ &\leq N^2 \mathbb{P}\left(\left| \frac{1}{m} \sum_{k=1}^m \tilde{\eta}_{ij}(X_k) \right|^2 \geq \epsilon^2/N^2\right) \\ &= N^2 \mathbb{P}\left(\left| \frac{1}{m} \sum_{k=1}^m \tilde{\eta}_{ij}(X_k) \right| \geq \epsilon/N\right) \\ &\leq 2N^2 \exp\left(-\frac{2(m\epsilon/N)^2}{m(4C^2)^2}\right) \\ &= 2N^2 \exp\left(-\frac{m\epsilon^2}{8N^2C^4}\right) \end{aligned}$$

Similarly, define  $\xi(X) := \Psi(X)^T \mathcal{L}_{N,n,m} \Psi(X)$ . Since

$$|\psi_i(X)\mathcal{L}\psi_j(X)| \leq C^2 \|\mathcal{L}_{N,n,m}\| \leq C^2 L,$$

we have

$$\mathbb{P}\left(\|\widehat{A} - A\|_F \geq \epsilon\right) \leq 2N^2 \exp\left(-\frac{m\epsilon^2}{8N^2C^4L^2}\right),$$

□

**Lemma 4** (Philipp, Lemma C.5). *Let  $G, A \in \mathbb{R}^{N \times N}$  be such that  $G$  is invertible and  $A \neq 0$ . Let  $\widehat{G}, \widehat{A} \in \mathbb{R}^{N \times N}$  be random matrices such that  $\widehat{G}$  is invertible a.s. Then for any sub-multiplicative matrix norm  $\|\cdot\|$  on  $\mathbb{R}^{N \times N}$  and any  $\epsilon > 0$  we have*

$$\mathbb{P}\left(\|G^{-1}A - \widehat{G}^{-1}\widehat{A}\| > \epsilon\right) \leq \mathbb{P}\left(\|A - \widehat{A}\| > \frac{\epsilon}{\tau} \|A\|\right) + \mathbb{P}\left(\|G - \widehat{G}\| > \frac{\epsilon}{\tau} \|G^{-1}\|^{-1}\right),$$

where  $\tau = 2\|G^{-1}\|\|A\| + \epsilon$ .

**Theorem 5.** Let  $\epsilon > 0$ . Define  $\epsilon_t = (\epsilon - O(t^2)) / t$ . Then, with same conditions defined in Theorem 3 and Lemma 4, we have

$$P\left(\|\hat{K}_{N,n,m} - K_{N,n,m}\|_F > \epsilon\right) \leq 2N^2 \left[ \exp\left(-\frac{m}{8} \left(\frac{\epsilon_t}{NC^2\tau\|G^{-1}\|}\right)^2\right) + \exp\left(-\frac{m}{8} \left(\frac{\epsilon_t\|A\|}{NC^2\tau L}\right)^2\right) \right]$$

*Proof.*

$$\begin{aligned} P\left(\|\hat{K}_{N,n,m} - K_{N,n,m}\|_F > \epsilon\right) &= P\left(t\|\hat{G}^{-1}\hat{A} - G^{-1}A\|_F + O(t^2) > \epsilon\right) \\ &= P\left(\|\hat{G}^{-1}\hat{A} - G^{-1}A\|_F > \epsilon_t\right) \\ &\leq \mathbb{P}\left(\|G - \hat{G}\| > \frac{\epsilon_t}{\tau}\|G^{-1}\|^{-1}\right) + \mathbb{P}\left(\|A - \hat{A}\| > \frac{\epsilon_t}{\tau}\|A\|\right) \\ &\leq 2N^2 \exp\left(-\frac{m(\frac{\epsilon_t}{\tau}\|G^{-1}\|^{-1})^2}{8N^2C^4}\right) + 2N^2 \exp\left(-\frac{m(\frac{\epsilon_t}{\tau}\|A\|)^2}{8N^2C^4L^2}\right) \\ &= 2N^2 \left[ \exp\left(-\frac{m}{8} \left(\frac{\epsilon_t\|G^{-1}\|^{-1}}{NC^2\tau}\right)^2\right) + \exp\left(-\frac{m}{8} \left(\frac{\epsilon_t\|A\|}{NC^2\tau L}\right)^2\right) \right] \end{aligned}$$

□

### 3 Convergence in zero-limit of sampling time

Now we have Koopman matrix approximation at discrete time  $K_{N,n}(1/n)$ . We will use it to construct the matrix  $A_{N,n}$ , which is the matrix representation of the discrete projected Koopman generators  $\mathcal{A}_{N,n}$  and find its limit in strong operator topology.

First, for each  $N > 0$ , construct the following sequence of matrices  $\{A_{N,n}\}_{n \geq 1}$ :

$$\begin{aligned} A_{N,n} &:= \frac{K_{N,n}\left(\frac{1}{n}\right) - I}{\frac{1}{n}} \\ &= \frac{\left[\Psi_X^\dagger \left(\Psi_X + \frac{1}{n} \cdot \mathcal{L}\Psi_X + O\left(\frac{1}{n^2}\right)\right)\right] - I}{\frac{1}{n}} \\ &= \frac{\left[I + \frac{1}{n}\Psi_X^\dagger \mathcal{L}\Psi_X + O\left(\frac{1}{n^2}\right)\right] - I}{\frac{1}{n}} \\ &= \Psi_X^\dagger \mathcal{L}\Psi_X + O\left(\frac{1}{n}\right) \end{aligned}$$

**Remark.** Here the first term  $\Psi_X^\dagger \mathcal{L}\Psi_X$  is not dependent on  $n$  since we choose the basis functions manually.

Choose  $f = \Psi_N \mathbf{a} \in C_b^2(\Omega)$ , then we have

$$\begin{aligned} &\lim_{n \rightarrow \infty} \mathcal{A}_{N,n} f \\ &= \lim_{n \rightarrow \infty} \Psi_N A_{N,n} \mathbf{a} \\ &= \lim_{n \rightarrow \infty} \Psi_N \left( \Psi_X^\dagger \mathcal{L}\Psi_X + O\left(\frac{1}{n}\right) \right) \mathbf{a} \\ &= \Psi_N \left( \Psi_X^\dagger \mathcal{L}\Psi_X \right) \mathbf{a} + \lim_{n \rightarrow \infty} \Psi_N O\left(\frac{1}{n}\right) \mathbf{a} \quad (\text{Here the } O\left(\frac{1}{n}\right) \text{ is a matrix}) \end{aligned}$$

Now, we consider the second term:

$$\begin{aligned} &\lim_{n \rightarrow \infty} \Psi_N O\left(\frac{1}{n}\right) \mathbf{a} \\ &= \lim_{n \rightarrow \infty} \begin{bmatrix} \psi_1 & \cdots & \psi_N \end{bmatrix} \begin{bmatrix} O\left(\frac{1}{n}\right) & \cdots & O\left(\frac{1}{n}\right) \\ \vdots & \ddots & \vdots \\ O\left(\frac{1}{n}\right) & \cdots & O\left(\frac{1}{n}\right) \end{bmatrix} \begin{bmatrix} a_1 \\ \vdots \\ a_N \end{bmatrix} \\ &= \lim_{n \rightarrow \infty} \begin{bmatrix} \psi_1 & \cdots & \psi_N \end{bmatrix} \begin{bmatrix} a'_1 \\ \vdots \\ a'_N \end{bmatrix} \\ &\quad (\text{where } a'_i = \sum_{j=1}^N [O\left(\frac{1}{n}\right)]_{ij} a_j) \\ &= \lim_{n \rightarrow \infty} \sum_{i=1}^N \psi_i a'_i \end{aligned}$$



$$\begin{aligned}
&= \lim_{n \rightarrow \infty} \sum_{i=1}^N \psi_i \left( \sum_{j=1}^N [O(\frac{1}{n})]_{ij} a_j \right) \\
&\leq \lim_{n \rightarrow \infty} \sum_{i=1}^N \psi_i \left( \left( N \cdot O(\frac{1}{n}) \right) \sum_{j=1}^N a_j \right) \\
&= \lim_{n \rightarrow \infty} \left( N \cdot O(\frac{1}{n}) \right) \sum_{i,j=1}^N \psi_i \left( \sum_{j=1}^N a_j \right) = 0.
\end{aligned}$$

Therefore, for  $f = \Psi_N \mathbf{a}$ , we have

$$\lim_{n \rightarrow \infty} \Psi_N A_{N,n} \mathbf{a} = \Psi_N A_N \mathbf{a},$$

where  $A_N := \Psi_X^\dagger \mathcal{L} \Psi_X$ . In other words,

$$\lim_{n \rightarrow \infty} \mathcal{A}_{N,n} f = \mathcal{A}_N f,$$

where  $\mathcal{A}_N = \mathcal{P}_N \mathcal{A}|_{\mathcal{F}_N}$ .

The above content is summarized in the next theorem:

**Theorem 6.** *For each  $N > 0$ , let  $\mathcal{A}_N = \mathcal{P}_N \mathcal{A}|_{\mathcal{F}_N}$  be the projected Koopman generator with its matrix representation  $A_N := \Psi_X^\dagger \mathcal{L} \Psi_X$  and  $\mathcal{A}_{N,n}$  be the discrete projected Koopman generator with its matrix representation  $A_{N,n}$  defined in the following:*

$$A_{N,n} := \frac{K_{N,n} \left( \frac{1}{n} \right) - I}{\frac{1}{n}}$$

Then,  $\mathcal{A}_{N,n} \rightarrow \mathcal{A}_N$  in strong operator topology as  $n \rightarrow \infty$ .

*Proof.*

$$\begin{aligned}
A_{N,n} &:= \frac{K_{N,n} \left( \frac{1}{n} \right) - I}{\frac{1}{n}} \\
&= \frac{\left[ \Psi_X^\dagger \left( \Psi_X + \frac{1}{n} \cdot \mathcal{L} \Psi_X + O(\frac{1}{n^2}) \right) \right] - I}{\frac{1}{n}} \\
&= \frac{\left[ I + \frac{1}{n} \Psi_X^\dagger \mathcal{L} \Psi_X + O(\frac{1}{n^2}) \right] - I}{\frac{1}{n}} \\
&= \Psi_X^\dagger \mathcal{L} \Psi_X + O(\frac{1}{n})
\end{aligned}$$

**Remark.** Here the first term  $\Psi_X^\dagger \mathcal{L} \Psi_X$  is not dependent on  $n$  since we choose the basis functions manually.

Choose  $f = \Psi_N \mathbf{a} \in C_b^2(\Omega)$ , then we have

$$\lim_{n \rightarrow \infty} \mathcal{A}_{N,n} f$$

$$\begin{aligned}
&= \lim_{n \rightarrow \infty} \Psi_N A_{N,n} \mathbf{a} \\
&= \lim_{n \rightarrow \infty} \Psi_N \left( \Psi_X^\dagger \mathcal{L} \Psi_X + O\left(\frac{1}{n}\right) \right) \mathbf{a} \\
&= \Psi_N \left( \Psi_X^\dagger \mathcal{L} \Psi_X \right) \mathbf{a} + \lim_{n \rightarrow \infty} \Psi_N O\left(\frac{1}{n}\right) \mathbf{a} \\
&= \Psi_N A_N \mathbf{a} + \lim_{n \rightarrow \infty} \Psi_N O\left(\frac{1}{n}\right) \mathbf{a}
\end{aligned}$$

Now, we consider the second term:

$$\begin{aligned}
&\lim_{n \rightarrow \infty} \Psi_N O\left(\frac{1}{n}\right) \mathbf{a} \\
&= \lim_{n \rightarrow \infty} \begin{bmatrix} \psi_1 & \cdots & \psi_N \end{bmatrix} \begin{bmatrix} O\left(\frac{1}{n}\right) & \cdots & O\left(\frac{1}{n}\right) \\ \vdots & \ddots & \vdots \\ O\left(\frac{1}{n}\right) & \cdots & O\left(\frac{1}{n}\right) \end{bmatrix} \begin{bmatrix} a_1 \\ \vdots \\ a_N \end{bmatrix} \\
&= \lim_{n \rightarrow \infty} \begin{bmatrix} \psi_1 & \cdots & \psi_N \end{bmatrix} \begin{bmatrix} a'_1 \\ \vdots \\ a'_N \end{bmatrix} \\
&\text{(where } a'_i = \sum_{j=1}^N [O\left(\frac{1}{n}\right)]_{ij} a_j \text{)} \\
&= \lim_{n \rightarrow \infty} \sum_{i=1}^N \psi_i a'_i \\
&= \lim_{n \rightarrow \infty} \sum_{i=1}^N \psi_i \left( \sum_{j=1}^N [O\left(\frac{1}{n}\right)]_{ij} a_j \right) \\
&\leq \lim_{n \rightarrow \infty} \sum_{i=1}^N \psi_i \left( \left( N \cdot O\left(\frac{1}{n}\right) \right) \sum_{j=1}^N a_j \right) \\
&= \lim_{n \rightarrow \infty} \left( N \cdot O\left(\frac{1}{n}\right) \right) \sum_{i,j=1}^N \psi_i \left( \sum_{j=1}^N a_j \right) = 0.
\end{aligned}$$

Therefore, for  $f = \Psi_N \mathbf{a}$ , we have

$$\lim_{n \rightarrow \infty} \mathcal{A}_{N,n} f = \lim_{n \rightarrow \infty} \Psi_N A_{N,n} \mathbf{a} = \Psi_N A_N \mathbf{a} = \mathcal{A}_N f.$$

□

## 4 Convergence in large dictionary size $N$

In this section, we want to show that  $\mathcal{P}_N \mathcal{A}|_{\mathcal{F}_N} = \mathcal{A}_N \rightarrow \mathcal{A}$  in strong operator topology as  $N \rightarrow \infty$ , under a similar mathematical framework established in gEDMD analysis paper . In addition, if we can assume  $e^{t\mathcal{A}_N}, e^{t\mathcal{A}}$  are exponentially bounded for all  $t \geq 0$ ,  $N \in \mathbb{N}$ , then we can use the Trotter-Kato Approximation theorem to obtain  $e^{t\mathcal{A}_N} \rightarrow e^{t\mathcal{A}}$  in strong operator topology as  $N \rightarrow \infty$ , uniformly for  $t$  in a compact interval.

### 4.1 Convergence of $\mathcal{A}_N$ to $\mathcal{A}$

Consider the state space  $(\Omega, \mathcal{B}, \mu)$ , where the set of observables is given by  $\mathcal{F} := L^2(\Omega, \mu)$ . The domain of the operator  $\mathcal{A}$  is defined as:

$$\mathcal{D} := \{f \in \mathcal{F} : \mathcal{A}f \in \mathcal{F}\}.$$

The operator  $\mathcal{A}$  is referred to as a *closed operator* if the graph of  $\mathcal{A}$ , defined by:

$$\{(f, \mathcal{A}f) \in \mathcal{F} \times \mathcal{F} : f \in \mathcal{D}\},$$

is a closed subspace of  $\mathcal{F} \times \mathcal{F}$ . In this context, if  $\mathcal{A}$  is closed, then  $\mathcal{D}$  becomes a Hilbert space equipped with the inner product:

$$\langle f, g \rangle_{\mathcal{D}} := \langle f, g \rangle_{\mathcal{F}} + \langle \mathcal{A}f, \mathcal{A}g \rangle_{\mathcal{F}}, \quad \forall f, g \in \mathcal{D},$$

and the corresponding norm:

$$\|f\|_{\mathcal{D}}^2 := \langle f, f \rangle_{\mathcal{D}}.$$

It follows directly from this structure that  $\|f\|_{\mathcal{F}} \leq \|f\|_{\mathcal{D}}$ , and the operator  $\mathcal{A} : \mathcal{D} \rightarrow \mathcal{F}$  is continuous with  $\|\mathcal{A}\| \leq 1$ .

In practice, if  $\mathcal{A}$  is the infinitesimal generator of a strongly continuous semi-group,  $\mathcal{D}$  is dense in  $\mathcal{F}$ .

An example is that when  $\mathcal{D}$  is a weighted Sobolev space  $H^2(\Omega, \mu)$ , containing all measurable functions  $\psi : \Omega \rightarrow \mathbb{R}$  with finite norm:

$$\|\psi\|_{H^2(X, \mu)} = \left( \sum_{|\alpha| \leq 2} \int_{\Omega} |D^{\alpha} \psi|^2 d\mu \right)^{1/2},$$

where  $D^{\alpha} \psi$  represents the weak derivative of order  $\alpha$ .

**Assumption 1.** *We assume the following:*

1. The basis functions  $\Psi = \{\psi_1, \dots, \psi_N\} \subset \mathcal{D}$  are linearly independent.
2. The functions  $\{\psi_i, \mathcal{A}\psi_i\}_{i=1}^N$  are continuous  $\mu$ -a.e..
3. The points  $\{x_i\}_{i=1}^m \subset \Omega$  are i.i.d. samples from  $\mu$ .

**Assumption 2.** *Assumption 1 holds and*

$$\lim_{N \rightarrow \infty} \|\mathcal{P}_N \phi - \phi\|_{\mathcal{F}} = 0, \quad \forall \phi \in \mathcal{F},$$

where  $\mathcal{P}_N$  is the projection of  $\mathcal{F}$  onto  $\mathcal{F}_N$  using the inner product on  $\mathcal{F}$ .

**Assumption 3.** *Assumption 1 holds,  $\mathcal{A}$  is a closed operator, and*

$$\lim_{N \rightarrow \infty} \|\mathcal{P}_{\mathcal{D}_N} f - f\|_{\mathcal{D}} = 0, \quad \forall f \in \mathcal{D}.$$

Here,  $\mathcal{P}_{\mathcal{D}_N}$  is the projection of  $\mathcal{D}$  onto  $\mathcal{F}_N$  using the inner product on  $\mathcal{D}$ .

**Theorem 7.** *Let  $\Psi$  satisfy Assumption 2 and 3, then*

$$\lim_{N \rightarrow \infty} \|\mathcal{A}_N \mathcal{P}_{\mathcal{D}_N} f - \mathcal{A}f\|_{\mathcal{F}} = 0, \quad \forall f \in \mathcal{D}.$$

*Proof.* By definition  $\mathcal{A}_N = \mathcal{P}_N \mathcal{A}|_{\mathcal{F}_N}$ , we obtain

$$\begin{aligned} \mathcal{A}_N \mathcal{P}_{\mathcal{D}_N} - \mathcal{A} &= (\mathcal{A}_N - \mathcal{A}) \mathcal{P}_{\mathcal{D}_N} + \mathcal{A} \mathcal{P}_{\mathcal{D}_N} - \mathcal{A} \\ &= (\mathcal{P}_N - \text{Id}) \mathcal{A} \mathcal{P}_{\mathcal{D}_N} + \mathcal{A} (\mathcal{P}_{\mathcal{D}_N} - \text{Id}) \\ &= (\mathcal{P}_N - \text{Id}) \mathcal{A} + (\mathcal{P}_N - \text{Id}) \mathcal{A} (\mathcal{P}_{\mathcal{D}_N} - \text{Id}) + \mathcal{A} (\mathcal{P}_{\mathcal{D}_N} - \text{Id}). \end{aligned}$$

Consider now  $f \in \mathcal{D}$ . By Assumptions 2, 3 and the fact that  $\mathcal{A}$  is continuous on its domain, we have

$$\begin{aligned} \|\mathcal{A}_N \mathcal{P}_{\mathcal{D}_N} f - \mathcal{A}f\|_{\mathcal{F}} &\leq \|(\mathcal{P}_N - \text{Id}) \mathcal{A}f\|_{\mathcal{F}} + \|(\mathcal{P}_N - \text{Id}) \mathcal{A}\| \|\mathcal{P}_{\mathcal{D}_N} f - f\|_{\mathcal{D}} \\ &\quad + \|\mathcal{A}\| \|\mathcal{P}_{\mathcal{D}_N} f - f\|_{\mathcal{D}} \rightarrow 0. \end{aligned}$$

□

## 4.2 Convergence of $\mathcal{K}_N(t)$ to $\mathcal{K}(t)$

Define the semigroup generated by  $\{\mathcal{A}_N\}_{N \geq 1}$  and  $\mathcal{A}$ :

$$\mathcal{K}_N(t) := e^{t\mathcal{A}_N}, \quad \mathcal{K}(t) := e^{t\mathcal{A}}$$

and assume that

$$\|\mathcal{K}_N(t)\|, \|\mathcal{K}(t)\| \leq M e^{wt} \quad \text{for all } t \geq 0, N \in \mathbb{N}$$

and some constants  $M \geq 1, w \in \mathbb{R}$ .

**Corollary 8.** *Let  $(\mathcal{K}_N(t))_{t \geq 0}$  and  $(\mathcal{K}(t))_{t \geq 0}$  be strongly continuous semigroups on a Banach space  $\Omega$  with generators  $\mathcal{A}_N$  and  $\mathcal{A}$ , respectively. Assume that for some constants  $M \geq 1, w \in \mathbb{R}$ , the semigroups satisfy*

$$\|\mathcal{K}_N(t)\|, \|\mathcal{K}(t)\| \leq M e^{wt} \quad \text{for all } t \geq 0, N \in \mathbb{N}.$$

*Furthermore, assume that for each  $x \in \mathcal{D}(\mathcal{A})$ ,  $\mathcal{A}_N x \rightarrow \mathcal{A}x$  as  $N \rightarrow \infty$ . Then*

$$\mathcal{K}_N(t) \rightarrow \mathcal{K}(t)$$

*in the strong operator topology, uniformly for  $t$  in compact intervals.*

*Proof.* By applying the First Trotter–Kato Approximation Theorem, the convergence result follows directly. □

### First Trotter–Kato Approximation Theorem.

(Trotter 1958, Kato 1959). Let  $(T(t))_{t \geq 0}$  and  $(T_n(t))_{t \geq 0}$ ,  $n \in \mathbb{N}$ , be strongly continuous semigroups on  $X$  with generators  $\mathcal{A}$  and  $\mathcal{A}_n$ , respectively, and assume that they satisfy the estimate

$$\|T(t)\|, \|T_n(t)\| \leq M e^{wt} \quad \text{for all } t \geq 0, n \in \mathbb{N},$$

and some constants  $M \geq 1$ ,  $w \in \mathbb{R}$ . Take  $\mathcal{D}$  to be a core for  $\mathcal{A}$  and consider the following assertions.

- (a)  $\mathcal{D} \subset \mathcal{D}(\mathcal{A}_n)$  for all  $n \in \mathbb{N}$  and  $\mathcal{A}_n x \rightarrow \mathcal{A}x$  for all  $x \in \mathcal{D}$ .
- (b) For each  $x \in \mathcal{D}$ , there exists  $x_n \in \mathcal{D}(\mathcal{A}_n)$  such that  $x_n \rightarrow x$  and  $\mathcal{A}_n x_n \rightarrow \mathcal{A}x$ .
- (c)  $R(\lambda, \mathcal{A}_n)x \rightarrow R(\lambda, \mathcal{A})x$  for all  $x \in X$  and some/all  $\lambda > w$ .
- (d)  $T_n(t)x \rightarrow T(t)x$  for all  $x \in X$ , uniformly for  $t$  in compact intervals.

Then the implications

$$(a) \implies (b) \iff (c) \iff (d)$$

hold, while (b) does not imply (a).

## A "Taylor" expansion of stochastic Koopman operator

By applying Itô's formula to both  $f(X_t)$  and  $\mathcal{A}f(X_t)$ , we can derive a "Taylor expansion" for  $\mathbb{E}[f(X_t)]$  as in (3).

First, we apply Itô's formula to  $f(X_t)$ :

$$f(X_t) = f(x) + \int_0^t (\mathcal{A}f)(X_s) ds + \int_0^t f'(X_s) \sigma(X_s) dW_s.$$

Next, we treat  $\mathcal{A}f$  as a function and apply Itô's formula to  $\mathcal{A}f(X_s)$ :

$$(\mathcal{A}f)(X_t) = (\mathcal{A}f)(x) + \int_0^t [\mathcal{A}(\mathcal{A}f)](X_s) ds + \int_0^t (\mathcal{A}f')(X_s) \sigma(X_s) dW_s.$$

Then, we substitute this expression for  $\mathcal{A}f(X_t)$  back into the formula for  $f(X_t)$ :

$$\begin{aligned} f(X_t) &= f(x) + \int_0^t (\mathcal{A}f)(X_s) ds + \int_0^t f'(X_s) \sigma(X_s) dW_s \\ &= f(x) + \int_0^t \left[ (\mathcal{A}f)(x) + \int_0^s [\mathcal{A}(\mathcal{A}f)](X_u) du + \int_0^s (\mathcal{A}f')(X_u) \sigma(X_u) dW_u \right] ds \\ &\quad + \int_0^t f'(X_s) \sigma(X_s) dW_s. \end{aligned}$$

After rearranging terms, we have:

$$\begin{aligned} f(X_t) &= f(x) + (\mathcal{A}f)(x) t + \int_0^t \int_0^s [\mathcal{A}(\mathcal{A}f)](X_u) du ds \\ &\quad + \int_0^t \int_0^s (\mathcal{A}f')(X_u) \sigma(X_u) dW_u ds + \int_0^t f'(X_s) \sigma(X_s) dW_s. \end{aligned}$$

Taking expectations on both sides and noting that the stochastic integrals have zero mean (assuming appropriate integrability conditions), we get:

$$\mathbb{E}[f(X_t)] = f(x) + (\mathcal{A}f)(x) t + \int_0^t \int_0^s \mathbb{E}[\mathcal{A}(\mathcal{A}f)(X_u)] du ds.$$

The double integral term represents the accumulated effect of the higher-order derivatives of  $f$  over time. To understand its order, consider that if  $\mathbb{E}[\mathcal{A}(\mathcal{A}f)(X_u)]$  is bounded by some constant  $M$ , then:

$$\left| \int_0^t \int_0^s \mathbb{E}[\mathcal{A}(\mathcal{A}f)(X_u)] du ds \right| \leq M \int_0^t \int_0^s du ds = M \int_0^t s ds = M \frac{t^2}{2}.$$

This shows that the double integral is of order  $O(t^2)$  when  $t$  is small.

Therefore, for small  $t$ , the expected value simplifies to:

$$\mathbb{E}[f(X_t)] = f(x) + (\mathcal{A}f)(x) t + O(t^2). \quad (7)$$