

MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG


DATA-DRIVEN MODELING OF
COMPLEX PHYSICAL SYSTEMS

Modeling Molecular Kinetics with Koopman Operators and Kernel-based Learning

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May 13, 2024

Metastable Systems

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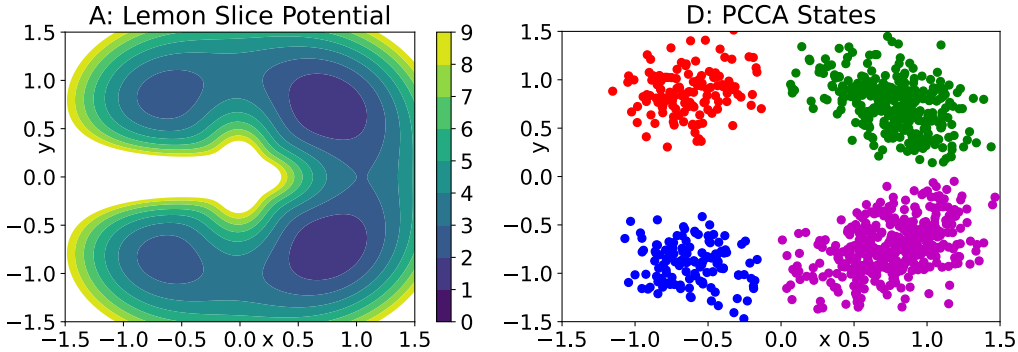
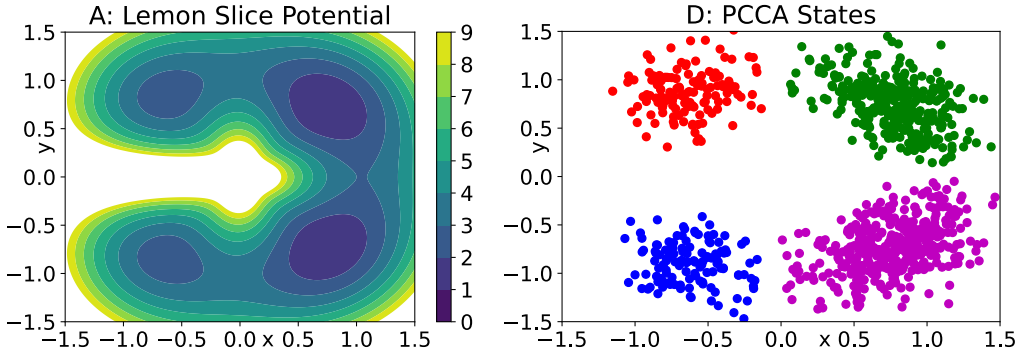


Metastable Systems

- **Goal:** Automatically analyse *metastable* systems based on simulation data.
- **Illustration**: Langevin Dynamics $dX_t = -\nabla V(X_t)\,\mathrm{d}t + \sqrt{2k_BT}\,\mathrm{d}W_t$.
- **Q:** What are metastable states? What are their transition rates? ...



Outline

1. The Koopman Operator and EDMD
2. Variational Approach
3. Kernel Methods and Random Features
4. Generator Learning

Extended Dynamic Mode Decomposition (EDMD)

Idea: Track dynamics of **observables** by means of a **linear map**:

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- Generate transformed snapshot matrices (x_k, y_k separated by **lag time** t):

$$\Psi(\mathbf{X}) = \left[\psi(x_1) \;\middle|\; \cdots \;\middle|\; \psi(x_m)\right], \quad \Psi(\mathbf{Y}) = \left[\psi(y_1) \;\middle|\; \cdots \;\middle|\; \psi(y_m)\right] \in \mathbb{R}^{n \times m}.$$

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- Solve **regression** problem (EDMD):

$$\begin{aligned}\mathbf{K}^t &= \operatorname{argmin}_{K \in \mathbb{R}^{n \times n}} \|\Psi(\mathbf{Y}) - \mathbf{K}^T \Psi(\mathbf{X})\|_F \\ &= (\Psi(\mathbf{X})^T \Psi(\mathbf{X}))^{-1} (\Psi(\mathbf{X})^T \Psi(\mathbf{Y})).\end{aligned}$$

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Why is this a good idea? Answer in two steps...

Williams et al, JNLS (2015)

1. Statistical Limit

- Infinite Data Limit:

$$\frac{1}{m}\left[\Psi(\mathbf{X})^T\Psi(\mathbf{X})\right]_{ij} \to \int_{\mathbb{X}} \psi_i(x)\,\psi_j(x)\,\mathrm{d}\rho(x),$$
$$\frac{1}{m}\left[\Psi(\mathbf{X})^T\Psi(\mathbf{Y})\right]_{ij} \to \int \psi_i(x)\,\mathbb{E}[\psi_j(\mathcal{X}_t)|\mathcal{X}_0 = x]\,\mathrm{d}\rho(x).$$

- EDMD learns a finite-dimensional projection of the **Koopman operator**:

$$\mathcal{K}^t\phi(x) = \mathbb{E}[\phi(\mathcal{X}_t)|\mathcal{X}_0 = x].$$

Reviews:
Klus, **FN**, et al, JNLS, 2018,
Mauroy, Suzuki, Mezic (eds), *Koopman operator in systems and control*, Springer 2020,
Berry, Giannakis, Harlim, Notices of the AMS, 2020,

Klus, **FN**, Peitz, et al, *Physica D*, 2020

2. Linear Dynamics

- Introduce the **generator** of the Koopman operator:

$$\mathcal{L}\psi = \lim_{t \to 0} \frac{1}{t} \left[\mathcal{K}^t - \mathrm{Id} \right] \psi.$$

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- Learning a linear model is justified.

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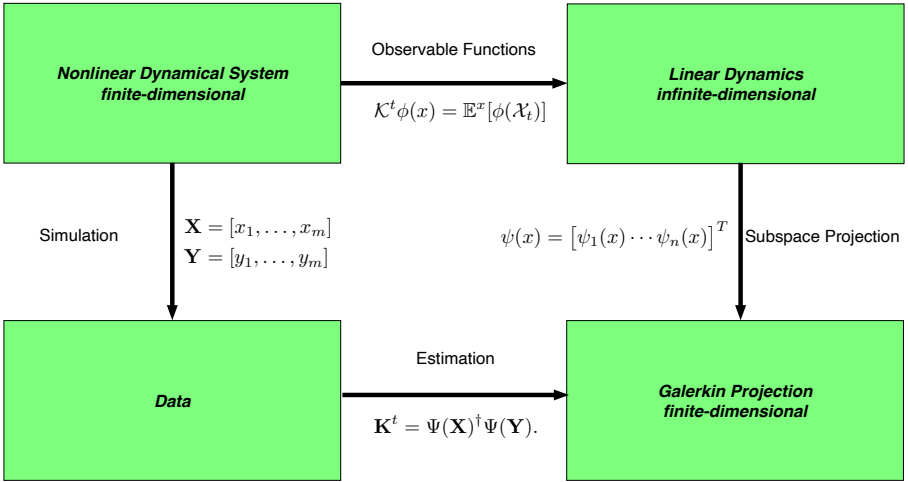
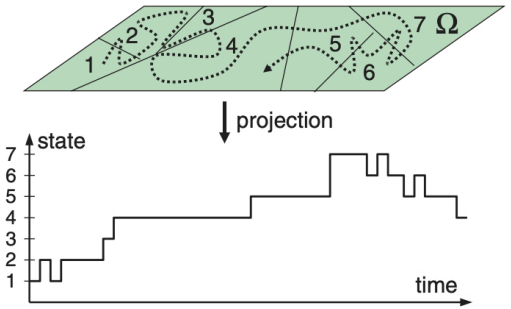
The Koopman Approach

Main Idea: **lifting** into an **infinite-dimensional** space where the dynamics become linear.



Special Case: MSM

Piece-wise constant basis functions lead to stochastic transition matrix:



$$\psi_i(x) = \begin{cases} 1 & x \in S_i \\ 0 & \text{else} \end{cases},$$

$$[\mathbf{K}^t]_{ij} = [\mathbf{T}^t]_{ij} \approx \mathbb{P}(X_t \in S_j \,|\, X_0 \in S_i).$$

Prinz et al, JCP (2011),

Bowman, Pande, Noé (eds.), Springer, 2014

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Variational Principle

- Metastability is encoded by *dominant eigenvalues* of the Koopman operator:

$$1 = \lambda_0(t) \geq \ldots \geq \lambda_M(t).$$

Davies, J. London. Math. Soc., 1982;
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- **Variational Characterization**:

$$\sum_{i=0}^{M} \left\langle \phi_i,\, \mathcal{K}^t \phi_i \right\rangle_\mu =: \mathcal{R}(\phi) \leq \sum_{i=0}^{M} \lambda_i(t) \tag{1}$$

$$\left\langle \phi_k,\, \phi_l \right\rangle_\mu = \delta_{kl}. \tag{2}$$

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- All quantities in (1-2) can be **estimated from simulation data**:

$$\left\langle \phi_i,\, \phi_i \right\rangle_\mu \approx \frac{1}{m} \sum_{k=1}^{m} \phi_i(x_k)\phi_i(x_k), \quad \left\langle \phi_i,\, \mathcal{K}^t \phi_i \right\rangle_\mu \approx \frac{1}{m} \sum_{k=1}^{m} \phi_i(x_k)\phi_i(y_k).$$

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Linear Variational Approach

- Applied to a finite-dimensional subspace $\left[\psi_1(x) \cdots \psi_n(x)\right]^T$., i.e. writing

$$\phi_i = \sum_{j=1}^{n} \mathbf{v}_{ji} \psi_j,$$

Noé and **FN**, SIAM MMS, 2013, **FN**, Keller, et al, JCTC, 2014
TICA: Pérez-Hernández et al, JCP, 2013,
Deep Learning: Mardt et al, Nat. Commun., 2018

Non-reversible systems: Wu and Noé, JNLS, 2020

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- leads to generalized eigenvalue problem for EDMD matrices:

$$\mathbf{C}^t \mathbf{V} = \mathbf{C}^0 \mathbf{V} \Lambda, \qquad \mathbf{C}^t = \frac{1}{m} \sum_{l=1}^{m} \psi(x_k) \otimes \psi(y_k), \qquad \mathbf{C}^0 = \sum_{l=1}^{m} \psi(x_k) \otimes \psi(x_k).$$

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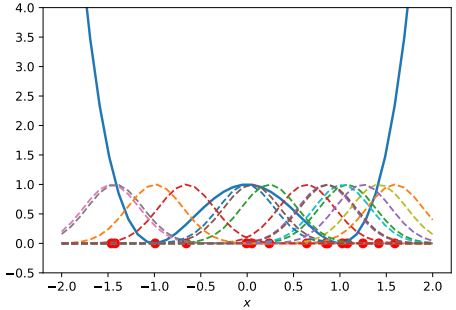
Data-driven Basis Sets

- Choosing a good basis set is hard.
- Idea: let the data define the basis.



- Typical choice: **radial basis functions**, e.g.

$$k(x_i, y) = \exp\left(-\frac{1}{2\sigma^2}\|x_i - y\|^2.\right)$$

EDMD and RKHS

- Kernel-based basis functions $k(x_i, \cdot)$ lead to matrices...

$$\mathbf{C}^0(r,s) = \mathbf{K}_X(r,s) = k(x_r, x_s), \qquad \mathbf{C}^t(r,s) = \mathbf{K}_X^t(r,s) = k(y_r, x_s).$$

- ... and the generalized eigenvalue problem:

$$\mathbf{K}_X^t \mathbf{w}_i = \lambda_i(t) \mathbf{K}_X \mathbf{w}_i.$$

- Both matrices scale with the data size $(m \times m)$.

Klus et al, JNLS, 2020; Klus, **FN**, and Hamzi, Entropy, 2020

RFF

- A translation invariant kernel $k(x, y) = \gamma(x - y)$ can be written as a superposition of complex plane waves:

$$k(x, y) = \mathbb{E}^{\omega \sim \rho} \left[e^{-i\omega^T (x-y)} \right] \approx \frac{1}{p} \sum_{u=1}^{p} e^{-i\omega_u^T x} \overline{e^{-i\omega_u^T y}},$$

where ρ is the **spectral measure** in frequency space (Bochner's theorem).

Rahimi and Recht, Advances in Neural Information Processing Systems, 2007

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  where ρ is the **spectral measure** in frequency space (Bochner's theorem).
- The spectral measure is known for most popular kernels (e.g. ρ is Gaussian for the Gaussian RBF kernel). Sampling from ρ is easy.

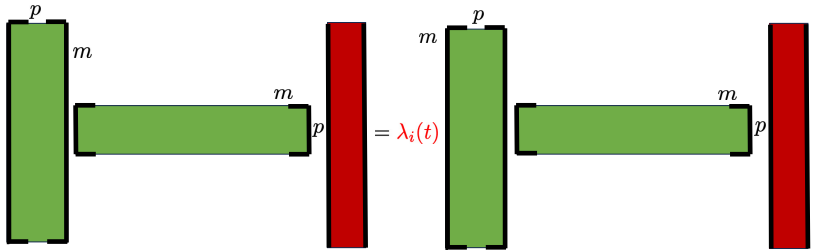
Rahimi and Recht, Advances in Neural Information Processing Systems, 2007

Low-Rank Kernel GEV

- **Low-rank** rep of kernel Koopman GEV:

$$\mathbf{K}_X = [k(x_r, x_s)]_{r,s} \approx \frac{1}{p}\left[\mathbf{M}\mathbf{M}^{\mathrm{H}}\right]_{r,s}, \qquad \mathbf{K}_X^t = [k(y_r, x_s)]_{r,s} \approx \frac{1}{p}\left[\mathbf{M}^t\mathbf{M}^{\mathrm{H}}\right]_{r,s},$$

$$\mathbf{M} = \left[e^{-ix_r^\top \omega_u}\right]_{r,u} \in \mathbb{C}^{m\times p}, \qquad \mathbf{M}^t = \left[e^{-iy_r^\top \omega_u}\right]_{r,u} \mathbb{C}^{m\times p}.$$



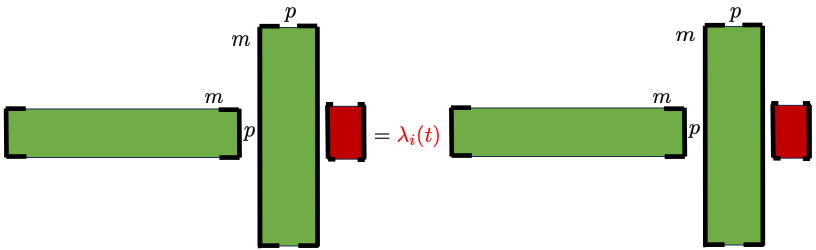
FN and Klus, JCP, 2023

Low-Rank Kernel GEV

- Non-zero eigenvalues can be obtained from dual problem

$$\mathbf{M}^{\mathrm{H}}\mathbf{M}^{t}\mathbf{v}_i = \hat{\lambda}_i(t)\mathbf{M}^{\mathrm{H}}\mathbf{M}\mathbf{v}_i,$$

which is of dimension $p \times p$.



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Algorithm

Algorithm 1 RFF-based Spectral Approximation of the Koopman Operator

Input: data matrices $\mathbf{X} = [x_1, \ldots, x_m] \in \mathbb{R}^{d \times m}$, $\mathbf{Y} = [y_1, \ldots, y_m] \in \mathbb{R}^{d \times m}$
kernel function k with spectral measure ρ,
number of features p, truncation rule for singular values.

Output: Approximate eigenpairs $(\hat{\lambda}_i(t), \hat{\psi}_i)$.

1: Draw p samples $\{\omega_u\}_{u=1}^{p}$ from the spectral measure ρ.
2: Form matrices $\mathbf{M} = \left[e^{-ix_r^\top \omega_u}\right]_{r,u}$, $\mathbf{M}^t = \left[e^{-iy_r^\top \omega_u}\right]_{r,u}$.
3: Compute SVD of $\mathbf{M}$, choose rank r according to truncation rule: $\mathbf{M} \approx \mathbf{U}\Sigma\mathbf{W}^{\mathrm{H}}$.
4: Form reduced matrix $\mathbf{R} = \mathbf{U}^{\mathrm{H}}\mathbf{M}^t\mathbf{W}\Sigma^{-1}$.
5: Compute eigenpairs of reduced problem $\mathbf{R}\mathbf{u}_i = \hat{\lambda}_i(t)\mathbf{u}_i$.
6: Transform to original RFF basis: $\mathbf{v}_i = \mathbf{W}\Sigma^{-1}\mathbf{u}_i$, $\hat{\psi}_i(x) = \mathbf{v}_i^{\mathrm{H}}\phi_{\mathrm{RFF}}(x)$.

Fip35

- Small protein, 35 amino acids.

Philipp, Schaller, Boshoff, Peitz, **FN**, Worthmann, arxiv 2402.02494, 2024

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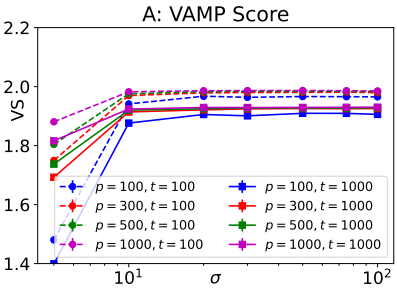
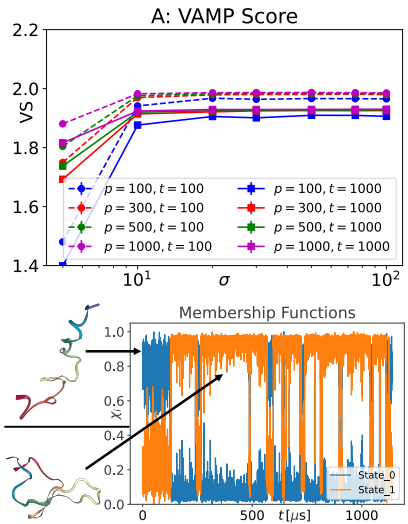


Philipp, Schaller, Boshoff, Peitz, **FN**, Worthmann, arxiv 2402.02494, 2024

Fip35

- Small protein, 35 amino acids.
- Use Gaussian kernel on 600 distances and angles.
- Tune Gaussian bandwidth and feature size p by variational approach.
- Compute leading 2 eigenvalues and eigenfunctions.
- Transform into membership functions indicating metastable states.

Philipp, Schaller, Boshoff, Peitz, **FN**, Worthmann, arxiv 2402.02494, 2024



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Generator Learning (gEDMD)

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- Learn a data-driven matrix model analogous to EDMD:

$$\Psi(\mathbf{X}) = \begin{bmatrix} \psi_1(x_1) & \dots & \psi_1(x_m) \\ \vdots & \ddots & \vdots \\ \psi_n(x_1) & \dots & \psi_n(x_m) \end{bmatrix}, \qquad \mathcal{L}\Psi(\mathbf{X}) = \begin{bmatrix} \mathcal{L}\psi_1(x_1) & \dots & \mathcal{L}\psi_1(x_m) \\ \vdots & \ddots & \vdots \\ \mathcal{L}\psi_n(x_1) & \dots & \mathcal{L}\psi_n(x_m) \end{bmatrix},$$

- matrix model:

$$\mathbf{L} = \left(\Psi(\mathbf{X})\Psi(\mathbf{X})^\top\right)^{-1}\left(\Psi(\mathbf{X})\mathcal{L}\Psi(\mathbf{X})^\top\right).$$

Coarse Grained Generator

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- Projected generator $\mathcal{L}^\xi = \mathcal{P}\mathcal{L}\mathcal{P}$ is **again the generator** of an **effective SDE** on $\mathbb{R}^m$.

$$d\mathcal{Z}_t = b^\xi(\mathcal{Z}_t)\,\mathrm{d}t + \sigma^\xi(\mathcal{Z}_t)\,\mathrm{d}W_t.$$

Legoll and Lelièvre, *Nonlinearity* (2010), Zhang, Hartmann, Schütte, *Faraday Disc.* (2016)

Learning the Reduced Generator

- Given a CG map ξ, choose basis functions **on CG space** $\psi_i = \psi_i(\xi(x))$.

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- We have the fundamental identity [1]

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- Therefore, gEDMD **simultaneously** provides a matrix approximation of $\mathcal{L}$ and $\mathcal{L}^\xi$. [2].

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Coarse Grained Equations

Learn effective SDE in two steps

FN, Boninsegna and Clementi, *JCP* (2019)

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- Obtain effective potential from thermodynamic models, e.g. force matching.

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- Obtain effective potential from thermodynamic models, e.g. force matching.
- Learn effective diffusion by matching it to CG generator models:

$$\left\langle \mathcal{L}_\theta^\xi \psi_i,\, f_j \right\rangle_\nu = -\frac{1}{2} \int \nabla\psi_i(z) \cdot A_\theta^\xi(z) \cdot \nabla f_j(z)\, \mathrm{d}\nu.$$

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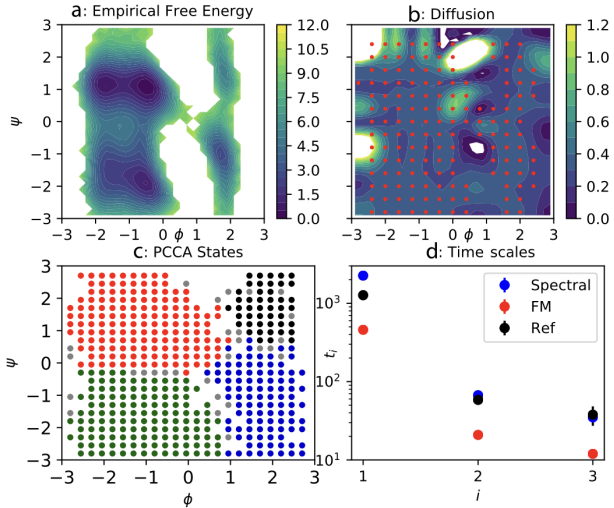
$$\left\langle \mathcal{L}_\theta^\xi \psi_i,\ f_j \right\rangle_\nu = -\frac{1}{2} \int \nabla\psi_i(z) \cdot A_\theta^\xi(z) \cdot \nabla f_j(z)\, \mathrm{d}\nu.$$

FN, Boninsegna and Clementi, *JCP* (2019)



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