

MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG


DATA-DRIVEN MODELING OF
COMPLEX PHYSICAL SYSTEMS

Dynamically Consistent Coarse-Graining with Koopman Operators

Feliks Nüske

September 26, 2024

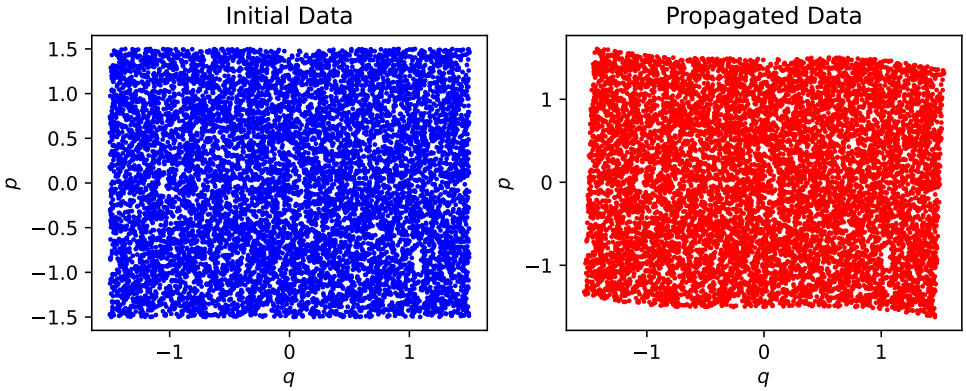
Outline

1. Koopman Models and Variational Approach

2. Dynamical Coarse Graining

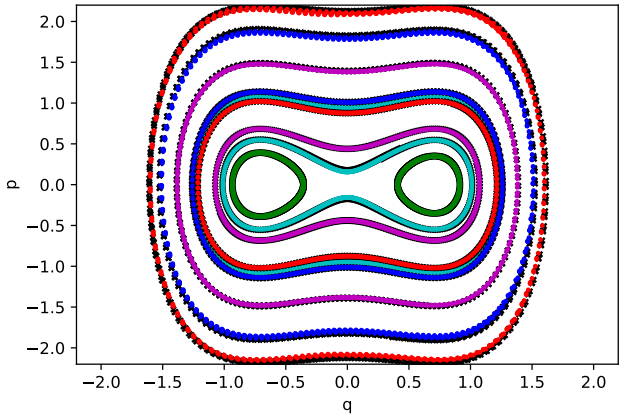
Motivation

Training Data for 2d Duffing Oscillator



Motivation

Forecasting with linear Koopman Model



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

Extended Dynamic Mode Decomposition (EDMD)

- Choose finitely many non-linear observables:

$$\psi(x) = \left[\psi_1(x) \cdots \psi_n(x)\right]^\top.$$

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

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

- Solve linear regression problem (EDMD):

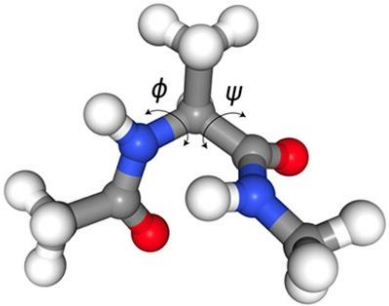
$$\begin{aligned}\mathbf{T}_t &= \operatorname{argmin}_{\mathbf{T}\in\mathbb{R}^{n\times n}} \|\Psi(\mathbf{Y}) - \mathbf{T}^\top\Psi(\mathbf{X})\|_F \\ &= (\Psi(\mathbf{X})^T\Psi(\mathbf{X}))^{-1}(\Psi(\mathbf{X})^T\Psi(\mathbf{Y})) = \hat{\mathbf{C}}_0^{-1}\hat{\mathbf{C}}_t^{-1}.\end{aligned}$$

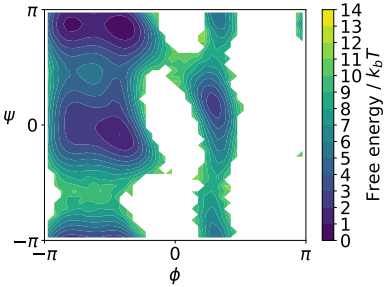
- Justified by Koopman theory for complete basis.

Williams et al, Journal of Nonlinear Science (2015)

Metastable Systems

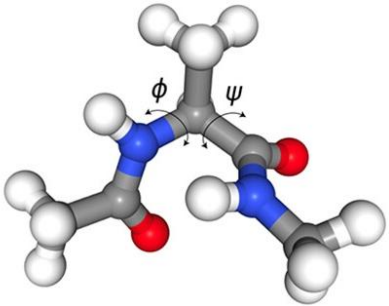
- **Goal:** Automatically analyse *metastable* systems based on simulation data (common in molecular systems, e.g. protein folding, ligand binding,...)

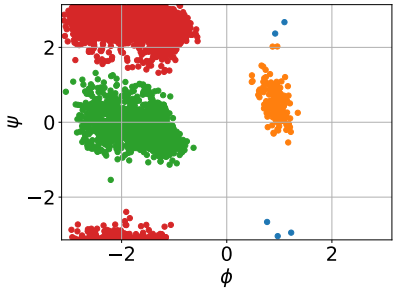




Metastable Systems

- **Goal:** Automatically analyse *metastable* systems based on simulation data (common in molecular systems, e.g. protein folding, ligand binding,...)
- **Q:** What are metastable states? What are their transition rates? ...





Linear Variational Approach

- Meta-stable states are encoded by *dominant eigenvectors* of Koopman matrix.
- Variational characterization for leading Koopman eigenvalues:

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

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

- Generalized eigenvalue problem for EDMD matrices:

$$\hat{\mathbf{C}}_t \mathbf{w}_i = \lambda_i(t) \hat{\mathbf{C}}_0 \mathbf{w}_i.$$

Noé and **FN**, SIAM MMS (2013),

FN, Keller, Pérez-Hernández, Mey, Noé, J. Chemical Theory Comput. (2014)

Application: Fip35

- Fast folding protein., 35 amino acids.

FN and Klus, J Chemical Physics (2023),

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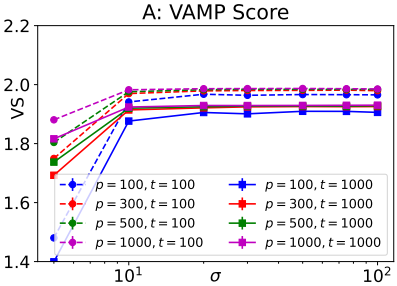
Application: Fip35

- Fast folding protein., 35 amino acids.
- Use Gaussian kernel on 600 distances and angles.
- Tune Gaussian bandwidth and random feature size by variational approach.



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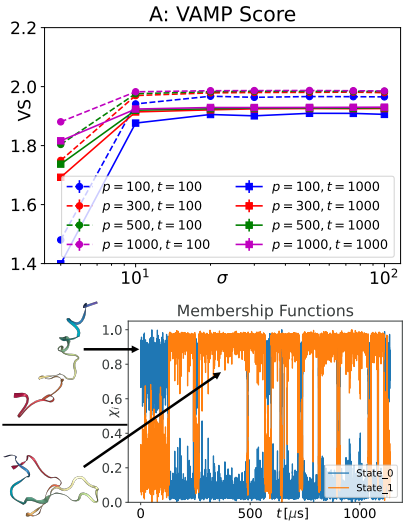
Application: Fip35

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



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1. Koopman Models and Variational Approach

2. Dynamical Coarse Graining

Coarse Grained Generator

- A **coarse graining (CG)** is a map to lower-dimensional space: $\xi : \mathbb{R}^d \mapsto \mathbb{R}^m$, $m \leq d$

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

Coarse Grained Generator

- A **coarse graining (CG)** is a map to lower-dimensional space: $\xi : \mathbb{R}^d \mapsto \mathbb{R}^m$, $m \leq d$
- Let $\mathcal{P}$ be the conditional expectation with respect to ξ:

$$\mathcal{P}\phi(z) = \frac{1}{\nu(z)}\mathbb{E}[\phi(x)|\xi(x) = z].$$

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

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

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- Ignores memory effects. Effective parameters must be *approximated / learned*.

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

Learning Coarse-Grained Dynamics

- Reversible SDEs can be parametrized by a potential and a diffusion field:

$$d\mathcal{Z}_t = \left[-a^{\xi}(\mathcal{Z}_t)\nabla F^{\xi}(\mathcal{Z}_t) + \nabla \cdot a^{\xi}(\mathcal{Z}_t)\right] \mathrm{d}t + \sigma^{\xi}(\mathcal{Z}_t)\,\mathrm{d}W_t.$$

Noid et al, J. Chemical Physics, (2008),

Nateghi and **FN**, arxiv 2409.16396 (2024)

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- Effective potential can be learned using *force matching*.

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- Effective potential can be learned using *force matching*.
- Our method: Effective diffusion can be learned by *diffusion learning*.

Noid et al, J. Chemical Physics, (2008),

Nateghi and **FN**, arxiv 2409.16396 (2024)

Diffusion Learning

- Generators for full and CG system are related:

$$\langle \psi_i \circ \xi,\, \mathcal{L}(\psi_j \circ \xi) \rangle_\mu = \left\langle \psi_i,\, \mathcal{L}^\xi \psi_j \right\rangle_\nu .$$

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- Data of the full system can be used to learn a model $\mathbf{L}_{\mathrm{ref}}$ for the full generator.

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- Matrix elements of effective generator are parametrized by effective diffusion:

$$\left\langle \psi_i,\, \mathcal{L}^\xi \psi_j \right\rangle_\nu = -\frac{1}{2} \int_{\mathbb{R}^m} \nabla_z \psi_i(z)\, a^\xi(z) \nabla_z \psi_j(z)\, \mathrm{d}\nu(z).$$

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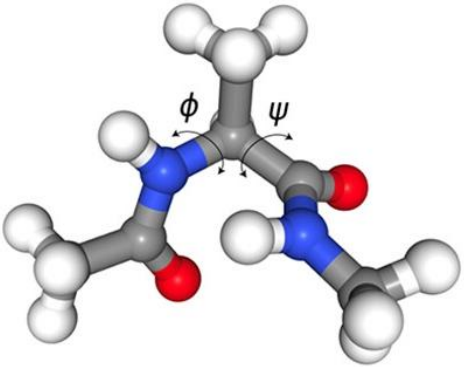
- Match these matrix elements against reference model:

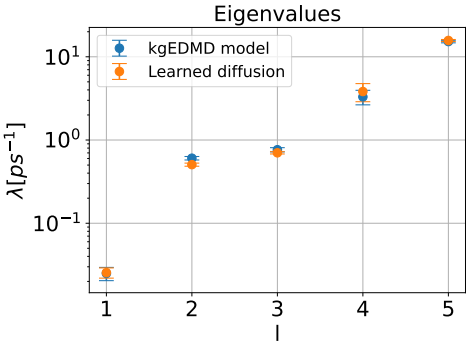
$$\alpha^* = \underset{\alpha \in \mathbb{R}^{d \times d \times r}}{\arg\min} \left[\left\| \hat{\mathbf{L}}^{\mathrm{ref}} - \mathbf{L}_\alpha \right\|_2^2 + \gamma \left\| \frac{\partial \sigma}{\partial z} \right\|_2^2 \right]$$

Nateghi and **FN**, arxiv 2409.16396 (2024)

Alanine Dipeptide

Learn CG Model in 2d dihedral angle space.





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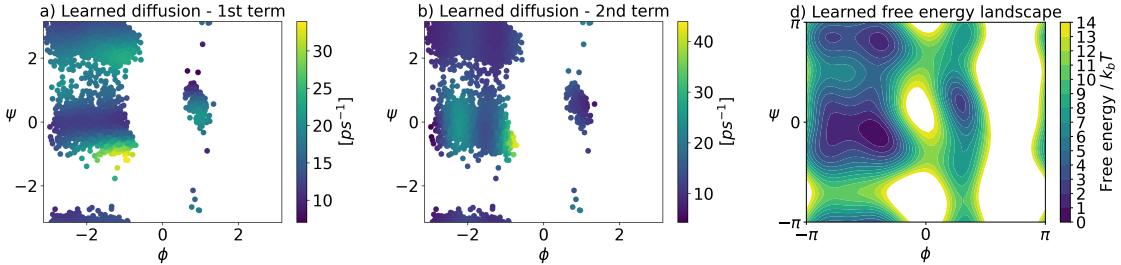

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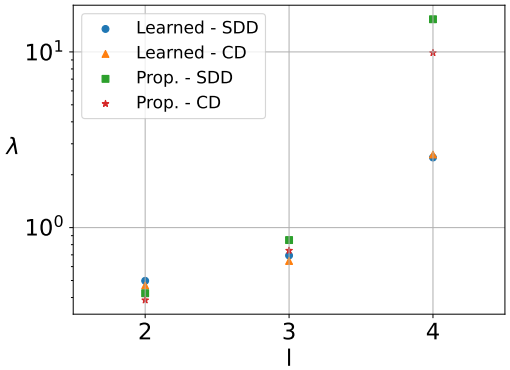
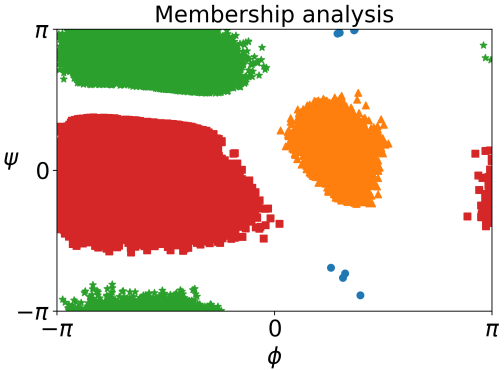
Alanine Dipeptide

Analysis of propagated CG model:





Nateghi and **FN**, arxiv 2409.16396 (2024)

Acknowledgments

Stefan Klus

Vahid Nateghi

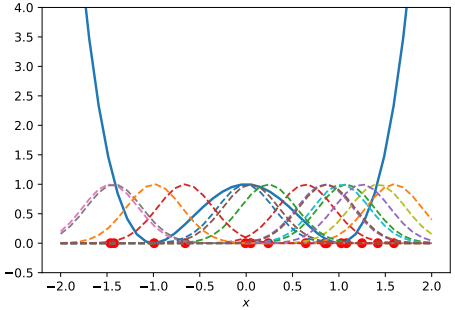
References:

- **FN**, Keller, Pérez-Hernández, Mey, Noé, *Variational Approach to Molecular Kinetics*, J Chemical Theory Comput 10 (4), 1739-1752 (2014)
- **FN** and Klus, *Efficient Approximation of Molecular Kinetics using Random Fourier Features*, J Chemical Physics 159, 074105 (2023)
- Nateghi and **FN**, arxiv 2409.16396 (2024)

`https://fnueske.github.io`

Kernel Basis Sets

- Let the data define the basis.



Klus, **FN**, and Hamzi, Entropy (2020)

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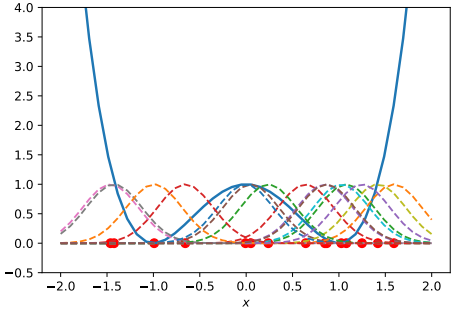

- Leads to a kernel $k(x, y)$ (symmetric positive-definite function) with features:

$$\psi_i = k(x_i, \cdot)$$

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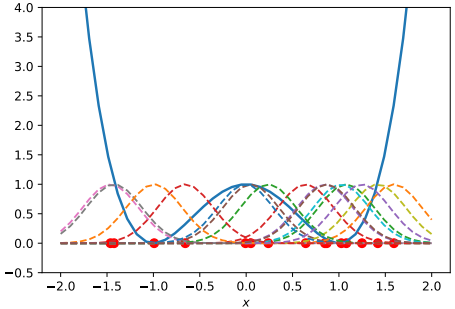

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- Kernel basis can be reduced using *random Fourier features*.

Klus, **FN**, and Hamzi, Entropy (2020)

Kernels and Random Features

- Translation invariant kernels $k(x, y) = \gamma(x - y)$ are superpositions of complex plane waves (Bochner's Theorem):

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

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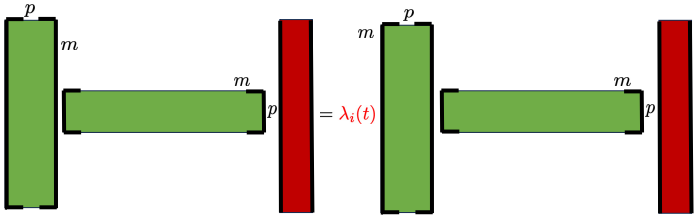
- Eigenvalue problem turns into low-rank format:



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