

MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG


DATA-DRIVEN MODELING OF
COMPLEX PHYSICAL SYSTEMS

Dimensionality Reduction and Metastability Analysis using the Koopman Operator

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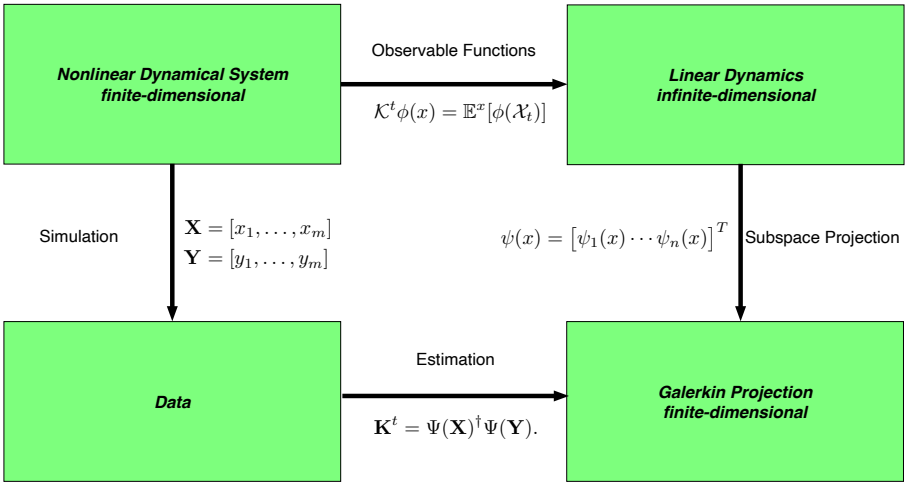
September 7, 2023

Outline

1. The Koopman Operator and EDMD
2. Variational Approach (VAC)
3. EDMD and Kernels
4. Random Fourier Features for EDMD

The Koopman Approach

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



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

$$\Psi(\mathbf{X}) = \begin{bmatrix}\psi(x_1) & | & \cdots & | & \psi(x_m)\end{bmatrix} \in \mathbb{R}^{n\times m},$$
$$\Psi(\mathbf{Y}) = \begin{bmatrix}\psi(y_1) & | & \cdots & | & \psi(y_m)\end{bmatrix} \in \mathbb{R}^{n\times m}.$$

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

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

Williams et al, *J. Nonlinear Sci.* (2015)

EDMD as a Statistical Method

- Assume x_k are **drawn from distribution** ρ:

$$\frac{1}{m}\left[\Psi(\mathbf{X})^T\Psi(\mathbf{X})\right]_{ij} = \frac{1}{m}\sum_{k=1}^{m}\psi_i(x_k)\psi_j(x_k)$$
$$\xrightarrow{m\to\infty} \mathbb{E}^{\mathcal{X}_0\sim\rho}[\psi_i(\mathcal{X}_0)\psi_j(\mathcal{X}_0)],$$

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- and similarly

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EDMD as a Galerkin Method

- Empirical **Gramian** in Hilbert space L^2_ρ:

$$\mathbb{E}^{\mathcal{X}_0\sim\rho}[\psi_i(\mathcal{X}_0)\psi_j(\mathcal{X}_0)] = \int_{\mathbb{X}} \psi_i(x)\,\psi_j(x)\,\mathrm{d}\rho(x) = \langle \psi_i,\, \psi_j \rangle_\rho\,,$$

- Empirical **Stiffness Matrix** in Hilbert space L^2_ρ:

$$\mathbb{E}^{\mathcal{X}_0\sim\rho}[\psi_i(\mathcal{X}_0)\psi_j(\mathcal{X}_t)] = \mathbb{E}^{x\sim\rho}[\psi_i(x)\,\mathbb{E}[\psi_j(\mathcal{X}_t)|\mathcal{X}_0 = x]\,].$$

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- Using the **Koopman operator**, EDMD becomes a Galerkin method:

$$\mathcal{K}^t\phi(x) = \mathbb{E}[\phi(\mathcal{X}_t)|\mathcal{X}_0 = x]$$
$$\Rightarrow \mathbb{E}^{\mathcal{X}_0\sim\rho}[\psi_i(\mathcal{X}_0)\psi_j(\mathcal{X}_t)] = \int_{\mathbb{X}} \psi_i(x)\,\mathcal{K}^t\psi_j(x)\,\mathrm{d}\rho(x) = \left\langle \psi_i,\, \mathcal{K}^t\psi_j \right\rangle_\rho.$$

Williams et al, *J. Nonlinear Sci.* (2015)

The Koopman Semigroup

- Koopman operators form a **semigroup**:

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

- Semigroup property gives rise to **infinitesimal generator**:

$$\mathcal{L} f = \lim_{t \to 0} \frac{1}{t} (\mathcal{K}^t - \mathrm{Id}) f.$$

- On the space of observables, the dynamics are linear:

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{K}^t \phi = \mathcal{L} \mathcal{K}^t \phi.$$

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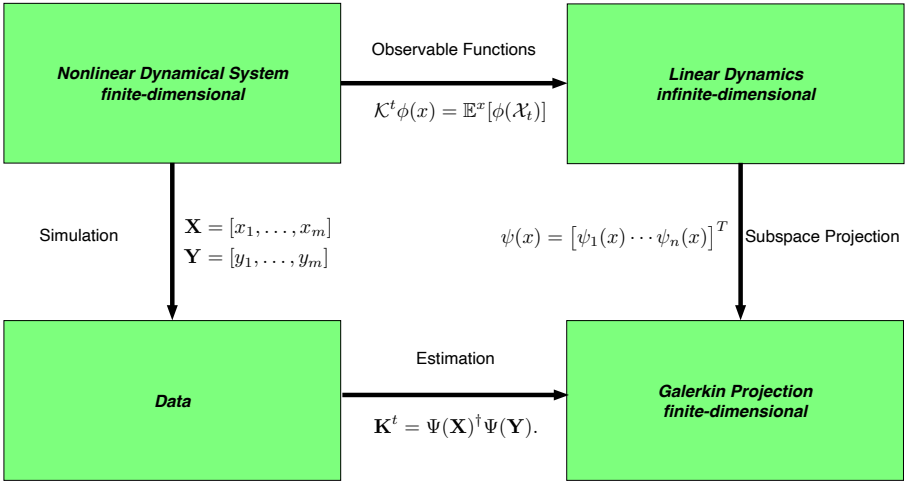

Summary

- Koopman framework uses a **lifting** into an **infinite-dimensional** space where the dynamics become **linear**.
- EDMD approximates a **Galerkin projection** of $\mathcal{K}^t$ in the **statistical limit**.
- EDMD matrix can be used to **forecast** expectations of ob system observables, potentially over **long timescales**.
- Applications in control, model reduction, metastability analysis, ...

Klus, **FN**, et al, *J. Nonlinear Sci.*, 2018,
Mauroy, Suzuki, Mezic (eds), *Koopman operator in systems and control*, Springer 2020,
Klus, **FN**, Peitz et al, *Physica D*, 2020,
Berry, Giannakis, Harlim, *Notices of the AMS*, 2020.

Outline

Variational Principle

- For **reversible** systems, Koopman operator $\mathcal{K}^t$ is **self-adjoint**.

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- **Rayleigh variational principle** (RVP) for dominant eigenvalues $1 = \lambda_0(t) \geq \ldots \geq \lambda_M(t)$:

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

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

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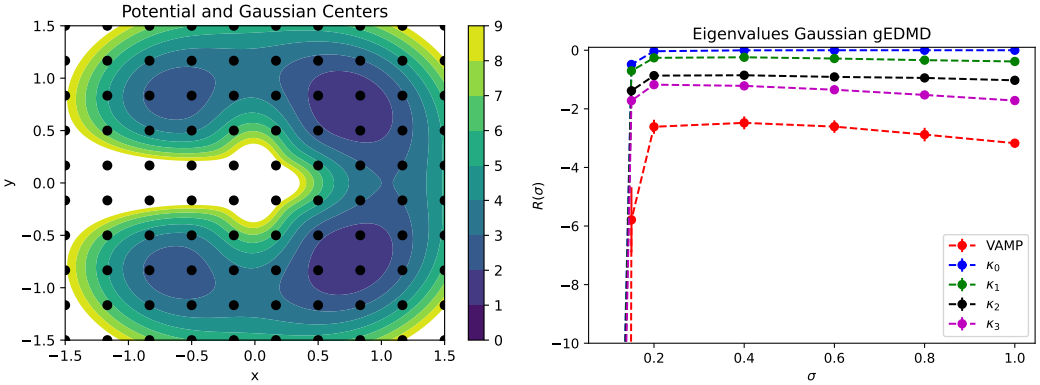
- $R(\psi)$ can be used as an **objective function**, subject to the constraint (2).
- All quantities in (1-2) can be **estimated from simulation data**:

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

Cross-Validation



Linear VAC: Noé and **FN**, *SIAM MMS*, 2013, **FN**, Keller, et al, *JCTC*, 2014,
TICA: Pérez-Hernández et al, *J. Chem. Phys.*, 2013, **Deep Learning**: Mardt et al, *Nat. Commun.*, 2018
Non-reversible systems: Wu and Noé, *J. Nonlinear Sci.*, 2020

Perspectives

- Learning from **short trajectories** and **renewal equations**,
  Noé, Schütte, et al, *PNAS* (2009)
  Cao, Huang, et al, *J. Chem. Phys.* 2020
- Models for the generator, **system identification**,
  Boninsegna, **FN**, Clementi, *J. Chem. Phys.* (2018)
  Klus, **FN**, Peitz, et al, *Physica D* (2020)
- Use Koopman models to **enhance exploration**,
  Hruska and Clementi, *J. Chem. Phys* (2018)
  Sidky, Chen, Ferguson, *Modern Physics*, 2020
  Shmilovich and Ferguson, *J Phys. Chem. A* (2023)
- **Error theory** based on concentration inequalities,
  Zhang and Zuazua, *Comptes Rendus Math.* (2022)
  FN et al, *J. Nonlinear Sci.* (2023)

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- Choosing a good basis set is hard.

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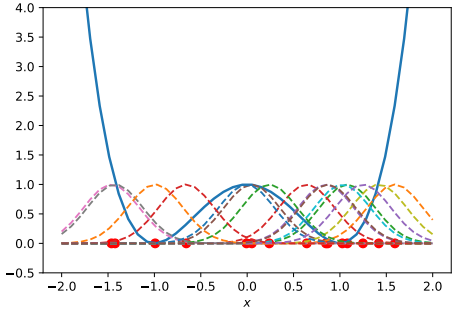

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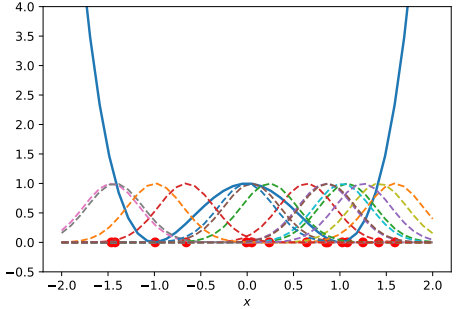

- Typical choice: **radial basis functions**, e.g.

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

RKHS

Theorem (Moore-Aronszajn, 1950)

Let $\mathbb{X}$ be a set and $k : \mathbb{X} \times \mathbb{X}$ be a continuous function such that

(*i*) $k(x, y) = k(y, x)$ *(symmetry)*

(*ii*) $\sum_{i,j=1}^{m} \alpha_i \alpha_j k(x_i, x_j) \geq 0$ *(positive definiteness).*

Then k generates a unique Hilbert space $\mathbb{H}$ of continuous functions such that

(*a*) $\mathbb{H} = \overline{\text{span}\{k(x, \cdot),\, x \in \mathbb{X}\}}$,

(*b*) $\langle f,\, k(x, \cdot)\rangle_{\mathbb{H}} = f(x) \quad \forall f \in \mathbb{H}$ *(reproducing property).*

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Facts:

- Gaussian RBF kernel is a valid kernel.
- Many popular kernels correspond to infinite-dimensional RKHSs.
- These RKHSs are dense in most L^2-spaces.

EDMD and RKHS

- Applying EDMD to kernel-based basis functions $k(x_i, \cdot)$ leads to matrices...

$$\mathbf{K}_{\mathbb{H}}^t = \mathbf{K}_X^{-1}\mathbf{K}_X^t, \qquad \mathbf{K}_X(r,s) = k(x_r, x_s), \qquad \mathbf{K}_X^t(r,s) = k(y_r, x_s).$$

- ... or to the generalized eigenvalue problem:

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

Klus et al, *J. Nonlinear Sci.*, 2020; Klus, **FN**, and Hamzi, *Entropy*, 2020

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- For infinite data, converges to cross-covariance operators:

$$\mathcal{K}_X f = \int_{\mathbb{X}} f(x)k(x,\cdot)\,\mathrm{d}\mu(x), \qquad \mathcal{K}_X^t f = \int_{\mathbb{X}} \mathcal{K}^t f(x)k(x,\cdot)\,\mathrm{d}\mu(x).$$

Klus et al, *J. Nonlinear Sci.*, 2020; Klus, **FN**, and Hamzi, *Entropy*, 2020

Outline

Motivation

- Recall kernelized eigenvalue problem:

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

- Kernel matrices are often low-rank; require **low-rank decomposition** of $\mathbf{K}_X$.
- Straightforward approach scales as $\mathcal{O}(m^3)$.
- Needs to be solved **many times** to accurately tune kernel parameters.
- Requires efficient low-rank approximation, e.g. Nyström methods, random linear algebra, random Fourier features,...

Intro RFF

- A translation invariant kernel with $k(x, x) = 1$ can be written as

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

  where ρ is the **spectral measure** in frequency space (Bochner's theorem).
- The spectral measure is known for most popular kernels, sampling from ρ is easy.

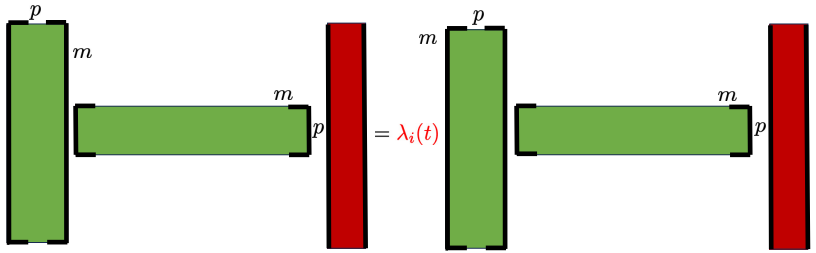
Rahimi and Recht, Advances in Neural Information Processing Systems, 2007

Low-Rank Kernel GEV

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

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

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



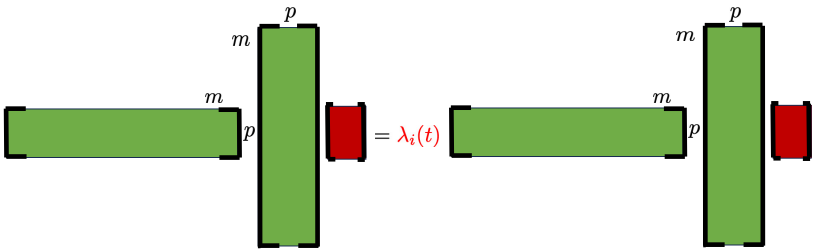
FN and Klus, J. Chem. Phys., 2023

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 $p \times p$.



FN and Klus, J. Chem. Phys., 2023

Low-Rank Kernel GEV

- The dual eigenvalue problem

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

  can be solved by operating only on $\mathbf{M}$, $\mathbf{M}^t$.
- If p is significantly smaller than m, cost is $\mathcal{O}(mp^2)$ instead of $\mathcal{O}(m^3)$.
- Dual GEV is the EDMD eigenvalue problem for a **randomized, complex-valued basis set** of plane waves:

$$\phi_{\mathrm{RFF}}(x) := \begin{bmatrix} \phi_1(x) \\ \vdots \\ \phi_p(x) \end{bmatrix} = \begin{bmatrix} e^{ix^\top \omega_1} \\ \vdots \\ e^{ix^\top \omega_p} \end{bmatrix}.$$

FN and Klus, J. Chem. Phys., 2023

NTL9

Small protein with 39 amino acids, use Gaussian kernel on 666 inter-residue distances, $m = 15.000$ data points in real space.

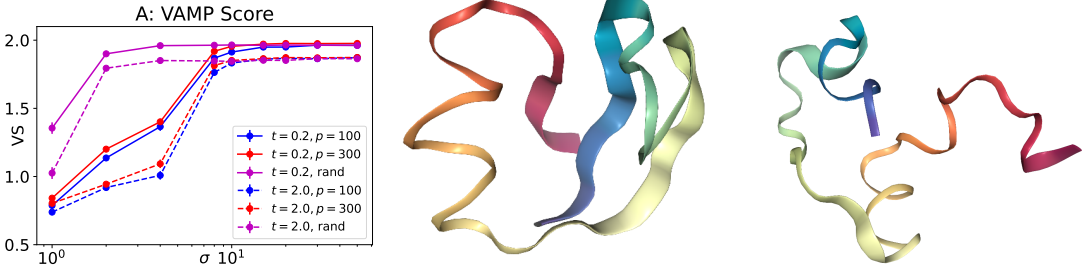


Figure: VAMP Score and Representatives of PCCA States for NTL9

FN and Klus, J. Chem. Phys., 2023

Conclusions

1. Koopman framework provides a linear view of dynamical systems, Galerkin projections can be learned consistently from simulation data.
2. Variational Score (VAMP) is a principled way of choosing model classes, especially for metastable systems.
3. Kernel Methods provide a powerful data-driven basis set with well-understood asymptotic properties.
4. Random Fourier features appear as a promising candidate for efficient low-rank approx. of resulting linear algebra problems.

Acknowledgments

Main Collaborators: Stefan Klus (Heriot-Watt U, Edinburgh), Sebastian Peitz (U Paderborn), Frank Noé (Freie U Berlin), Cecilia Clementi (Freie U Berlin)

References:

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