Stochastic Koopman Operator and the Numerical Approximations of its Spectral Objects

Operator Theoretic Methods in Dynamic Data Analysis,
IPAM Workshop

February 11-15, 2019

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Outline of the talk

Stochastic Koopman Operator

Koopman eigenvalues and eigenfunctions, Linear RDS

Semigroup property of the Koopman operator family

Numerical approximations of the stochastic Koopman operator

sHankel-DMD algorithm

The continuation of the research

Koopman Operator

$(\varphi^t)_{t\in\mathbb{T}}$ - a nonlinear dynamical flow over $M \subseteq \mathbb{R}^n$ with the cocycle property

$$\varphi^{t+s}(\mathbf{x}) = \varphi^t(\varphi^s(\mathbf{x})).$$

Koopman operator: linear infinite-dimensional operator defined by

$$U^t f(\mathbf{x}) = f(\varphi^t(\mathbf{x})). \tag{1}$$

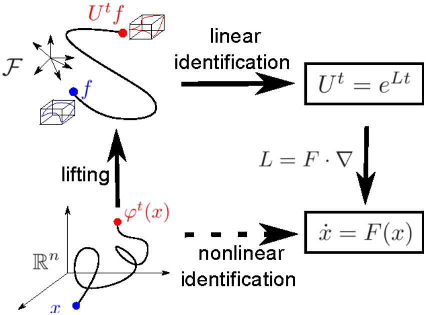

Figure: Source: http://homepages.laas.fr/henrion/ecc15/mezic-workshop-ecc15.pdf by I. Mezić and A. Mauroy

Koopman eigenvalues and eigenfunctions, Linear RDS

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Stochastic Koopman Operator

Random dynamical system (RDS) φ consists of two ingredients:

- **Model of noise:** A driving flow $\theta := (\theta(t))_{t\in\mathbb{T}}$ over $(\Omega, \mathcal{F}, P)$ with cocycle property, where $\theta(t)$ are measurable and measure preserving, i.e. $\theta(t)P = P$.
- **Model for the evolution:** A measurable mapping $\varphi : \mathbb{T} \times \Omega \times M \to M$ ($M \subseteq \mathbb{R}^d$) over θ such that $\varphi(t,\omega) = \varphi(t,\omega,\cdot) : M \to M$ satisfies cocycle property:

$$\varphi(0,\omega) = id_M, \;\; \varphi(t+s,\omega) = \varphi(t,\theta(s)\omega) \circ \varphi(s,\omega), \;\; s,t \in \mathbb{T}, \omega \in \Omega. \tag{2}$$

$\mathbb{T}$ is the group (or semigroup) and we call it time.

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  $\mathbb{T}$ is the group (or semigroup) and we call it time.

For each $\mathbf{x} \in M$, $(\varphi(t,\omega)\mathbf{x})_{t\in T,\omega\in\Omega}$ is a stochastic process, so that the initial distribution over Ω induces a probability measure on $M^{\mathbb{T}}$.

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Definition

The **stochastic Koopman operator** $\mathcal{K}^t$ associated with the RDS φ is defined on functions $f : M \to \mathbb{C}$ (observables) by

$$\mathcal{K}^t f(x) = \mathbb{E}[f(\varphi(t,\omega)x)]. \quad (3)$$

$(\mathcal{K}^t)_{t\in\mathbb{T}}$ - stochastic Koopman operator family

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Types of RDS (Arnold: RDS, Springer, 1998.)

Discrete time RDS ($\mathbb{T} = \mathbb{Z}$ or $\mathbb{T} = \mathbb{Z}^+ \cup \{0\}$)

$$\varphi(n, \omega) = T(\psi^{n-1}(\omega), \cdot) \circ \cdots \circ T(\psi(\omega), \cdot) \circ T(\omega, \cdot), \quad n \geq 1, \quad \psi = \theta(1). \quad (4)$$

- $(T(\psi^i(\omega), \cdot))_{i \in \mathbb{T}}$ - stationary sequence of random maps on M
- the sequence $\mathbf{x}_n = \varphi(n, \omega)\mathbf{x}_0$, $n = 0, 1, \ldots$ solves the random difference equation

$$\mathbf{x}_{n+1} = T(\psi^n(\omega), \mathbf{x}_n), \; n \geq 0, \quad \mathbf{x}_0 = \mathbf{x}. \quad (5)$$

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Continuous time RDS generated by random differential eq. (RDE)

$$\dot{\mathbf{x}} = F(\theta(t)\omega, \mathbf{x}), \quad \theta(t)\omega - \text{real noise} \tag{6}$$

This RDE generates an RDS φ over θ:

$$\varphi(t,\omega)\mathbf{x} = \mathbf{x} + \int_0^t F(\theta(s)\omega, \varphi(s,\omega)\mathbf{x})ds, \quad \varphi(0,\omega)\mathbf{x} = \mathbf{x}. \tag{7}$$

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Continuous time RDS generated by stochastic differential eq. (SDE)

$$dX_t = G(X_t)dt + \sigma(X_t)dW_t, \quad \theta(t)\omega(\cdot) = \omega(t+\cdot) - \omega(t). \quad (8)$$

- $G : M \to M$, $\sigma : M \to \mathbb{R}^{d\times r}$ - L^2 measurable
- $W_t = (W_t^1, \ldots, W_t^r)$ r-dimensional Wiener process

$$\varphi(t,\omega)\mathbf{x} = X_t(\omega) = \mathbf{x} + \int_0^t G(X_s(\omega))ds + \int_0^t \sigma(X_s(\omega))dW_s. \quad (9)$$

Stochastic Koopman Eigenvalues and Eigenfunctions

Definition

The observables $\phi^t : M \to \mathbb{C}$ that satisfy equation

$$\mathcal{K}^t \phi^t(\mathbf{x}) = \lambda^S(t)\phi^t(\mathbf{x}) \tag{10}$$

are the **eigenfunctions** of the stochastic Koopman operator (3) and $\lambda^S(t)$ are its **eigenvalues**.

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Proposition 1. - **Discrete Linear RDS**

Let be $M \subseteq \mathbb{R}^d$ and $\Phi(n, \omega)$ the linear RDS generated by $T(\omega, \mathbf{x}) = \mathbf{A}(\omega)\mathbf{x}$, so that $T^n(\omega, \mathbf{x}) = \Phi(n, \omega)\mathbf{x}$ and

$$\Phi(n, \omega) = \mathbf{A}(\psi^{n-1}(\omega)) \cdots \mathbf{A}(\psi(\omega))\mathbf{A}(\omega).$$

Assume that $\hat{\Phi}(n) := \mathbb{E}[\Phi(n, \omega)]$ are diagonalizable, with simple eigenvalues $\hat{\lambda}_j(n)$ and left eigenvectors $\hat{\mathbf{w}}_j^n$, $j = 1, \ldots, d$. Then the eigenfunctions of the stochastic Koopman operator $\mathcal{K}^n$ are

$$\phi_j^n(\mathbf{x}) = \langle \mathbf{x}, \hat{\mathbf{w}}_j^n \rangle, \quad j = 1, \ldots, d, \tag{11}$$

with the corresponding eigenvalues $\lambda_j^S(n) = \hat{\lambda}_j(n)$.
Moreover, if matrices $\mathbf{A}(\omega)$, $\omega \in \Omega$ are simultaneously diagonalizable with simple eigenvalues $\lambda_j(\omega)$ and left eigenvectors $\mathbf{w}_j$, $j = 1, \ldots, d$, then

$$\hat{\mathbf{w}}_j^n = \mathbf{w}_j \quad \text{and} \quad \lambda_j^S(n) = \mathbb{E}\left[\prod_{i=1}^{n} \lambda_j(\psi^{i-1}(\omega))\right].$$

Linear RDS generated by RDE

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Proposition 2.

If $\mathbf{A} : \Omega \to \mathbb{R}^{d\times d}$ and $\mathbf{A} \in L^1(\Omega, \mathcal{F}, P)$ then RDE

$$\dot{\mathbf{x}} = \mathbf{A}(\theta(t)\omega)\mathbf{x}, \tag{12}$$

generates a linear RDS Φ satisfying

$$\Phi(t, \omega) = \mathbf{I} + \int_0^t \mathbf{A}(\theta(s)\omega)\Phi(s, \omega)ds. \tag{13}$$

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Assume that $\hat{\Phi}(t) = \mathbb{E}[\Phi(t, \omega)]$ is diagonalizable, with simple eigenvalues $\hat{\mu}_j^t$ and left and right eigenvectors $\hat{\mathbf{w}}_j^t$, $\hat{\mathbf{v}}_j^t$ $j = 1, \dots, d$. Then

$$\phi_j^t(\mathbf{x}) = \langle \mathbf{x}, \hat{\mathbf{w}}_j^t \rangle, \quad j = 1, \dots, d, \tag{14}$$

are the principal eigenfunctions of $\mathcal{K}^t$ with eigenvalues $\lambda_j^S(t) = \hat{\mu}_j^t$. Moreover, if matrices $\mathbf{A}(\omega)$ commute and are diagonalizable with the simple eigenvalues $\lambda_j(\omega)$ and corresponding left eigenvectors $\mathbf{w}_j$, $j = 1, \dots, d$, then

$$\hat{\mathbf{w}}_j^t = \mathbf{w}_j \quad \text{and} \quad \lambda_j^S(t) = \mathbb{E}\left[\mathrm{e}^{\int_0^t \lambda_j(\theta(s)\omega) ds} \right].$$

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Koopman mode decomposition of the full-state observable:

$$\mathcal{K}^t\mathbf{x} = \sum_{j=1}^{d} \lambda_j^S(t)\langle \mathbf{x}, \hat{\mathbf{w}}_j^t \rangle \hat{\mathbf{v}}_j^t. \tag{15}$$

Linear RDS generated by SDE

Consider the nonautonomous SDE of the form

$$dX_t = G(t, X_t)dt + \sigma(t, X_t)dW_t, \quad (16)$$

where $G : [0, T] \times \mathbb{R}^d \to \mathbb{R}^d$ and $\sigma : [0, T] \times \mathbb{R}^d \to \mathbb{R}^{d\times r}$ are L^2 measurable. The driving flow $\theta(t)$ is defined by "Wiener shifts":

$$\theta(t)\omega(\cdot) = \omega(t + \cdot) - \omega(t). \quad (17)$$

The solution $X_t(\omega)$ with the initial condition $X_{t_0}(\omega) = \mathbf{x}$ is formally defined in terms of Itô integral as

$$\varphi(t, t_0, \omega)\mathbf{x} = X_t(\omega) = X_{t_0}(\omega) + \int_{t_0}^{t} G(s, X_s(\omega))ds + \int_{t_0}^{t} \sigma(s, X_s(\omega))dW_s. \quad (18)$$

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Definition

The stochastic Koopman operator family $\mathcal{K}^{t,t_0}$ related to this RDS is defined by

$$\mathcal{K}^{t,t_0} f(\mathbf{x}) = \mathbb{E}[f(\varphi(t, t_0, \omega)\mathbf{x})]. \tag{19}$$

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In this more general setting with the two-parameter family of Koopman operators (19), the eigenfunctions $\phi^{t,t_0} : M \to \mathbb{C}$ and eigenvalues $\lambda^S(t, t_0)$ of the Koopman operator $\mathcal{K}^{t,t_0}$ defined on a finite-time interval satisfy

$$\mathcal{K}^{t,t_0}\phi^{t,t_0}(\mathbf{x}) = \lambda^S(t, t_0)\phi^{t,t_0}(\mathbf{x}). \tag{20}$$

Linear RDS generated by SDE

Proposition 3.

Let the linear SDE with **additive noise** be defined by

$$dX_t = \mathbf{A}(t)X_t dt + \sum_{i=1}^{r} b^i(t)dW_t^i, \quad \mathbf{A}(t) \in \mathbb{R}^{d\times d}, b^i(t) \in \mathbb{R}^d, i = 1, \ldots, r. \quad (21)$$

Assume that the fundamental matrix $\Phi(t, t_0)$ satisfying the matrix differential equation

$$\dot{\Phi} = \mathbf{A}(t)\Phi, \quad \Phi(t_0) = \mathbf{I} \quad (22)$$

is diagonalizable, with simple eigenvalues $\hat{\mu}_j^{t,t_0}$ and left eigenvectors $\hat{\mathbf{w}}_j^{t,t_0}$. Then $\phi_j^{t,t_0}(\mathbf{x}) = \langle \mathbf{x}, \hat{\mathbf{w}}_j^{t,t_0} \rangle$, $j = 1, \ldots, d$, are the eigenfunctions of $\mathcal{K}^{t,t_0}$ with the eigenvalues $\lambda_j^S(t, t_0) = \hat{\mu}_j^{t,t_0}$.
If matrices $\mathbf{A}(t)$ commute and are diagonalizable with the simple eigenvalues $\lambda_j(t)$ and corresponding left eigenvectors $\mathbf{w}_j$, $j = 1, \ldots, d$, then

$$\hat{\mathbf{w}}_j^{t,t_0} = \mathbf{w}_j \quad \text{and} \quad \lambda_j^S(t, t_0) = e^{\int_{t_0}^t \lambda_j(s)ds}. \quad (23)$$

Sketch of the proof.

Follows from $X_t(\omega) = \Phi(t, t_0)\left(\mathbf{x} + \sum_{i=1}^{r} \int_{t_0}^{t} \Phi^{-1}(s, t_0) b^i(s) dW_s^i\right)$.

Linear RDS generated by SDE

Proposition 4.

Let the linear SDE with **multiplicative noise** be defined by

$$dX_t = \mathbf{A}(t)X_t dt + \sum_{i=1}^{r} \mathbf{B}^i(t)X_t\, dW_t^i, \quad \mathbf{A}(t), \mathbf{B}^i(t) \in \mathbb{R}^{d\times d}, i = 1, \ldots, r. \tag{24}$$

Denote with $\Phi(t, t_0)$ the fundamental matrix satisfying the matrix SDE

$$d\Phi = \mathbf{A}\Phi\, dt + \sum_{i=1}^{r} \mathbf{B}^i(t)\Phi\, dW_t^i, \quad \Phi(t_0) = \mathbf{I} \tag{25}$$

and assume that $\hat{\Phi}(t, t_0) = \mathbb{E}\left[\Phi(t, t_0)\right]$ is diagonalizable, with simple eigenvalues $\hat{\mu}_j^{t,t_0}$ and left eigenvectors $\hat{\mathbf{w}}_j^{t,t_0}$. Then

$$\phi_j^{t,t_0}(\mathbf{x}) = \langle \mathbf{x}, \hat{\mathbf{w}}_j^{t,t_0} \rangle, \quad j = 1, \ldots, d, \tag{26}$$

are the eigenfunctions of $\mathcal{K}^{t,t_0}$ with the eigenvalues $\lambda_j^S(t, t_0) = \hat{\mu}_j^{t,t_0}$.

If the matrices $\mathbf{A}(t), \mathbf{B}^i(t)$, $i = 1, \ldots, r$ commute and if the matrices $\mathbf{A}(t)$ are diagonalizable with the simple eigenvalues $\lambda_j(t)$ and left eigenvectors $\mathbf{w}_j$, then

$$\hat{\mathbf{w}}_j^{t,t_0} = \mathbf{w}_j \quad \text{and} \quad \lambda_j^S(t, t_0) = e^{\int_{t_0}^{t} \lambda_j(s)ds}. \tag{27}$$

Sketch of the proof. Follows from $X_t(\omega) = \Phi(t, t_0)\mathbf{x}$.

Semigroup property of the Koopman operator family

Let suppose that the generated RDS is **homogeneous Markovian**, i.e., that for any $\mathbf{x} \in M$, $(\varphi(t,\omega)\mathbf{x})_{t\in\mathbb{T},\omega\in\Omega}$ is time-homogeneous Markov process.
This will happen in the following cases:

- discrete RDS with i.i.d. increments
- continuous time RDS generated by an autonomous SDE (8)

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Let $\mathcal{F}_t^{\mathbf{x},\omega} = \sigma(\varphi(s,\omega)\mathbf{x}, \theta(s)(\omega), 0 \le s \le t)$ be σ-algebras induced by a solution and a driving system. Moreover, assume that $\varphi(t,\cdot)$ and $\theta(t)(\cdot)$ are independent for each $t \in \mathbb{T}$.
The **Markov property** implies that for every $s \le t$ and every random variable Y, measurable with respect to filtration $\mathcal{F}_t^{\mathbf{x},\omega}$,

$$\mathbb{E}[Y|\mathcal{F}_s^{\mathbf{x},\omega}] = \mathbb{E}[Y|\varphi(s,\omega)\mathbf{x}]. \tag{28}$$

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Proposition 5.

If RDS is time-homogeneous Markovian, the stochastic Koopman operator family satisfies the **semigroup** property, i.e.

$$\mathcal{K}^{t+s} = \mathcal{K}^s \circ \mathcal{K}^t.$$

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Koopman operator semigroup for discrete time RDS

Let the one step map be: $T(\omega, \cdot) = T_0(\pi(\omega), \cdot), \pi(\omega) = \omega_0$, so that

$$\varphi(n, \omega) = T_0(\pi(\psi^{n-1}(\omega)), \cdot) \circ \cdots \circ T_0(\pi(\psi(\omega)), \cdot) \circ T_0(\pi(\omega), \cdot), \quad n \geq 1.$$

If ω is i.i.d. stochastic process, $\{(\varphi(n, \omega)\mathbf{x})_{t \in \mathbb{T}, \omega \in \Omega}, \mathbf{x} \in M\}$ is homogeneous Markov process realized on M and

$$\mathcal{K}^n = (\mathcal{K}^1)^n.$$

We call $\mathcal{K}^S = \mathcal{K}^1$ the **generator** of the Koopman semigroup.

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Example: A perturbed rotation on circle

Suppose that a driving flow is defined by shift transformations:

$$\theta(t)\omega(\cdot) = \omega(\cdot + t).$$

The one-step map $T : \Omega \times S^1 \to S^1$ is defined by

$$T(\omega,x) = x + \vartheta + \pi(\omega), \quad \pi(\omega) = \omega_0, \tag{29}$$

$\vartheta \in S^1 \setminus Q$, $(\omega_i)_{i\in\mathbb{Z}}$ i.i.d random variables $\sim U[-\delta/2,\delta/2]$, $\delta > 0$.

- $\phi_j(x) = \exp(i2\pi jx)$ and $\lambda_j^S = \dfrac{\sin(j\pi\delta)}{j\pi\delta}\exp(i2\pi j\vartheta)$.
- $f : L^2(S^1) \to \mathbb{C}$: $\mathcal{K}^n f(x) = \sum_{j\in\mathbb{Z}} c_j \left(\dfrac{\sin(j\pi\delta)}{j\pi\delta}\right)^n \exp(i2\pi jn\vartheta)\exp(i2\pi jx)$.

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Example: A rotation on circle

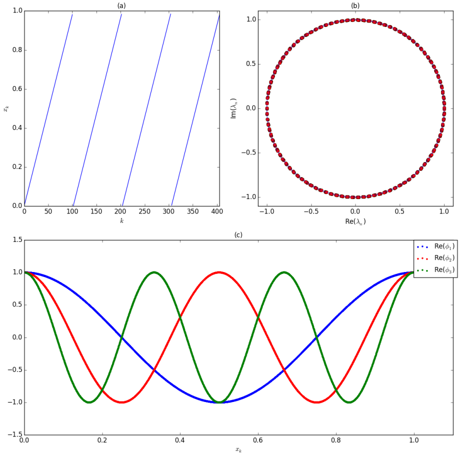

Figure: Rotation on circle, $\vartheta = \pi/320$ - deterministic case: (a) solution; (b) eigenvalues; (c) real part of eigenfunctions.

Example: A perturbed rotation on circle

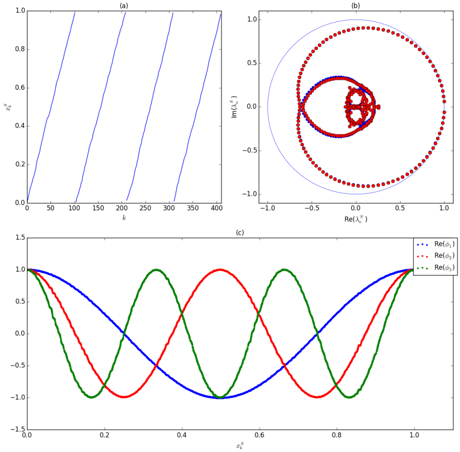

Figure: Rotation on circle, $\vartheta = \pi/320$, $\delta = 0.01$ - stochastic case: (a) solution; (b) eigenvalues; (c) real part of eigenfunctions.

Koopman operator semigroup for continous time RDS

The action of the **generator** of the stochastic Koopman semigroup $(\mathcal{K}^t)_{t\in\mathbb{T}}$ is given by

$$\mathcal{K}^S f(\mathbf{x}) = \lim_{t\to 0+} \frac{\mathcal{K}^t f(\mathbf{x}) - f(\mathbf{x})}{t}. \tag{30}$$

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Koopman operator semigroup for continous time RDS

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Proposition 6. - **RDS generated by RDE**

If the solution of RDE $\dot{\mathbf{x}} = F(\theta(t)\omega, \mathbf{x})$ is differentiable with respect to t and if $(\mathcal{K}^t)_{t\in\mathbb{T}}$ is a semigroup, for $f \in C_b^1(\mathbb{R}^d)$:

$$\mathcal{K}^S f(\mathbf{x}) = \mathbb{E}\left[F(\omega, \mathbf{x})\right] \cdot \nabla f(\mathbf{x}). \tag{31}$$

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Proposition 7. - **RDS generated by SDE**

If the RDS generated by SDE $dX_t = G(X_t)dt + \sigma(X_t)dW_t$, $(\mathcal{K}^t)_{t\in\mathbb{T}}$ is a semigroup. For $f \in C_b^2(\mathbb{R}^d)$

$$\mathcal{K}^S f(\mathbf{x}) = G(\mathbf{x})\nabla f(\mathbf{x}) + \frac{1}{2}\mathrm{Tr}\left(\sigma(\mathbf{x})(\nabla^2 f(\mathbf{x}))\sigma(\mathbf{x})^T\right). \tag{32}$$

Let $\phi \in C_b^2(\mathbb{R}^d)$ be an eigenfunction of $\mathcal{K}^S$ with the eigenvalue λ. Then

$$d\phi(X_t) = \lambda\phi(X_t)dt + \nabla\phi(X_t)\sigma(X_t)dW_t \qquad \text{and} \tag{33}$$

$$\mathcal{K}^t\phi(\mathbf{x}) = e^{\lambda t}\phi(\mathbf{x}). \tag{34}$$

The application of DMD algorithms on RDS

Different approaches are used: **standard** DMD approach using snapshot pairs and **sHankel** DMD applied on stochastic Hankel matrix

- $\mathbf{f} = (f_1, \ldots, f_n)^T : M \to \mathbb{C}^n$ - vector valued observable
- $\mathbf{f}^k(\omega, \mathbf{x}) = \mathbf{f} \circ T^k(\omega, \mathbf{x}), k = 0, 1, 2, \ldots$

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- Define

$$\mathbf{X}_m = \begin{pmatrix} \mathbf{f}^0(\mathbf{x}_1) & \mathbf{f}^0(\mathbf{x}_2) & \ldots & \mathbf{f}^0(\mathbf{x}_m) \end{pmatrix}, \ \mathbf{Y}_m = \begin{pmatrix} \mathbf{f}^k(\mathbf{x}_1) & \mathbf{f}^k(\mathbf{x}_2) & \ldots & \mathbf{f}^k(\mathbf{x}_m) \end{pmatrix}.$$

or

$$\mathbf{X}_m = \begin{pmatrix} \mathbf{f}^0(\mathbf{x}_0) & \mathbf{f}^1(\mathbf{x}_0) & \ldots & \mathbf{f}^{m-1}(\mathbf{x}_0) \end{pmatrix}, \ \mathbf{Y}_m = \begin{pmatrix} \mathbf{f}^1(\mathbf{x}_0) & \mathbf{f}^2(\mathbf{x}_0) & \ldots & \mathbf{f}^m(\mathbf{x}_0) \end{pmatrix}.$$

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- **Output:** $(\lambda_i, \mathbf{v}_i)$ obtained from Rayleigh quotient of $\mathbb{K}$ with respect to $\mathbf{X}_m$ where $\mathbb{K}$ is the matrix representation of the projection of the stochastic Koopman operator (or its generator) satisfying

$$\mathbf{Y}_m = \mathbb{K}\mathbf{X}_m \approx \mathbb{K}\mathbf{U}_k \boldsymbol{\Sigma}_k \mathbf{V}_k^*, \quad \text{where} \quad \mathbf{X}_m = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^*. \tag{35}$$

$\rightarrow$ approximations of Koopman eigenvalues and eigenvectors

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DMD algorithms on RDS

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Schmid, P.J., Dynamic mode decomposition of numerical and experimental data, J. Fluid Mech., 656(1) (2010), pp. 5-28
basic algorithm

Tu, J. H., Rowley, C. W., Luchtenburg, D. M., Brunton, S. L., Kutz, J. N., On dynamic mode decomposition: theory and applications, J. Comp. Dyn., 2(1) (2014), pp. 391-421
analysis, improvements and applications

Drmač, Z., Mezić, I., Mohr, R., Data driven modal decompositions: analysis and enhancements, SIAM J. Sci. Comput., 40(4) (2018), pp. A2253-A2285
enhancements: scaling, residual computation
$\eta = \|\mathbb{K}(\mathbf{U}_r\mathbf{w}) - \lambda(\mathbf{U}_r\mathbf{w})\|_2 = \|(\mathbf{Y}_m\mathbf{V}_r\Sigma_r^{-1})\mathbf{w} - \lambda(U_r\mathbf{w})\|_2,$

Takeishi, N., Kawahara, Y., Yairi, T., Subspace dynamic mode decomposition for stochastic Koopman analysis, Phys. Rev. E, 96:033310 (2017)
convergence of the algorithm in the stochastic framework

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Numerical approximations of the transfer operators for stochastic DS

Literature:

- Williams, M., Kevrekidis, I., Rowley, C., A data-driven approximation of the Koopman operator: extending dynamic mode decomposition, J. Nonlinear Sci., 25(6) (2015), pp. 1307-1346
  The eigenvalues and eigenfunctions of backward Kolmogorov equation are computed by EDMD algorithm
- Klus, S., Koltai, P., Schütte, C., On the numerical approximation of the Perron-Frobenius and Koopman operator, J. Comp. Dyn., 3(1) (2016), pp. 51-79
- Klus, S., Schütte, C., Towards tensor-based methods for the numerical approximation of the Perron-Frobenius and Koopman operator, J. Comp. Dyn., 3(2) (2016), pp. 139-161
  The spectral objects of the Koopman and Perron-Frobenious operator are computed using Ulam's method and EDMD algorithm
- Klus, S., Nüske, F., Koltai, P., Wu, H., Kevrekidis, I., Schütte, C., Noé, F., Data-driven model reduction and transfer operator approximation, J. Nonlinear Sci., 28(3) (2018), pp. 985-1010
  A review of different numerical techniques for approximating the spectral objects of different transfer operators

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Example: A perturbed rotation on circle

Observables: $f_j(x) = \cos(j2\pi x), g_j(x) = \sin(j2\pi x),\ j = 1, \dots, n_1,$

$$\mathbf{f} = (f_1, \dots, f_{n_1}, g_1, \dots, g_{n_1})^T.$$

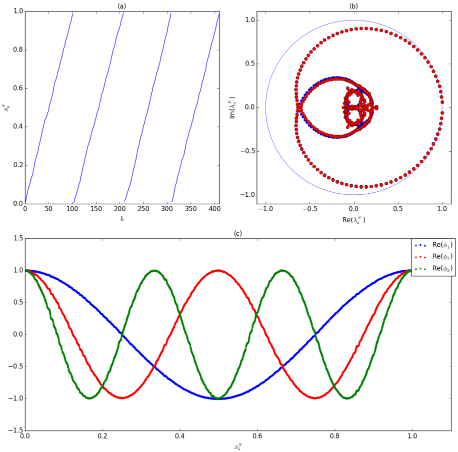

Figure: Rotation on circle, $\vartheta = \pi/320$, $\delta = 0.01$ - stochastic case: (a) solution; (b) eigenvalues; (c) real part of eigenfunctions.

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Example: Linear RDS generated by SDE

$$dX = \mu x\, dt + \sigma dW_t, \quad \mu < 0 \tag{36}$$

In deterministic case, i.e. when $\sigma = 0$, the Koopman eigenvalues are equal to

$$\lambda_n = n\mu,$$

and the related Koopman eigenfunctions are

$$\phi_n(x) = \frac{1}{n!} x^n.$$

In stochastic case, i.e. when $\sigma > 0$, the eigenvalues are same as in deterministic case, while the eigenfunctions are

$$\phi_n(x) = a_n H_n(\alpha x), \quad \alpha = \sqrt{\frac{|\mu|}{\sigma}}.$$

Here a_n denotes normalizing parameter and H_n are Hermite polynomials.

- Numerical approximations: DMD RRR algorithm
- Observable functions: $f_j(x) = x^j, j = 1, \dots, n$

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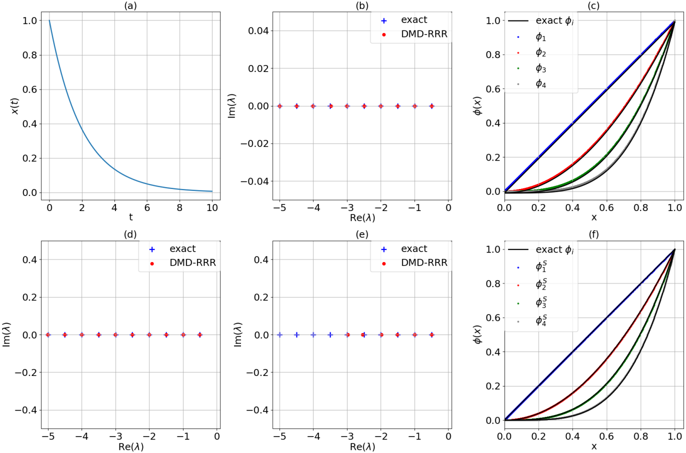

Figure: Linear scalar equation (36). Deterministic case $\mu = -0.5$: (a) solution; (b) Koopman eigenvalues; (c) Koopman eigenfunctions; Stochastic case $\mu = -0.5$ $\sigma = 0.001$: (d) stochastic Koopman eigenvalues - 1st approach: DMD RRR with values determined along trajectory; (e) stochastic Koopman eigenvalues - 2nd approach: DMD RRR with multiple initial conditions; (f) stochastic Koopman eigenfunctions.

Stochastic Hankel DMD algorithm (sHankel DMD)

$$\mathbf{f}_n(\omega, \mathbf{x}) = \left(f(\mathbf{x}), f(T(\omega, \mathbf{x})), \ldots, f(T^{n-1}(\omega, \mathbf{x})) \right)^T$$

$$\mathbf{f}_n^k = \mathbb{E}\left[\mathbf{f}_n(\theta(k)\omega, T^k(\omega, \mathbf{x})) \right] = \left(\mathcal{K}^k f(\mathbf{x}), \mathcal{K}^k f(T(\omega, \mathbf{x})), \ldots, \mathcal{K}^k f(T^{n-1}(\omega, \mathbf{x})) \right)^T$$

Observe: $\mathbf{f}_n^k$ are values of $\mathcal{K}^k f$ along the trajectory of length n starting at $\mathbf{x}$.

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Observe: $\mathbf{f}_n^k$ are values of $\mathcal{K}^k f$ along the trajectory of length n starting at $\mathbf{x}$.

The stochastic Hankel matrix of dimension $n \times m$: associated with the trajectories starting at $\mathbf{x} \in M$, generated by the map T is defined by

$$\mathbf{H}_{n\times m}(\omega, \mathbf{x}) = \begin{pmatrix} \mathbf{f}_n^0 & \mathbf{f}_n^1 & \ldots & \mathbf{f}_n^{m-1} \end{pmatrix} \tag{37}$$

$$= \begin{pmatrix} f(\mathbf{x}) & \mathcal{K}f(\mathbf{x}) & \ldots & \mathcal{K}^{m-1}f(\mathbf{x}) \\ f(T(\omega, \mathbf{x})) & \mathcal{K}f(T(\omega, \mathbf{x})) & \ldots & \mathcal{K}^{m-1}f(T(\omega, \mathbf{x})) \\ \vdots & \vdots & \ddots & \vdots \\ f(T^{n-1}(\omega, \mathbf{x})) & \mathcal{K}f(T^{n-1}(\omega, \mathbf{x})) & \ldots & \mathcal{K}^{m-1}f(T^{n-1}(\omega, \mathbf{x})) \end{pmatrix}.$$

Note that the columns of $\mathbf{H}_{n\times m}(\omega, \mathbf{x})$ are approximations of functions in the Krylov subspace

$$\mathbb{K}_m(\mathcal{K}, f) = \begin{pmatrix} f & \mathcal{K}f & \ldots & \mathcal{K}^{m-1}f \end{pmatrix} \tag{38}$$

obtained by sampling values of functions $\mathcal{K}^j f$, $j = 0, \ldots, m-1$ along the trajectory of length n starting at $\mathbf{x} \in M$.

Convergence of the stochastic Hankel DMD algorithm

Assume that the **skew-product DS** $\Theta(n)(\omega, x) = (\theta(n)\omega, T^n(\omega, x))$ generated by T and $\theta(t)$ is **ergodic** on $\Omega \times A$ w.r.t. some invariant measure ν.

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Birckhoff's ergodic theorem

For $f \in L^2(\Omega \times A; \nu)$:

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} f(\theta(k)\omega, T^k(\omega, \mathbf{x})) = \int_{\Omega\times A} f(\omega, x) d\nu, \quad \text{a. e. on } \Omega \times A. \tag{39}$$

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The measure ν is **invariant (resp. ergodic)** for RDS φ if it is invariant (resp. ergodic) for the skew product flow, i.e., if $\Theta(n)\nu = \nu$ and if $\pi_\Omega \nu = P$.

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If A is a Polish space: $d\nu(\omega, x) = d\mu_\omega(x) dP(\omega)$, i.e. for $f \in L^1(\nu)$

$$\int_{\Omega\times A} f d\nu = \int_\Omega \int_A f(\omega, x) d\mu_\omega(x) dP(\omega).$$

Convergence of the stochastic Hankel DMD algorithm

Assume that the **skew-product DS** $\Theta(n)(\omega, x) = (\theta(n)\omega, T^n(\omega, x))$ generated by T and $\theta(t)$ is **ergodic** on $\Omega \times A$ w.r.t. some invariant measure ν.

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$$\int_{\Omega\times A} f d\nu = \int_\Omega \int_A f(\omega, x) d\mu_\omega(x) dP(\omega).$$

Let suppose φ is ergodic with respect to the invariant measure ν and that $\mu = \pi_A \nu = \mathbb{E}_P(\nu) = \mathbb{E}_P(\mu_\omega)$.

Convergence of the stochastic Hankel DMD algorithm

Assume that the **skew-product DS** $\Theta(n)(\omega, x) = (\theta(n)\omega, T^n(\omega, x))$ generated by T and $\theta(t)$ is **ergodic** on $\Omega \times A$ w.r.t. some invariant measure ν.

Birckhoff's ergodic theorem

For $f \in L^2(\Omega \times A; \nu)$:

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} f(\theta(k)\omega, T^k(\omega, \mathbf{x})) = \int_{\Omega\times A} f(\omega, x) d\nu, \quad \text{a. e. on } \Omega \times A. \tag{39}$$

The measure ν is **invariant (resp. ergodic)** for RDS φ if it is invariant (resp. ergodic) for the skew product flow, i.e., if $\Theta(n)\nu = \nu$ and if $\pi_\Omega \nu = P$.
If A is a Polish space: $d\nu(\omega, x) = d\mu_\omega(x) dP(\omega)$, i.e. for $f \in L^1(\nu)$

$$\int_{\Omega\times A} f d\nu = \int_\Omega \int_A f(\omega, x) d\mu_\omega(x) dP(\omega).$$

Let suppose φ is ergodic with respect to the invariant measure ν and that $\mu = \pi_A \nu = \mathbb{E}_P(\nu) = \mathbb{E}_P(\mu_\omega)$.

Consider the observables $f : A \to \mathbb{R}$, $f \in \mathcal{H} = L^2(A, \mu)$. It follows from (39):

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} f(T^k(\omega, \mathbf{x})) = \int_{\Omega\times A} f(x) d\nu = \int_\Omega \int_A f(x) d\mu_\omega(x) dP(\omega) = \int_A f d\mu. \tag{40}$$

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Proposition 8.

Suppose that the dynamics on the compact invariant set $A \subseteq M$ is given by the one step map $T(\omega, \cdot) : A \to A$ for each $\omega \in \Omega$ and that the associated discrete time RDS φ **is ergodic** with respect to the **invariant measure** ν. Assume additionally that the processes $\{\varphi(n, \omega)\mathbf{x}, \mathbf{x} \in A\}$ form a **Markov family**. Denote by μ the marginal measure $\mu = \mathbb{E}_{\mathbb{P}}(\nu)$ on A.
Let the Krylov subspace $\mathbb{K}_m(\mathcal{K}, f)$ span an ***r*-dimensional subspace** of the Hilbert space $\mathcal{H} = L^2(A, \mu)$, with $r < m$, invariant under the action of the stochastic Koopman operator. Then for almost every $\mathbf{x} \in A$, as $n \to \infty$, the eigenvalues and eigenfunctions obtained by applying DMD algorithm to the first $r + 1$ columns of the $n \times (m + 1)$ dimensional stochastic Hankel matrix, **converge** to the true eigenvalues and eigenfunctions of the stochastic Koopman operator.

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Sketch of the proof.

Arbabi, H. and Mezić, I., Ergodic theory, Dynamic Mode Decomposition and Computation of Spectral Properties of the Koopman operator, SIAM J. Appl. Dyn. Syst., 16(4) (2017), pp. 2096-2126

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Since $\mathbb{K}_m(\mathcal{K}, f)$ spans r-dimensional subspace of $\mathcal{H}$, invariant under the action of $\mathcal{K}$, its representation in the basis $\begin{pmatrix} f, & \mathcal{K}f, & \dots, & \mathcal{K}^{r-1}f \end{pmatrix}$ is

$$\mathbf{C} = \begin{pmatrix} 0 & 0 & \dots & 0 & c_0 \\ 1 & 0 & \dots & 0 & c_1 \\ 0 & 1 & \dots & 0 & c_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & c_{r-1} \end{pmatrix} \quad \text{companion matrix} \tag{41}$$

The vector $\mathbf{c} = \begin{pmatrix} c_0 & c_1 & \dots & c_{r-1} \end{pmatrix}^T$ is equal to:

$$\mathbf{c} = \mathbf{G}^{-1} \begin{pmatrix} < f, \mathcal{K}^r f >_{\mathcal{H}}, & < \mathcal{K}^1, \mathcal{K}^r f >_{\mathcal{H}}, & \dots, & < \mathcal{K}^{r-1} f, \mathcal{K}^r f >_{\mathcal{H}} \end{pmatrix}^T. \tag{42}$$

where $\mathbf{G} = (G_{ij})_{i,j=1}^r$ and $G_{ij} =< \mathcal{K}^{i-1}, \mathcal{K}^{j-1} f >_{\mathcal{H}}$.

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where $\mathbf{G} = (G_{ij})_{i,j=1}^r$ and $G_{ij} =< \mathcal{K}^{i-1}, \mathcal{K}^{j-1} f >_{\mathcal{H}}$.

For $f, g \in \mathcal{H}$, let denote by $< \mathbf{f}_n(\omega, \mathbf{x}), \mathbf{g}_n(\omega, \mathbf{x}) >$ the data-driven inner product. We have

$$\lim_{n\to\infty} \frac{1}{n} < \mathbf{f}_n(\omega, \mathbf{x}), \mathbf{g}_n(\omega, \mathbf{x}) >= \lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} f(T^k(\omega, \mathbf{x}))\, g^*(T^k(\omega, \mathbf{x}))$$

$$= \lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} f\, g^* \left(T^k(\omega, \mathbf{x}) \right) = \int_A f\, g^*\, d\mu =< f, g >_{\mathcal{H}} . \tag{43}$$

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Convergence of the stochastic Hankel DMD algorithm

Consider the stochastic Hankel matrix $\mathbf{H}_{n\times(r+1)}(\omega,\mathbf{x})$ of dimension $n\times(r+1)$ along a trajectory starting at $\mathbf{x}$ and the companion matrix algorithm [Arbabi, Mezić 2017; Drmač 2018] applied to

$$\mathbf{X}_r = \left(\mathbf{f}_n^0(\mathbf{x})\ \mathbf{f}_n^1(\mathbf{x})\ \ldots\ \mathbf{f}_n^{r-1}(\mathbf{x})\right) \text{ and } \mathbf{Y}_r = \left(\mathbf{f}_n^1(\mathbf{x})\ \mathbf{f}_n^2(\mathbf{x})\ \ldots\ \mathbf{f}_n^{r}(\mathbf{x})\right).$$

Then numerical companion matrix solves

$$\tilde{\mathbf{C}} = \arg\min_{\mathbf{B}\in\mathbb{C}^{r\times r}} \|\mathbf{Y}_r - \mathbf{X}_r\mathbf{B}\|.$$

Since $\mathbf{X}_r$ has a full column rank, $\mathbf{X}_r^\dagger = (\mathbf{X}_r^*\mathbf{X}_r)^{-1}\mathbf{X}_r^*$, thus

$$\begin{aligned}\tilde{\mathbf{C}} &= \mathbf{X}_r^\dagger\mathbf{Y}_r = (\mathbf{X}_r^*\mathbf{X}_r)^{-1}\mathbf{X}_r^*\mathbf{Y}_r \\ &= \left(\frac{1}{n}\mathbf{X}_r^*\mathbf{X}_r\right)^{-1}\left(\frac{1}{n}\mathbf{X}_r^*\mathbf{Y}_r\right) = \tilde{\mathbf{G}}^{-1}\left(\frac{1}{n}\mathbf{Y}_r\mathbf{X}_r^*\right).\end{aligned} \tag{44}$$

Here $\tilde{\mathbf{G}} = (\tilde{G}_{ij}(\omega,\mathbf{x}))_{i,j=1}^r$ and

$$\begin{aligned}\tilde{G}_{ij}(\omega,\mathbf{x}) &= \tfrac{1}{n} < \mathbf{f}_n^{i-1}(\mathbf{x}), \mathbf{f}_n^{j-1}(\mathbf{x}) >= \frac{1}{n}\sum_{k=0}^{n-1}\mathcal{K}^{i-1}f(T^k(\omega,\mathbf{x}))\mathcal{K}^{j-1}f^*(T^k(\omega,\mathbf{x})) \\ &= \frac{1}{n}\sum_{k=0}^{n-1}(\mathcal{K}^{i-1}f)(\mathcal{K}^{j-1}f^*)(T^k(\omega,\mathbf{x})),\ i,j=1,\ldots,r.\end{aligned} \tag{45}$$

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From (44) we get that the elements in the last column of $\tilde{\mathbf{C}}$ are equal to

$$\tilde{\mathbf{c}} = \tilde{\mathbf{G}}^{-1}\frac{1}{n}\left(< \mathbf{f}_n^0(\mathbf{x}), \mathbf{f}_n^r(\mathbf{x}) >, \; < \mathbf{f}_n^1(\mathbf{x}), \mathbf{f}_n^r(\mathbf{x}) >, \; \ldots, \; < \mathbf{f}_n^{r-1}(\mathbf{x}), \mathbf{f}_n^r(\mathbf{x}) >\right)^T. \tag{46}$$

Now, by using (43), we conclude that

$$\lim_{n\to\infty} \tilde{G}_{ij}(\omega, \mathbf{x}) = < \mathcal{K}^{i-1}f, \mathcal{K}^{j-1}f >_{\mathcal{H}}, \quad i, j = 1, \ldots, r \tag{47}$$

and

$$\lim_{n\to\infty} < \mathbf{f}_n^{j-1}(\mathbf{x}), \mathbf{f}_n^r(\mathbf{x}) > = < \mathcal{K}^{j-1}f, \mathcal{K}^r f >_{\mathcal{H}} \quad j = 1, \ldots, r, \quad \text{for a.e. } \mathbf{x} \tag{48}$$

$$\Longrightarrow \tilde{\mathbf{C}} \xrightarrow{n\to\infty} \mathbf{C}$$

As proved in [Drmač 2018], the eigenvalues and eigenvectors provided by DMD RRR algorithm are obtained from the eigenvalues and eigenvectors of the matrix that is similar to the companion matrix $\tilde{\mathbf{C}}$. □

Example: Stuart-Landau equations

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The deterministic case:

$$\begin{aligned} dr &= (\delta r - r^3)dt \\ d\theta &= (\gamma - \beta r^2)dt. \end{aligned} \tag{49}$$

For $\delta > 0$ the system has the limit cycle $\Gamma : r = \sqrt{\delta}$ with the base frequency $\omega_0 = \gamma - \beta\delta$ and eigenvalues $\lambda_{ln} = -2l\delta + in\omega_0, l \in \mathbb{N}, n \in \mathbb{Z}$.

The stochastic case:

$$\begin{aligned} dr &= (\delta r - r^3 + \frac{\epsilon^2}{r})dt + \epsilon\, dW_r \\ d\theta &= (\gamma - \beta r^2)dt + \frac{\epsilon}{r}\, dW_\theta, \end{aligned} \tag{50}$$

where W_r and W_θ satisfy SDE system

$$\begin{aligned} dW_r &= \cos\theta dW_x + \sin\theta dW_y \\ dW_\theta &= -\sin\theta dW_x + \cos\theta dW_y, \end{aligned}$$

and dW_x and dW_y are independent Wiener processes. For small noise and $\delta > 0$ the system has the stable limit cycle Γ and the eigenvalues are

$$\lambda_{ln} = \begin{cases} -\frac{n^2\epsilon^2(1+\beta^2)}{2\delta} + in\omega_0 + \mathcal{O}(\epsilon^4), l = 0 \\ -2l\delta + in\omega_0 + \mathcal{O}(\epsilon^2), l > 0 \end{cases}. \tag{51}$$

(Tantet et. al., ArXiv 2017)

Example: Stuart-Landau equations

Observable: $f(r,\theta) = \sum^{K} \mathrm{e}^{\pm ik(\theta - \beta \log(r/\delta))}$

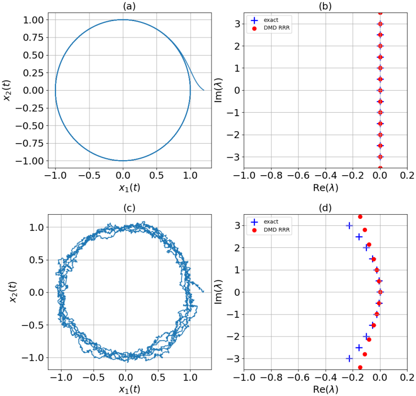

Figure: $\delta = 0.5, \beta = 1, \gamma = 1$. Deterministic case: (a) solution; (b) Koopman eigenvalues. Stochastic case: (c) solution; (d) stochastic Koopman eigenvalues. Algorithm: **sHankel-DMD**; The threshold for the residuals: 0.001.

Example: Noisy Van der Pol oscillator

$$dX_1 = X_2 dt \tag{52}$$

$$dX_2 = \left(\mu(1 - X_1^2)X_2 - X_1\right) dt + \sqrt{2\varepsilon} dW_t \tag{53}$$

Deterministic case: $\mu = 0.3$, $\varepsilon = 0$

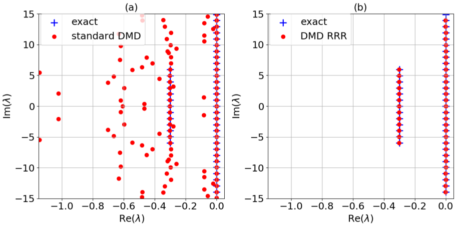

Figure: (a) eigenvalues obtained by using standard DMD algorithm; (b) eigenvalues obtained by using **DMD-RRR algorithm**; The threshold for the residuals: 10^{-2}.

Example: Noisy Van der Pol oscillator

Observable: $f(X_1, X_2) = X_1 + X_2 + \sqrt{X_1^2 + X_2^2}$

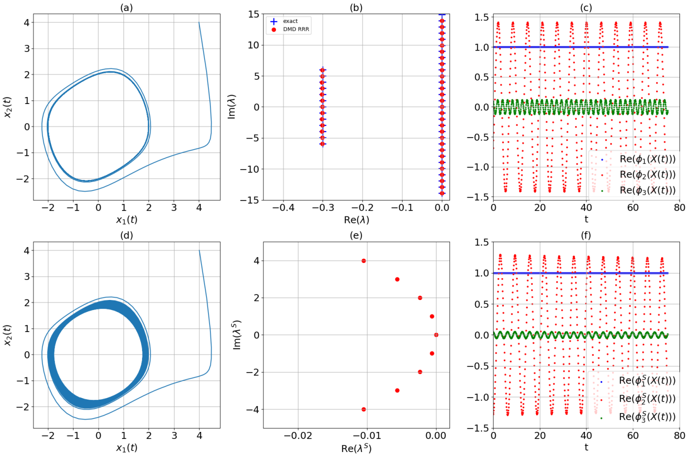

Figure: Deterministic case: (a) solution; (b) Koopman eigenvalues; (c) Koopman eigenfunctions along trajectories. Stochastic case $\epsilon = 0.005$: (d) solution; (e) stochastic Koopman eigenvalues; (f) stochastic Koopman eigenfunctions along trajectories. Algorithm: **sHankel-DMD**; The threshold for the residuals: 0.001.

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Example: Noisy Lotka-Volterra predator-prey system

$$dX_1 = (a_1 - b_1 X_2 - c_1 X_1)\, X_1 dt + \sigma_1 X_1 dW_t^1 \quad (54)$$
$$dX_2 = (-a_2 + b_2 X_1 - c_2 X_2)\, X_2 dt + \sigma_2 X_2 dW_t^2. \quad (55)$$

The model parameters $a_1, b_1, c_1, a_2, b_2, c_2 > 0$ depend on the particular species under consideration. The intensity of the noise is modeled by nonnegative parameters σ_1 and σ_2.

Deterministic case:

- $a_1 = 1.0$, $b_1 = 0.5$, $c_1 = 0.01$, $a_2 = 0.75$, $b_2 = 0.25$, $c_2 = 0.01$
- Equilibrium point: $(x_1^*, x_2^*) = (3.07754, 1.93845)$
- $\lambda_{1,2} = -0.02500799 \pm 0.863524i$
- System has exponentially stable fixed point and is conjugate to the linear one

Stochastic case:

- Stochastic case: $\sigma_1 = \sigma_2 = 0.05$
- Equilibrium point:$(\bar{x}_1^*, \bar{x}_2^*) = (3.08243, 1.93585)$
- $\lambda_{1,2}^S = -0.02509 \pm 0.86363i$

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Example: Noisy Lotka-Volterra predator-prey system

Observable: $f(X_1, X_2) = X_1 + X_2$

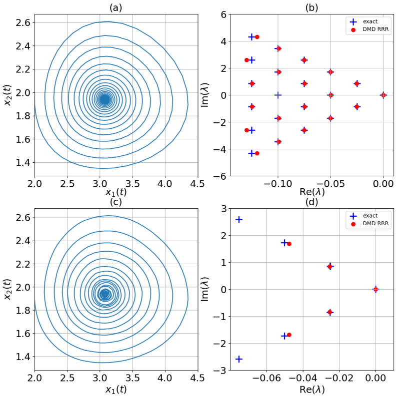

Figure: Deterministic case: (a) solution; (b) Koopman eigenvalues. Stochastic case: (a) solution; (b) stochastic Koopman eigenvalues - the exact eigenvalues refer to the determined eigenvalues $\lambda^S_{1,2}$ that we heuristically expect to be valid. Algorithm: **sHankel-DMD**; The threshold for the residuals: 0.001.

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What's next

- The application of the data-driven algorithms in nonautonomous systems with noise

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Thank you for your attention!

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