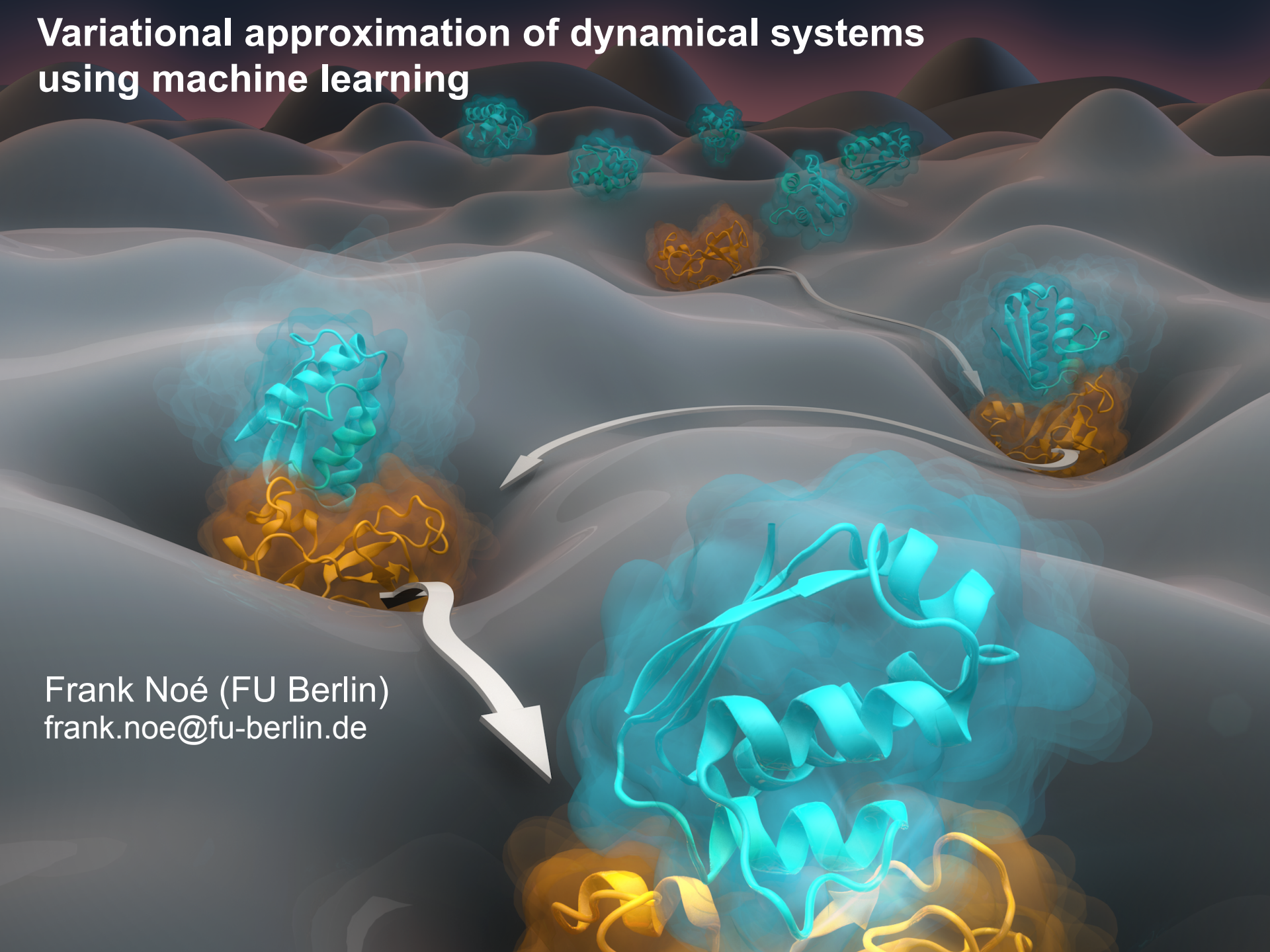
Variational approximation of dynamical systems using machine learning



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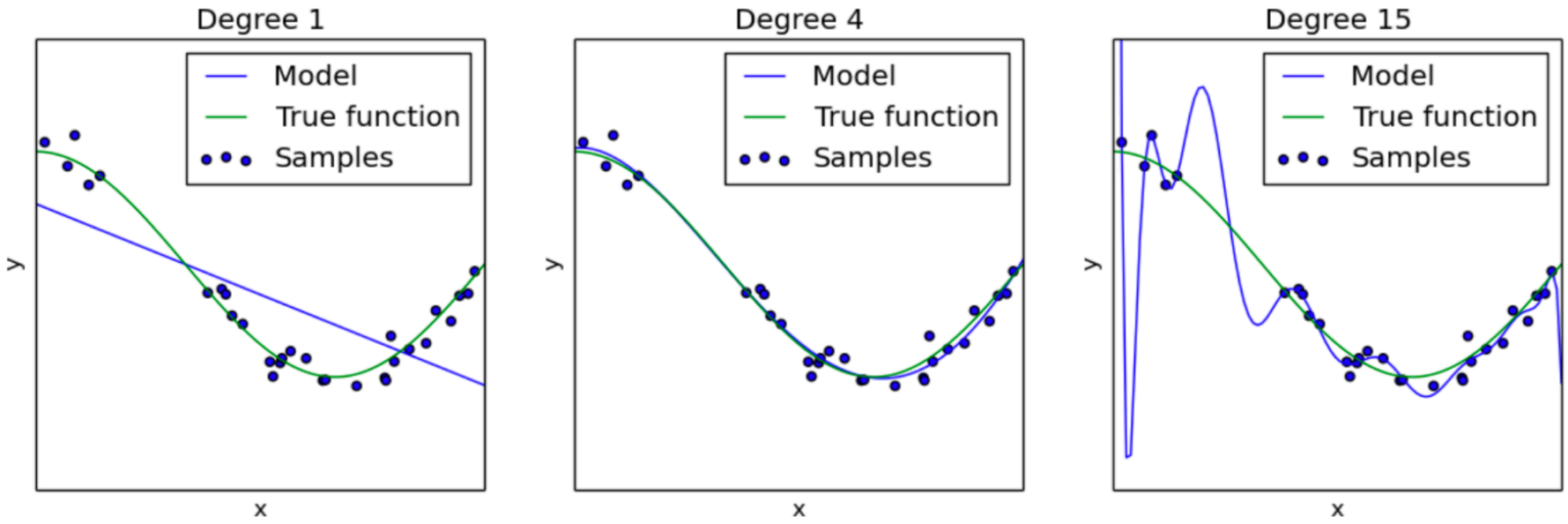
Choices…

Aim: learn model of dynamical system from observations x_t, $x_{t+\tau}$

How do we choose?

- Method / Representation (DMD, EDMD, TICA, VAMPnets, time-Autoencoder, …)
- Type of Basis Set (polynomial, cos/sin, characteristic functions, …)
- Number of Basis Functions
- Type of Kernel in a Kernel approach
- Regularization Hyperparameters
- Type of Neurons and Architecture of Neural Net



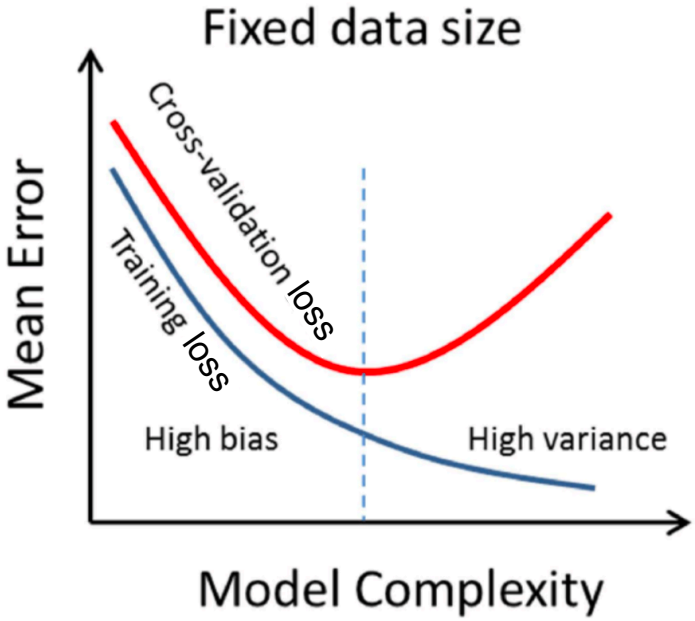
Machine Learning Answer

Cost or **loss function** C quantifies performance of network with parameters θ to predict observations $\mathbf{X}$.

Learning network weights

$$\hat{\theta} = \arg\min_\theta C(\mathbf{X}, \mathbf{Y}, \theta)$$

Minimimizing *cost* $C \equiv$ maximizing *score* $-C$. Often we just write $C(\theta)$.

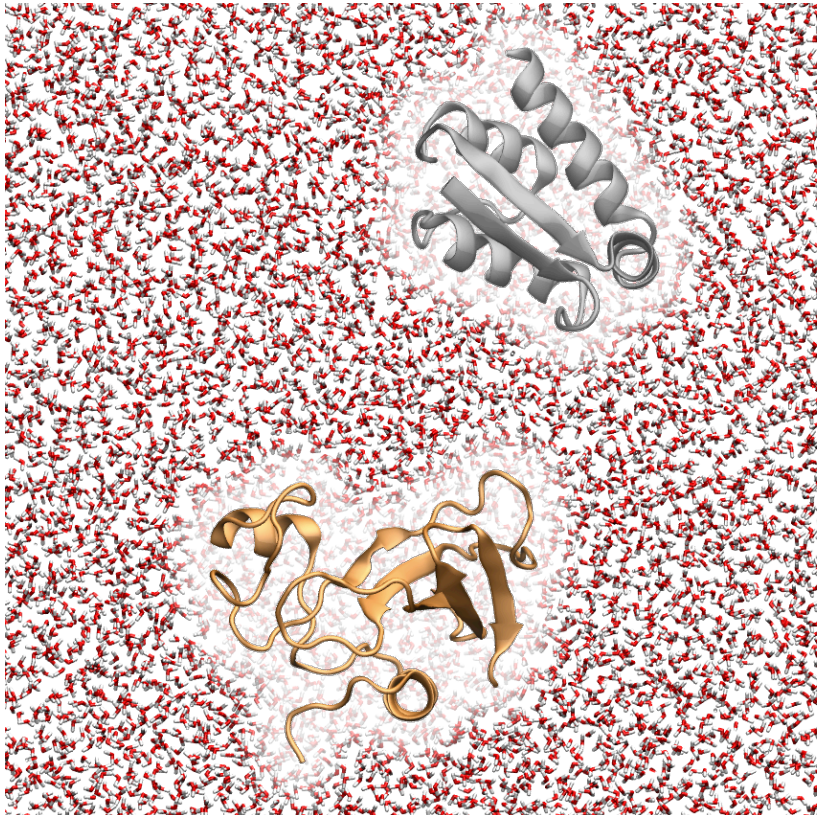


Standard approach (general and flexible):

- Parameter optimization: Training data
- Hyperparameter optimization: Validation data
- Quantifying model performance: Test data
- Details: **Statistical Estimator Theory** (e.g., Vapnik and others)

Simulating biological timescales at atomic resolution

Microsecond
MD Trajectories



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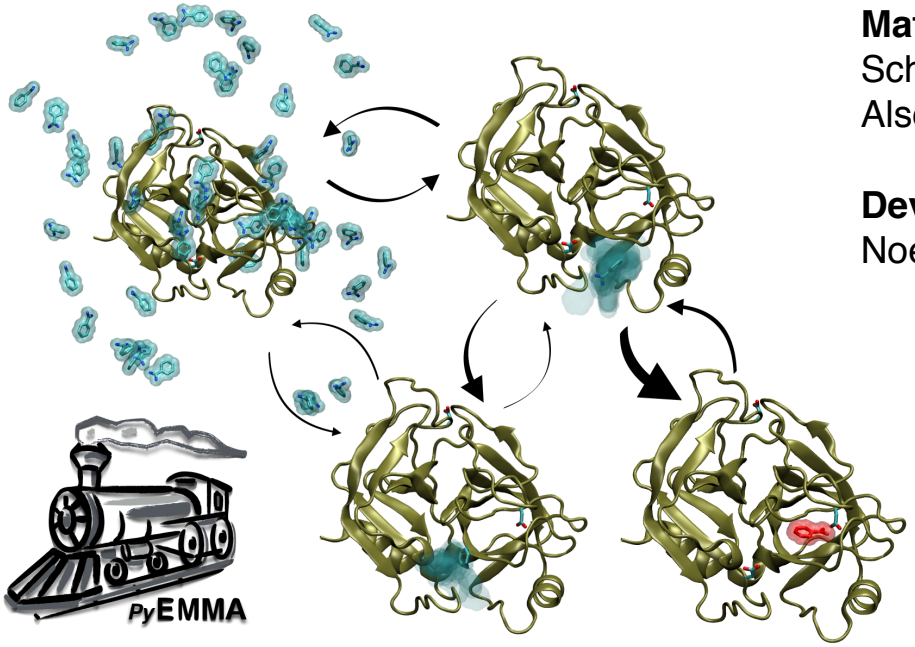


Mathematical theory:
Schütte et al, **J Comp Phys** 1999,
Also: Weber, Deuflhard, Friesecke, Dellnitz …

Developments for high-throuput molecular dynamics:
Noé, Pande, Swope, Hummer (mid 2000's)

Dynamical operators

Propagator

$$\rho_{t+\tau} = \mathcal{P}_\tau \rho_t = \int p_\tau(y \mid x)\, \rho_t(x)\, \mathrm{d}x$$

Transfer operator / Perron-Frobenius operator

= propagator for densities $u(x) = \frac{\rho(x)}{\pi(x)}$ with stationary density $\pi(x)$.

$$u_{t+\tau} = \mathcal{T}_\tau u_t = \int \frac{\pi(x)}{\pi(y)} p_\tau(y \mid x)\, \rho_t(x)\, \mathrm{d}x$$

Koopman operator

Adjoint to $\mathcal{P}$, adjoint to $\mathcal{T}$ with respect to π

$$f_{t+\tau} = \mathcal{K}_\tau f_t = \int p_\tau(y \mid x)\, f_t(y)\, \mathrm{d}y = \mathbb{E}[f_{t+\tau}(x)]$$

with detailed balance: $\pi(x)p_\tau(y \mid x) = \pi(y)p_\tau(x \mid y)$ we have $\mathcal{K}_\tau \equiv \mathcal{T}_\tau$

See: Mesic **Nonlinear Dyn.** 41, 309 (2005).

Slow processes (unique equilibrium distribution, detailed balance)

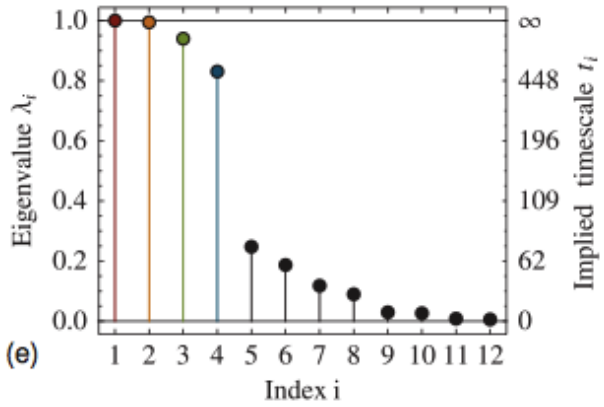
Backward propagator

$$\rho_\tau = \mathcal{T}(\tau)\rho_0$$

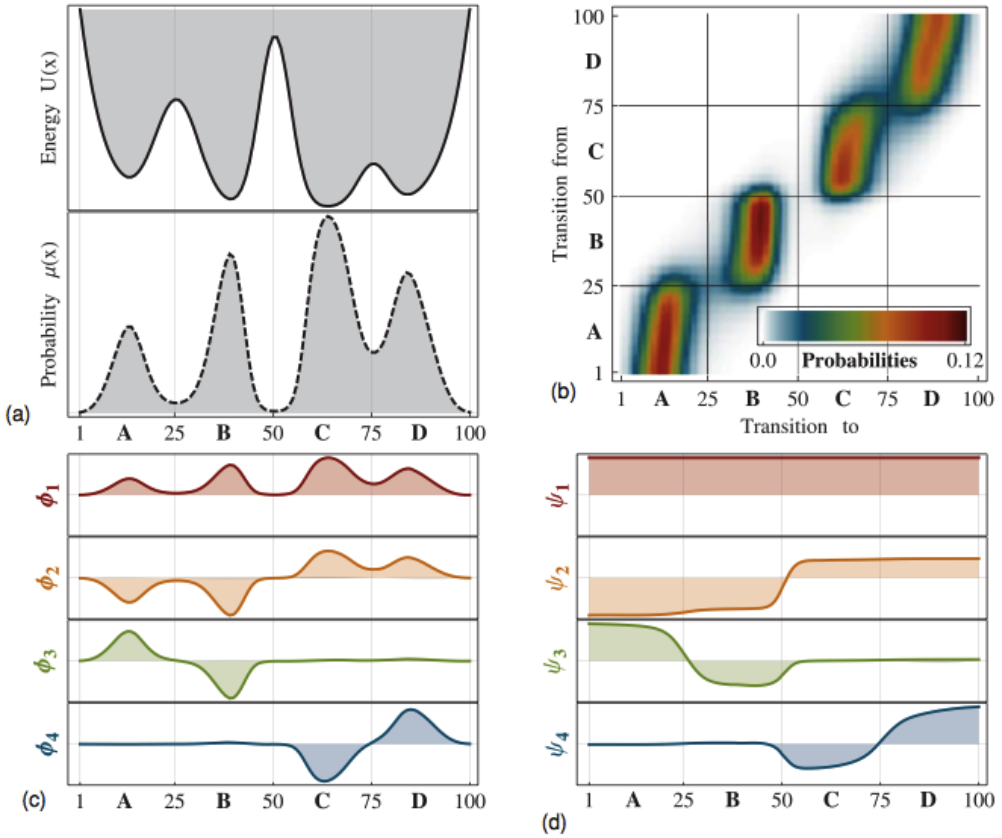
Spectral decomposition

$$\rho_\tau = \sum_{i=1}^{\infty} \mathrm{e}^{-\tau\kappa_i} \langle \psi_i \mid \rho_0 \rangle \psi_i \quad \text{+ fast part}$$

Eigenvalues / timescales κ_i^{-1}



Processes:



Schütte et al: **J. Comput. Phys.** (1999), Prinz et al.: **J. Chem. Phys.** 134, p174105 (2011)

Variational approach for Markov processes

Data-based version of: Fan, **PNAS** 35, 652-655 (1949)

The first m eigenfunctions $\psi_1, \ldots, \psi_m$ are the solution to the problem

$$\max_{f_1,\ldots,f_m} \sum_{i=1}^{m} \mathbb{E}\left[f_i\left(\mathbf{x}_t\right) f_i\left(\mathbf{x}_{t+\tau}\right)\right] \tag{1}$$

$$\text{s.t.} \quad \mathbb{E}\left[f_i\left(\mathbf{x}_t\right)^2\right] = 1$$

$$\mathbb{E}\left[f_i\left(\mathbf{x}_t\right) f_j\left(\mathbf{x}_{t+\tau}\right)\right] = 0, \ \textit{for } i \neq j$$

and the maximum value is the sum of $\lambda_1, \ldots, \lambda_m$

Properties:

- ψ_i and ψ_j are uncorrelated for $i \neq j$.
- ψ_i are the directions of slow kinetics with maximal autocorrelations $\mathbb{E}_\mu\left[\psi_i\left(\mathbf{x}_t\right) \psi_i\left(\mathbf{x}_{t+\tau}\right)\right] = \lambda_i\left(\tau\right)$.
- Population changes along ψ_i coordinates decay with $\lambda_i\left(\tau\right) = \mathrm{e}^{-\frac{\tau}{t_i}}$.
- For every other set of functions, the eigenvalues will be underestimated $\hat{\lambda}_i\left(\tau\right) \leq \lambda_i\left(\tau\right)$.

Noé and Nüske, **MMS** 11, 635-655 (2013)
Nüske et al, **JCTC** 10, 1739-1752 (2014)

Variational approach for reversible Markov processes

Method of linear variation

Ansatz: Define Basis set $\boldsymbol{\chi} = [\chi_1(\mathbf{x}), ..., \chi_n(\mathbf{x})]^\top$ and seek the linear expansions:

$$\hat{\psi}_i(\mathbf{x}) = \sum_j r_{ij}\chi_j(\mathbf{x})$$

Noé and Nüske, **MMS** 11, 635-655 (2013)
Nüske et al, **JCTC** 10, 1739-1752 (2014)

Variational approach for reversible Markov processes: Estimator

1. Define

$$\mathbf{X}_0 = \begin{bmatrix} \chi_1(\mathbf{x}_0) & \cdots & \chi_n(\mathbf{x}_0) \\ \vdots & & \vdots \\ \chi_1(\mathbf{x}_{T-\tau}) & \cdots & \chi_n(\mathbf{x}_{T-\tau}) \end{bmatrix} \qquad \mathbf{X}_\tau = \begin{bmatrix} \chi_1(\mathbf{x}_\tau) & \cdots & \chi_n(\mathbf{x}_\tau) \\ \vdots & & \vdots \\ \chi_1(\mathbf{x}_T) & \cdots & \chi_n(\mathbf{x}_T) \end{bmatrix}$$

2. Empirical covariance matrices: $\mathbf{C}^0$ and $\mathbf{C}^\tau$ with:

$$\mathbf{C}^0 = \mathbf{X}_0^\top \mathbf{X}_0$$
$$\mathbf{C}^\tau = \mathbf{X}_0^\top \mathbf{X}_\tau$$

3. Solve

$$\mathbf{C}^\tau \mathbf{r}_i = \mathbf{C}^0 \hat{\lambda}_i \mathbf{r}_i$$

4. The projections

$$\mathbf{\Psi} = \mathbf{X}\mathbf{R}$$

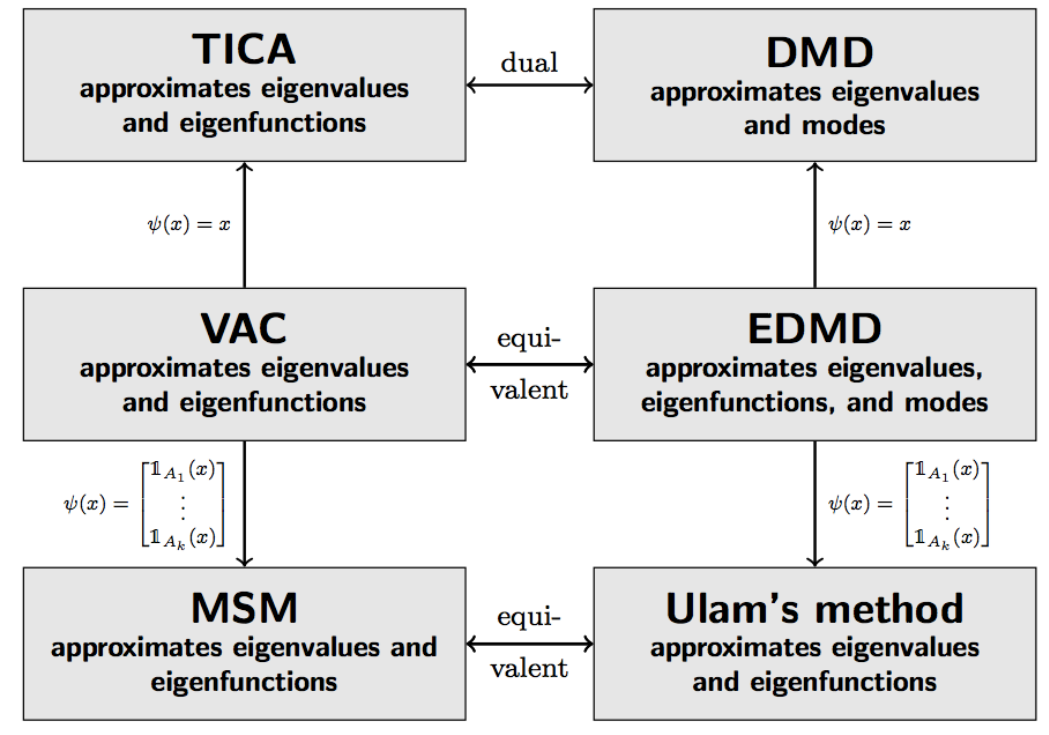
approximate the transfer operator eigenfunctions on the sampled configurations x_t.

Noé and Nüske, **MMS** 11, 635-655 (2013)
Nüske et al, **JCTC** 10, 1739-1752 (2014)

Comparison between methods

Molgedey and Schuster, **PRL** 72 3634-3637 (1994)
Pérez-Hernández et al, **JCP** 139, 015102 (2013)

Schmidt, Sesterhenn,
Ann. Meet. APS Div. Fluid Mech. (2008)



Noé & Nüske **MMS** 11, 635-655 (2013)

Nüske et al, **JCTC** 10, 1739-1752 (2014)

Williams, Kevrikidis, Rowley
J. Nonlinear Sci. 6, 1-40 (2015)

Schütte et al: **J. Comput. Phys.** (1999)
also: Noé, Pande, Hummer, Weber, Swope, …

Klus, Nüske, Koltai, Wu, Krevrekidis, Schütte, Noé: Data-driven model reduction and transfer operator approximation (**J. Nonlin. Sci.** 2018 / **arXiv**:1703.10112)

Variational approach for Markov processes (VAMP)

Koopman operator

$$\begin{aligned} \mathcal{K}_\tau f(x) &= \mathbb{E}\left[f(x_{t+\tau}) \,|x_t = x\right] \\ &= \int p_\tau(x,y)\, f(y)\, \mathrm{d}y \end{aligned}$$

Wu and Noé, **arXiv**:1707.04659 (2017)

Variational approach for Markov processes (VAMP)

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Singular value decomposition:

$$\mathcal{K}_\tau f = \sum_i \sigma_i \left\langle \phi_i, f \right\rangle_{\rho_1} \psi_i$$

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- ρ_0, ρ_1 : empirical distribution of x_t, $x_{t+\tau}$
- If data are in equilibrium: stationary distribution $\mu = \rho_0 = \rho_1$
- $\{\phi_i\}$ and $\{\psi_i\}$ are both orthonormal bases with respect to $\langle \cdot, \cdot \rangle_{\rho_1}$ and $\langle \cdot, \cdot \rangle_{\rho_0}$,
- σ_i denotes the ith largest singular value.

Wu and Noé, **arXiv**:1707.04659 (2017)

Variational approach for Markov processes (VAMP)

Theorem **VAMP variational principle.** *The k dominant singular components of a Koopman operator are the solution of the following maximization problem:*

$$\sum_{i=1}^{k} \sigma_i^r = \max_{\mathbf{f},\mathbf{g}} \mathcal{R}_r\left[\mathbf{f},\mathbf{g}\right], \quad s.t. \left\langle f_i, f_j \right\rangle_{\rho_0} = 1_{i=j}, \quad \left\langle g_i, g_j \right\rangle_{\rho_1} = 1_{i=j}, \tag{10}$$

where $r \geq 1$ can be any positive integer. The maximal value is achieved by the singular functions $f_i = \psi_i$ and $g_i = \phi_i$ and

$$\mathcal{R}_r\left[\mathbf{f},\mathbf{g}\right] = \sum_{i=1}^{k} \left\langle f_i, \mathcal{K}_\tau g_i \right\rangle_{\rho_0}^r \tag{11}$$

is called the VAMP-r score of $\mathbf{f}$ and $\mathbf{g}$.

Wu and Noé, **arXiv**:1707.04659 (2017)

Implementation: time-lagged canonical covariance analysis (TCCA)

1. Compute

$$\mathbf{C}_{00} = \frac{1}{T-\tau}\mathbf{X}^\top\mathbf{X}$$
$$\mathbf{C}_{01} = \frac{1}{T-\tau}\mathbf{X}^\top\mathbf{Y}$$
$$\mathbf{C}_{11} = \frac{1}{T-\tau}\mathbf{Y}^\top\mathbf{Y}$$

with

$$\mathbf{X} = \left(\boldsymbol{\chi}_0\left(\mathbf{x}_1\right), \boldsymbol{\chi}_0\left(\mathbf{x}_2\right), \ldots, \boldsymbol{\chi}_0\left(\mathbf{x}_{T-\tau}\right)\right)^\top$$
$$\mathbf{Y} = \left(\boldsymbol{\chi}_1\left(\mathbf{x}_{1+\tau}\right), \boldsymbol{\chi}_1\left(\mathbf{x}_{2+\tau}\right), \ldots, \boldsymbol{\chi}_1\left(\mathbf{x}_T\right)\right)^\top$$

Wu and Noé, **arXiv**:1707.04659 (2017)

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2. Perform the truncated SVD

$$\mathbf{C}_{00}^{-\frac{1}{2}}\mathbf{C}_{01}\mathbf{C}_{11}^{-\frac{1}{2}} \approx \mathbf{U}_k\hat{\boldsymbol{\Sigma}}_k\mathbf{V}_k^\top$$

3. Output $\hat{\boldsymbol{\Sigma}}_k$, $\boldsymbol{\psi} = \mathbf{U}_k^\top\mathbf{C}_{00}^{-\frac{1}{2}}\boldsymbol{\chi}_0$ and $\boldsymbol{\phi} = \mathbf{V}_k^\top\mathbf{C}_{11}^{-\frac{1}{2}}\boldsymbol{\chi}_1$

Wu and Noé, **arXiv**:1707.04659 (2017)

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3. Output $\hat{\boldsymbol{\Sigma}}_k$, $\boldsymbol{\psi} = \mathbf{U}_k^\top\mathbf{C}_{00}^{-\frac{1}{2}}\boldsymbol{\chi}_0$ and $\boldsymbol{\phi} = \mathbf{V}_k^\top\mathbf{C}_{11}^{-\frac{1}{2}}\boldsymbol{\chi}_1$

For the choice $\boldsymbol{\chi}_0 = \boldsymbol{\chi}_1$, TCCA is consistent with EDMD:

$$\mathbf{K}_\tau^\top = \mathbf{C}_{01}^\top\mathbf{C}_{00}^{-1}$$

Wu and Noé, **arXiv**:1707.04659 (2017)

VAMP: Koopman approximation error

Theorem (Koopman approximation error): For an operator $\hat{\mathcal{K}}_\tau$ defined by

$$\hat{\mathcal{K}}_\tau h = \sum_i \hat{\sigma}_i \left\langle g_i, h \right\rangle_{\rho_1} f_i$$

we have

- R_E (VAMP-E score)

$$\left\| \hat{\mathcal{K}}_\tau - \mathcal{K}_\tau \right\|_{\mathrm{HS}}^2 = \mathrm{tr}\left[\hat{\mathbf{\Sigma}} \mathbf{C}_{00} \hat{\mathbf{\Sigma}} \mathbf{C}_{11} - 2 \hat{\mathbf{\Sigma}} \mathbf{C}_{01} \right] + \sum_i \sigma_i^2$$

where $\|\cdot\|_{\mathrm{HS}}$ denotes the Hilbert-Schmidt norm, $\hat{\mathbf{\Sigma}} = \mathrm{diag}\left(\hat{\sigma}_1, \hat{\sigma}_2, \ldots\right)$, and

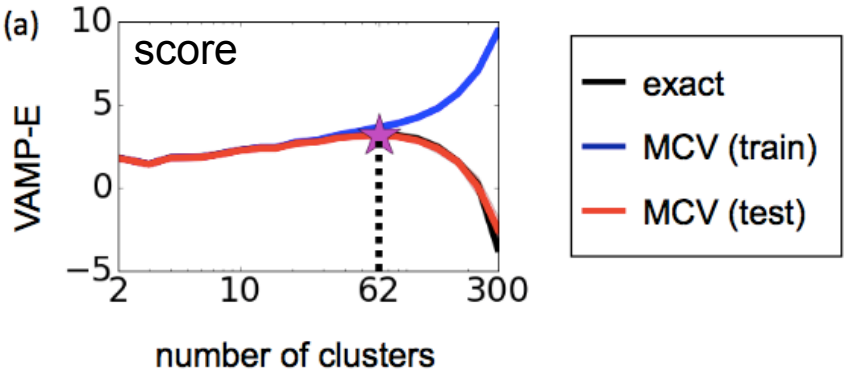
$$\begin{aligned}
\left[\mathbf{C}_{00}\right]_{ij} &= \mathbb{E}_{\rho_0}\left[f_i\left(\mathbf{x}\left(t\right)\right) f_j\left(\mathbf{x}\left(t\right)\right) \right] \\
\left[\mathbf{C}_{01}\right]_{ij} &= \mathbb{E}_{\rho_0}\left[f_i\left(\mathbf{x}\left(t\right)\right) g_j\left(\mathbf{x}\left(t+\tau\right)\right)^\top \right] \\
\left[\mathbf{C}_{11}\right]_{ij} &= \mathbb{E}_{\rho_1}\left[g_i\left(\mathbf{x}\left(t\right)\right) g_j\left(\mathbf{x}\left(t\right)\right)^\top \right].
\end{aligned}$$

Wu and Noé, **arXiv**:1707.04659 (2017)

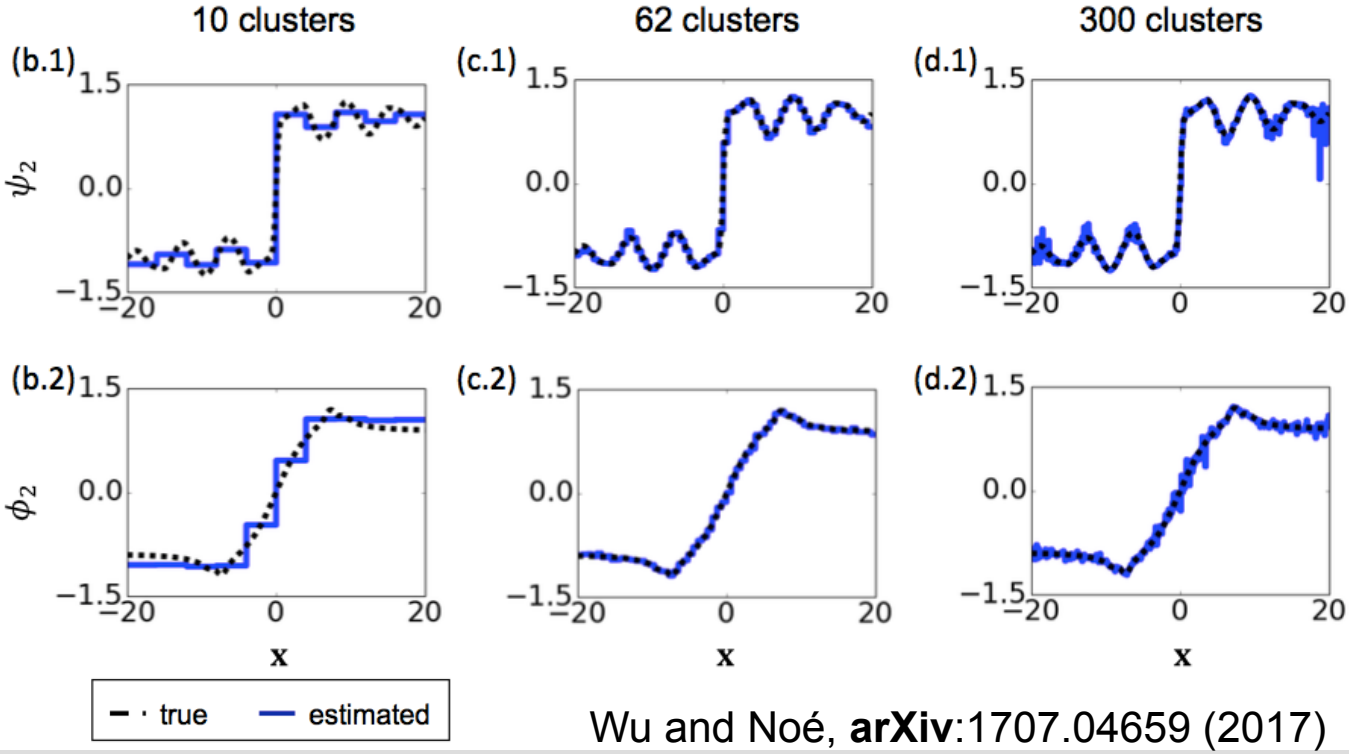
1D-Example

Markov process with Gaussian noise w_t

$$x_{t+1} = \frac{x_t}{2} + \frac{25x_t}{1+x_t^2} + \sqrt{10}\,(1.1 + \cos(x_t))\,w_t$$



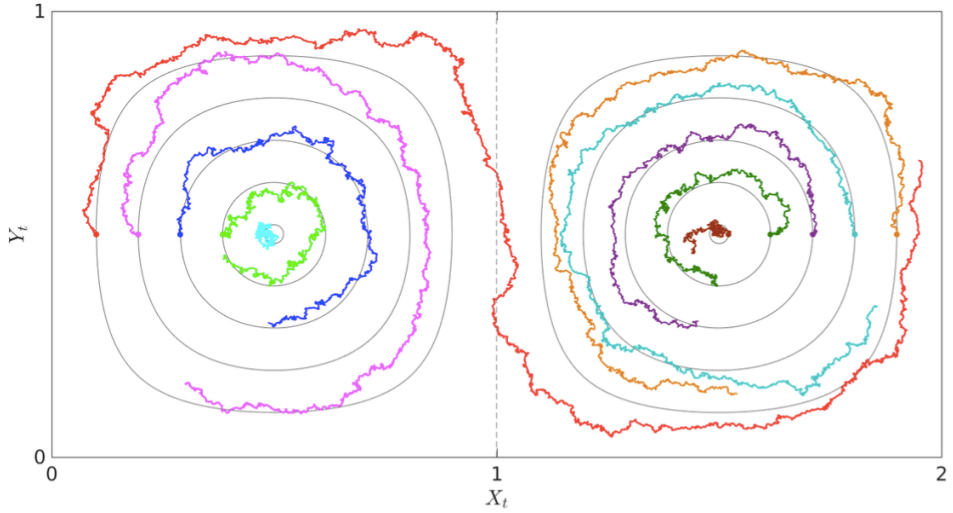
Eigenfunctions

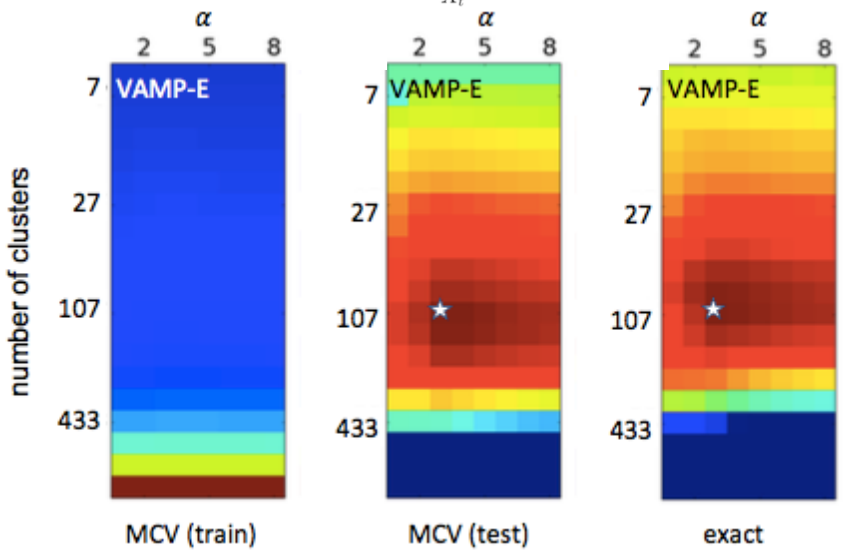


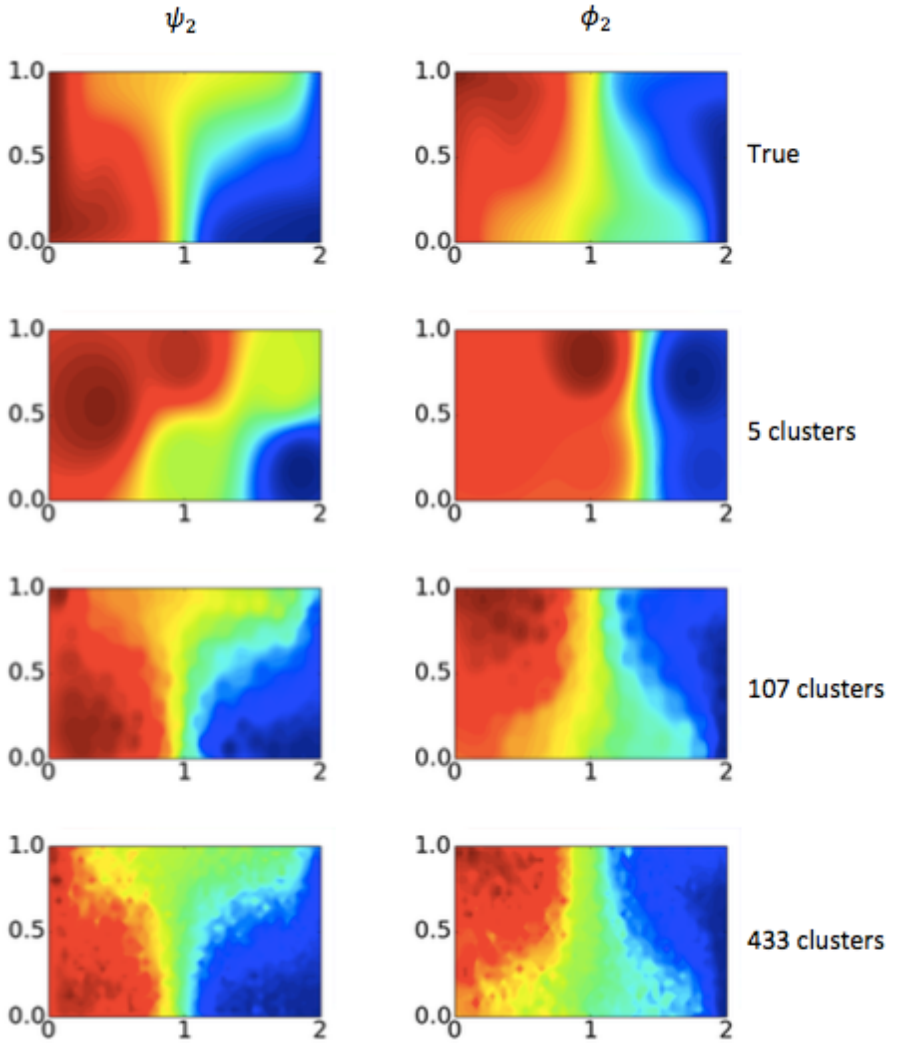
Wu and Noé, **arXiv**:1707.04659 (2017)

Generalization: VAMP reduces nonequilibrium processes

$$dx_t = -\pi\, A\, \sin(\pi\, x_t)\, \cos(\pi\, y_t) - \epsilon(2y_t - 1) + \varepsilon\, d\mathbf{W}_{t,1},$$
$$dy_t = \quad \pi\, A\, \cos(\pi\, x_t)\, \sin(\pi\, y_t) - \epsilon(2x_t - 3) + \varepsilon\, d\mathbf{W}_{t,2}$$

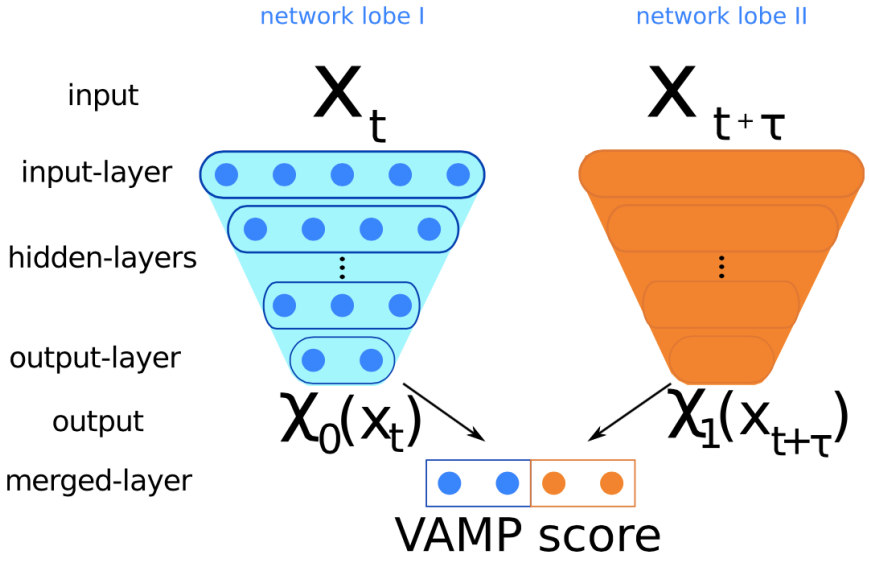






Wu and Noé, **arXiv**:1707.04659 (2017)

VAMPnets



VAMP variational principle (subspace version)

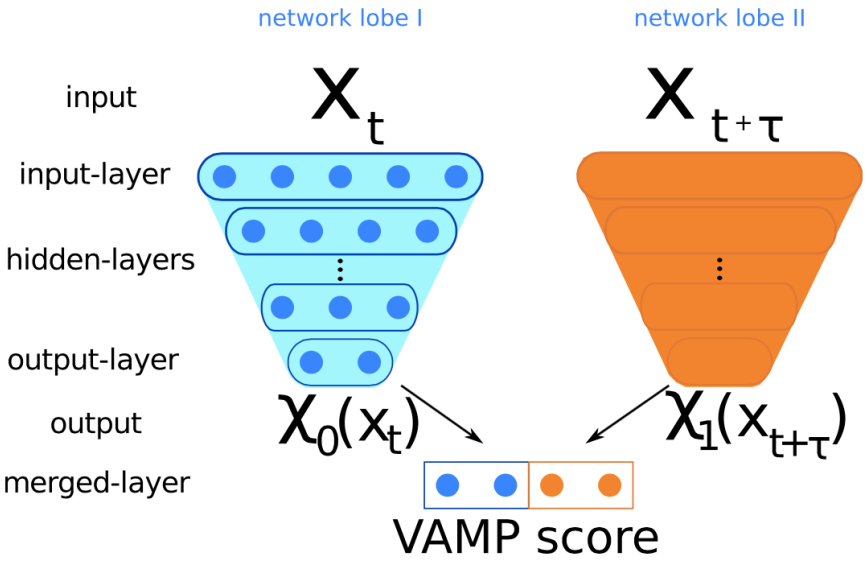
For any two sets of linearly independent functions $\boldsymbol{\chi}_0(\mathbf{x}) = (\chi_{01}(\mathbf{x}), ..., \chi_{0n}(\mathbf{x}))$ *and* $\boldsymbol{\chi}_1(\mathbf{x}) = (\chi_{11}(\mathbf{x}), ..., \chi_{1n}(\mathbf{x}))$*, let us call*

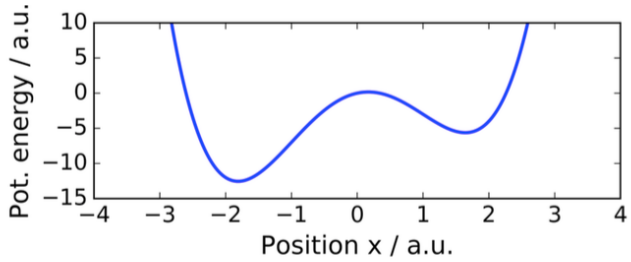
$$\hat{R}_2[\boldsymbol{\chi}_0, \boldsymbol{\chi}_1] = \left\| \mathbf{C}_{00}^{-\frac{1}{2}} \mathbf{C}_{01} \mathbf{C}_{11}^{-\frac{1}{2}} \right\|_F^2$$

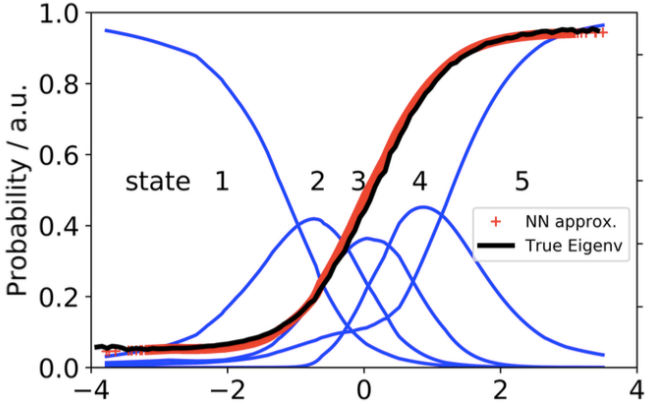
their VAMP-2 score, where $\mathbf{C}_{00}$*,* $\mathbf{C}_{01}$*,* $\mathbf{C}_{11}$ *are the feature correlation matrices as defined earlier and* $\|\cdot\|_F$ *indicates the Frobenius norm. The maximum value of the VAMP-2 score is achieved when the top n left and right Koopman singular functions belong to* $\mathrm{span}(\boldsymbol{\chi}_0)$ *and* $\mathrm{span}(\boldsymbol{\chi}_1)$*, respectively.*

Mardt, Pasquali, Wu, Noé **Nat. Commun.** 9, 5 (2018)

VAMPnets



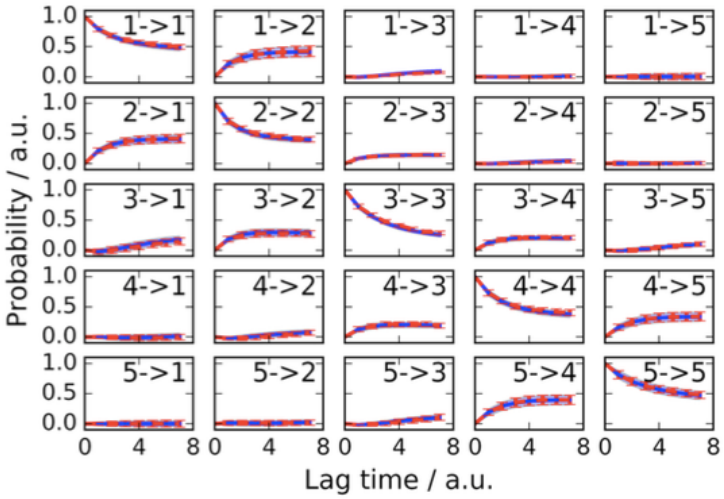




Resulting Markov model: $\mathbf{K} = \mathbf{C}_{00}^{-1}\mathbf{C}_{01}.$

Relaxation timescales: $t_i(\tau) = -\frac{\tau}{\ln|\lambda_i(\tau)|},$

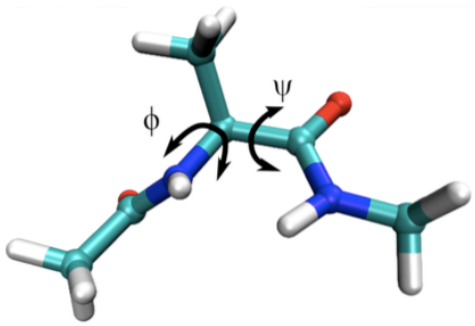
Validate (Chapman-Kolmogorov test): $\mathbf{K}(n\tau) = \mathbf{K}^n(\tau),$

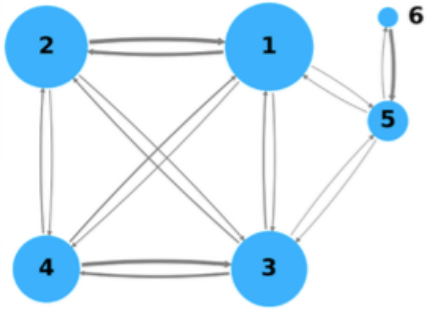


Mardt, Pasquali, Wu, Noé **Nat. Commun.** 9, 5 (2018)

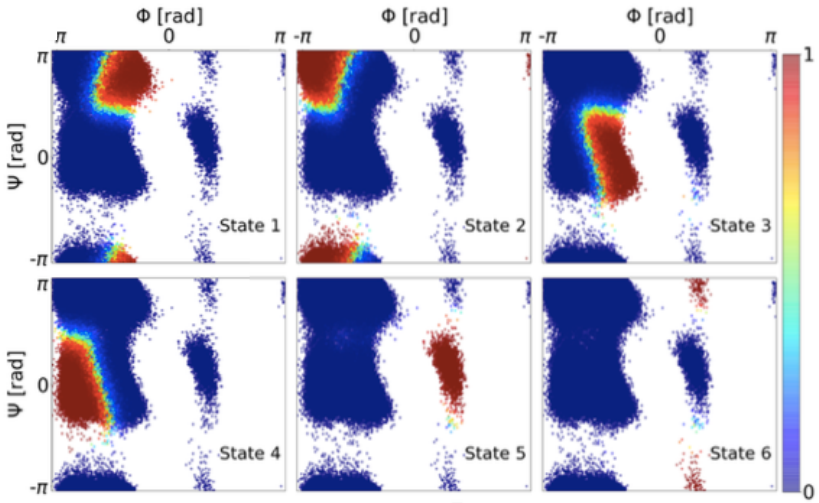
VAMPnets

Alanine dipeptide

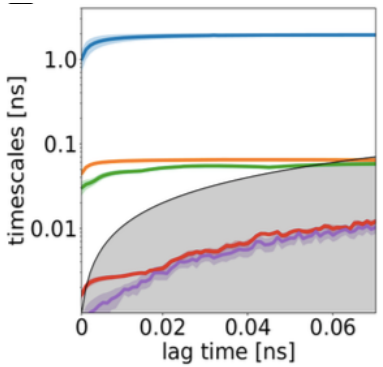


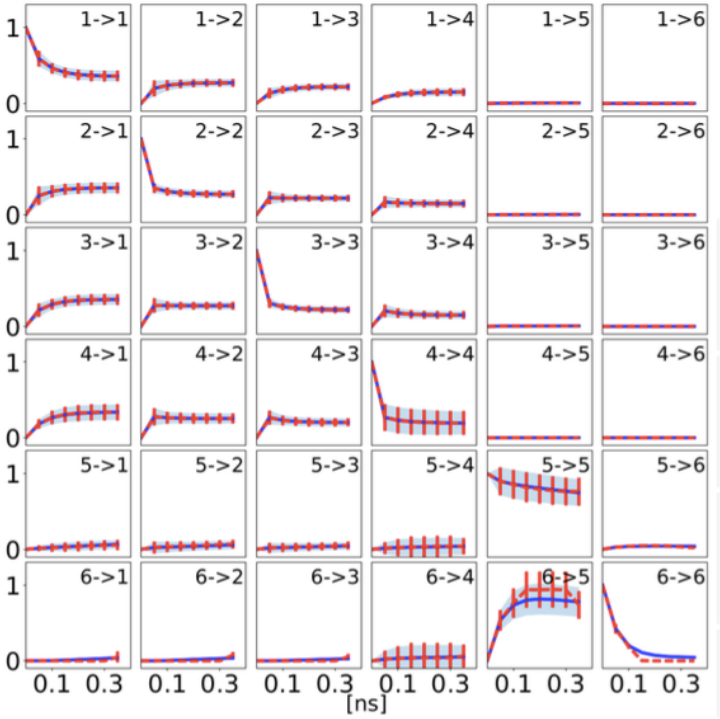


Max. transition probability: 41%
Min. transition probability: 0.5%



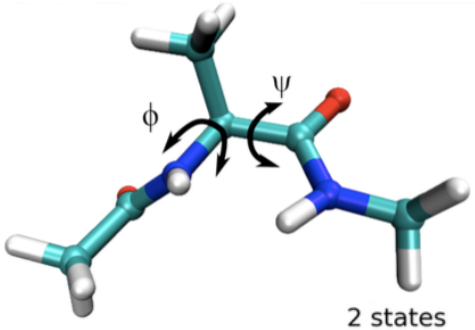
Validation



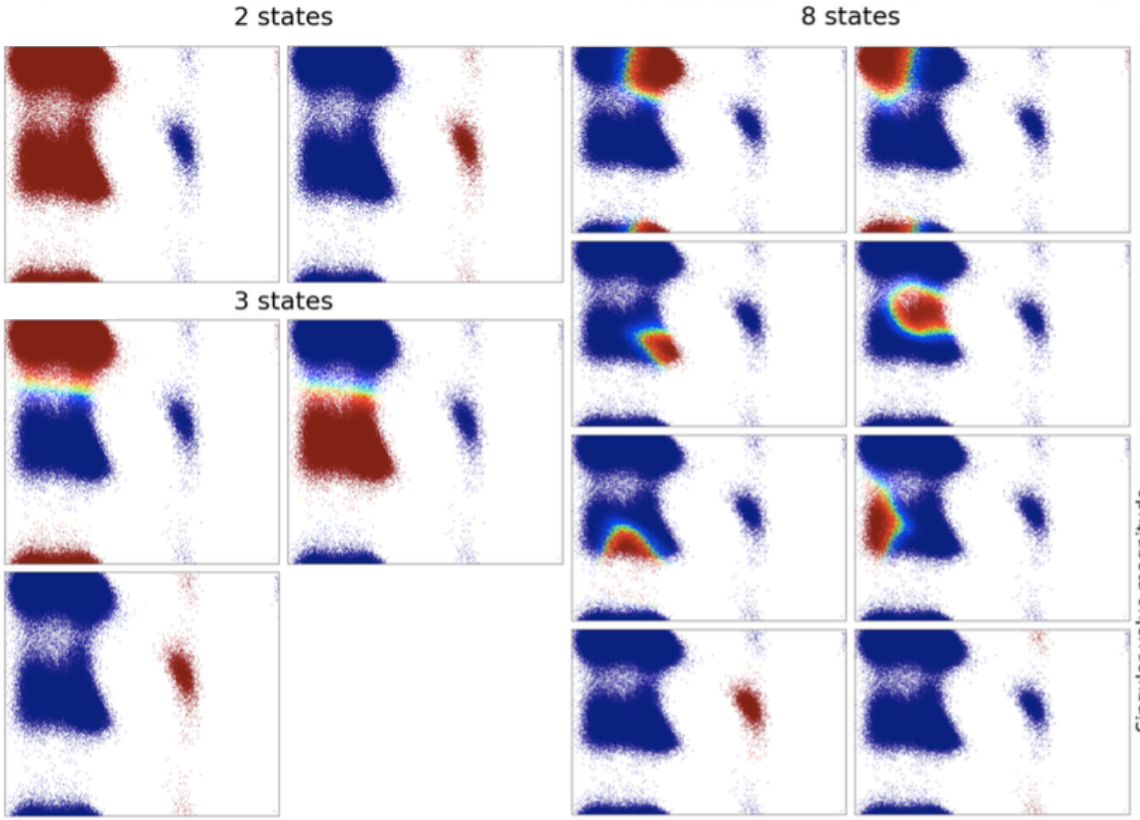


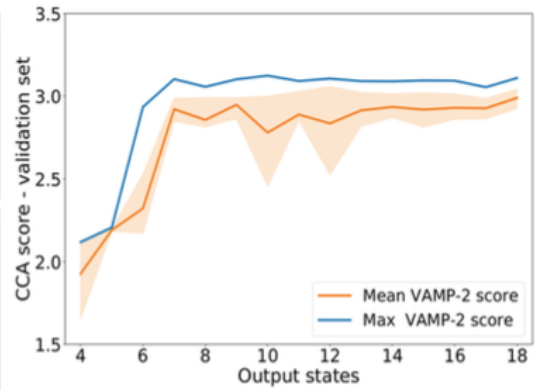
Mardt, Pasquali, Wu, Noé **Nature Communications** (2018)

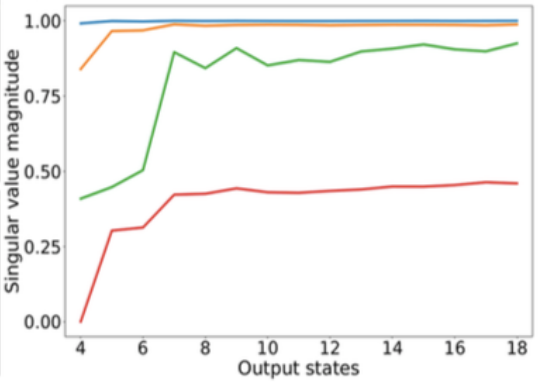
VAMPnets



Results as a function of the number of states



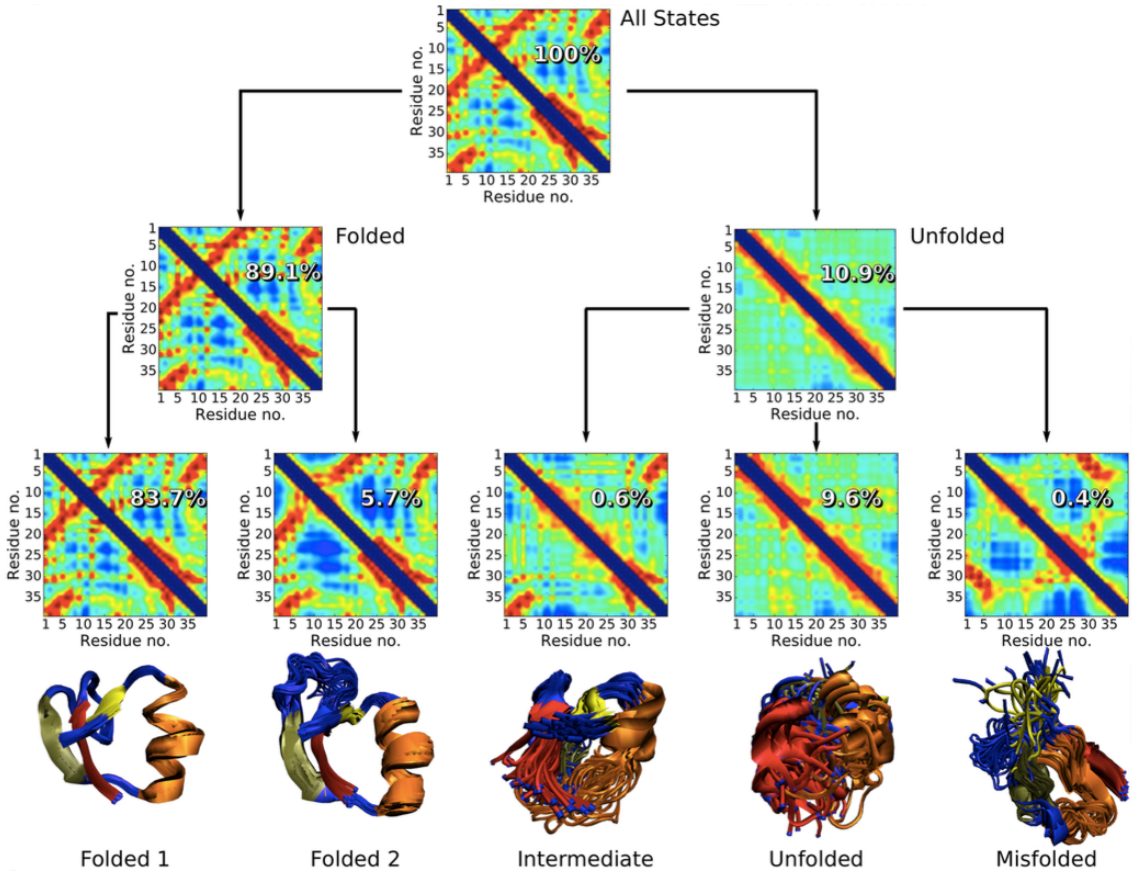




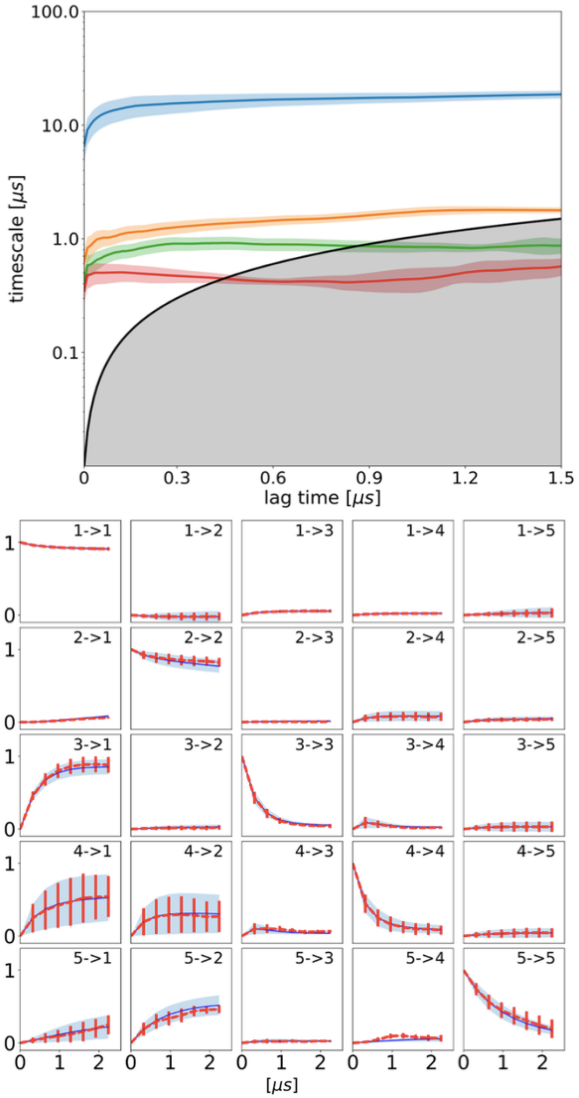
Mardt, Pasquali, Wu, Noé **Nature Communications** (2018)

VAMPnets

NTL9 Protein folding

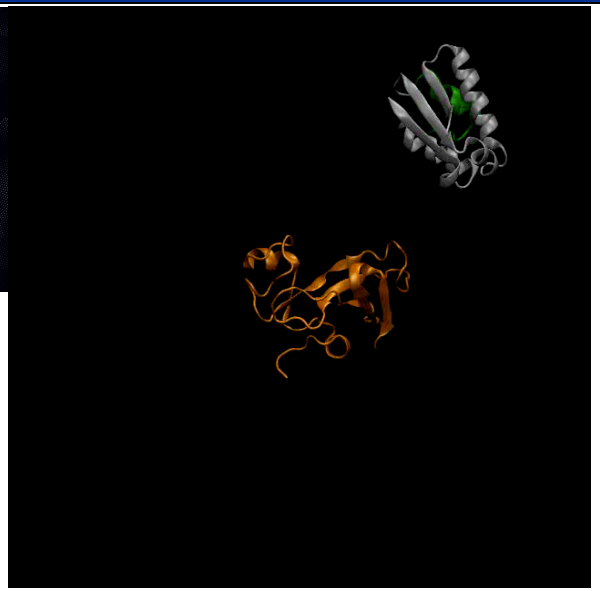


Validation

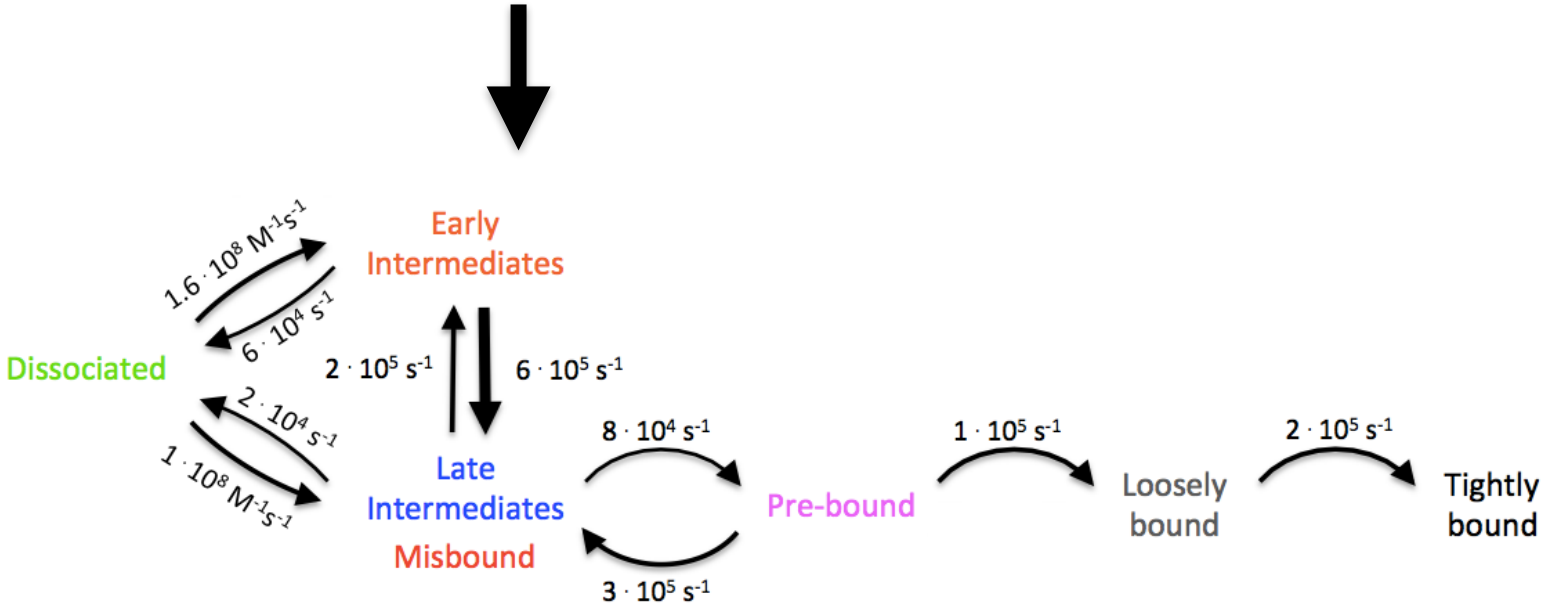


Mardt, Pasquali, Wu, Noé **Nature Communications** (2018)

Simulating biological timescales at atomic resolution

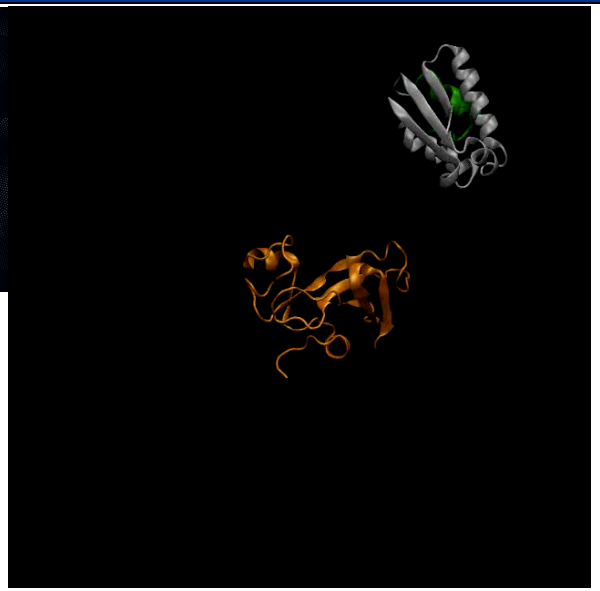


1000's of
Microsecond
MD Trajectories

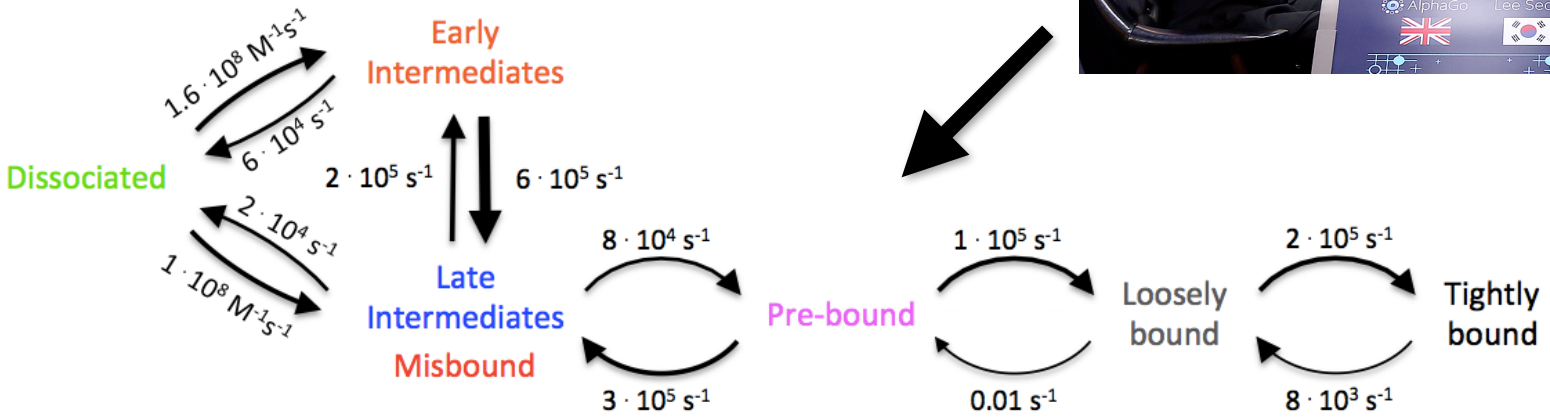


Markov State Model — **Millisecond kinetics**

Simulating biological timescales at atomic resolution

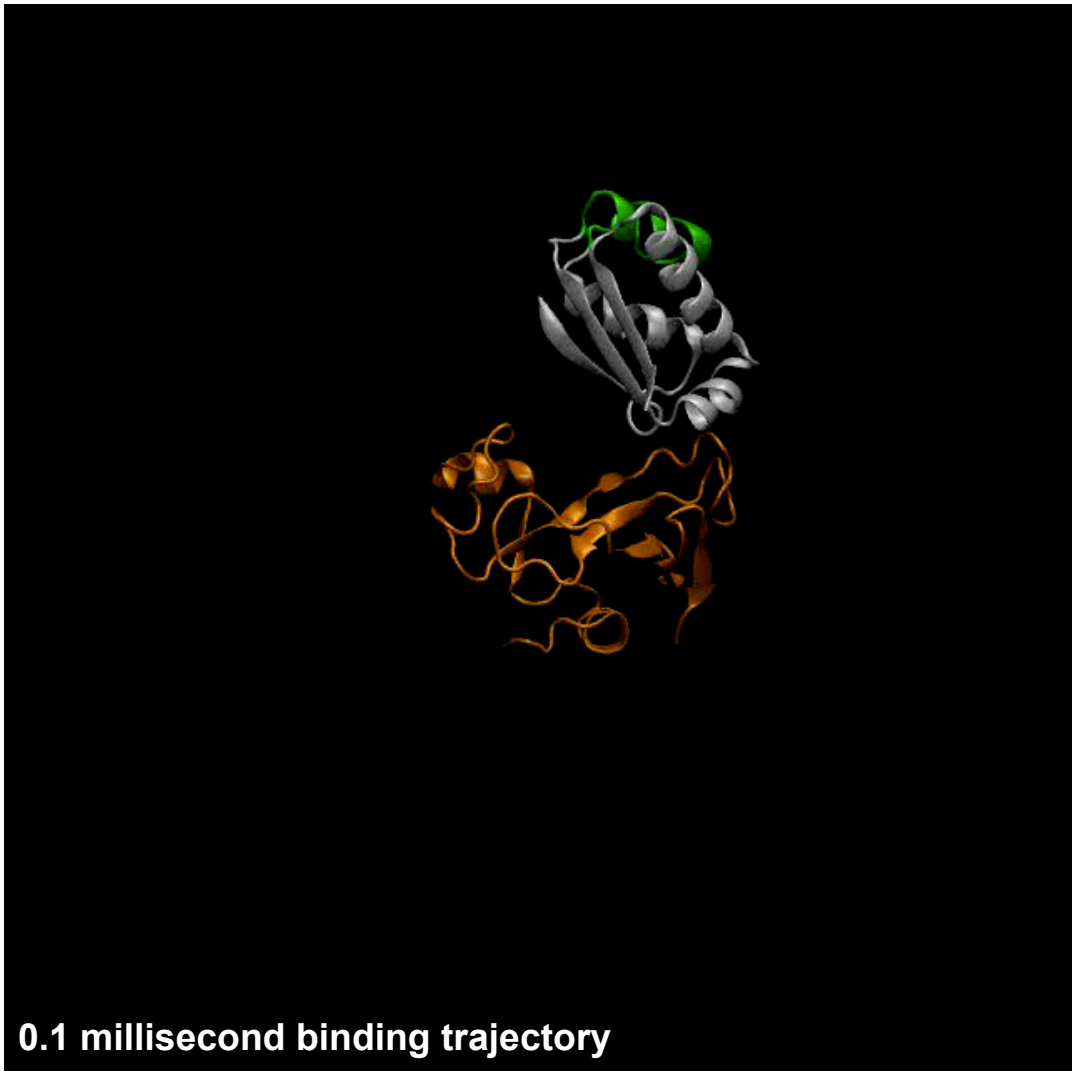


Reinforcement learning



Adaptive Markov State Model — **seconds to hours kinetics**

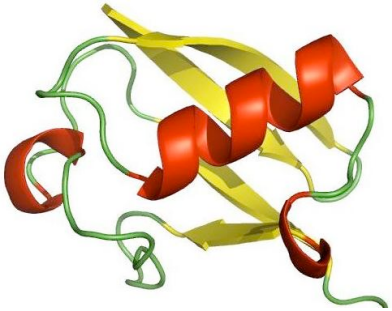
Sampling biological timescales at atomic resolution

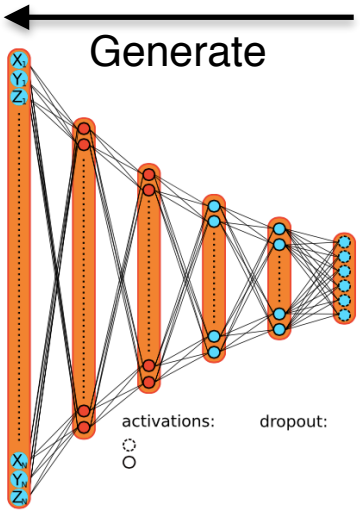


Plattner, Doerr, De Fabritiis, Noé
Nature Chemistry 9, 1005 (2017)

Generative learning and molecular design

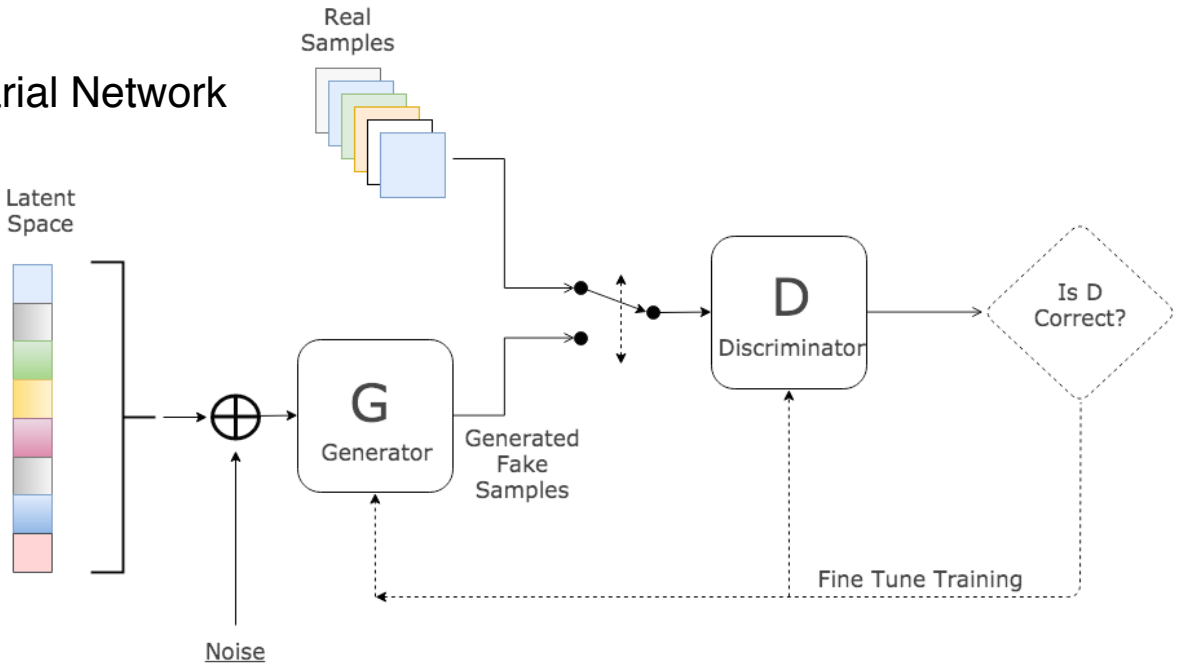
Structure and dynamics
from MD Simulation data
Experimental data …



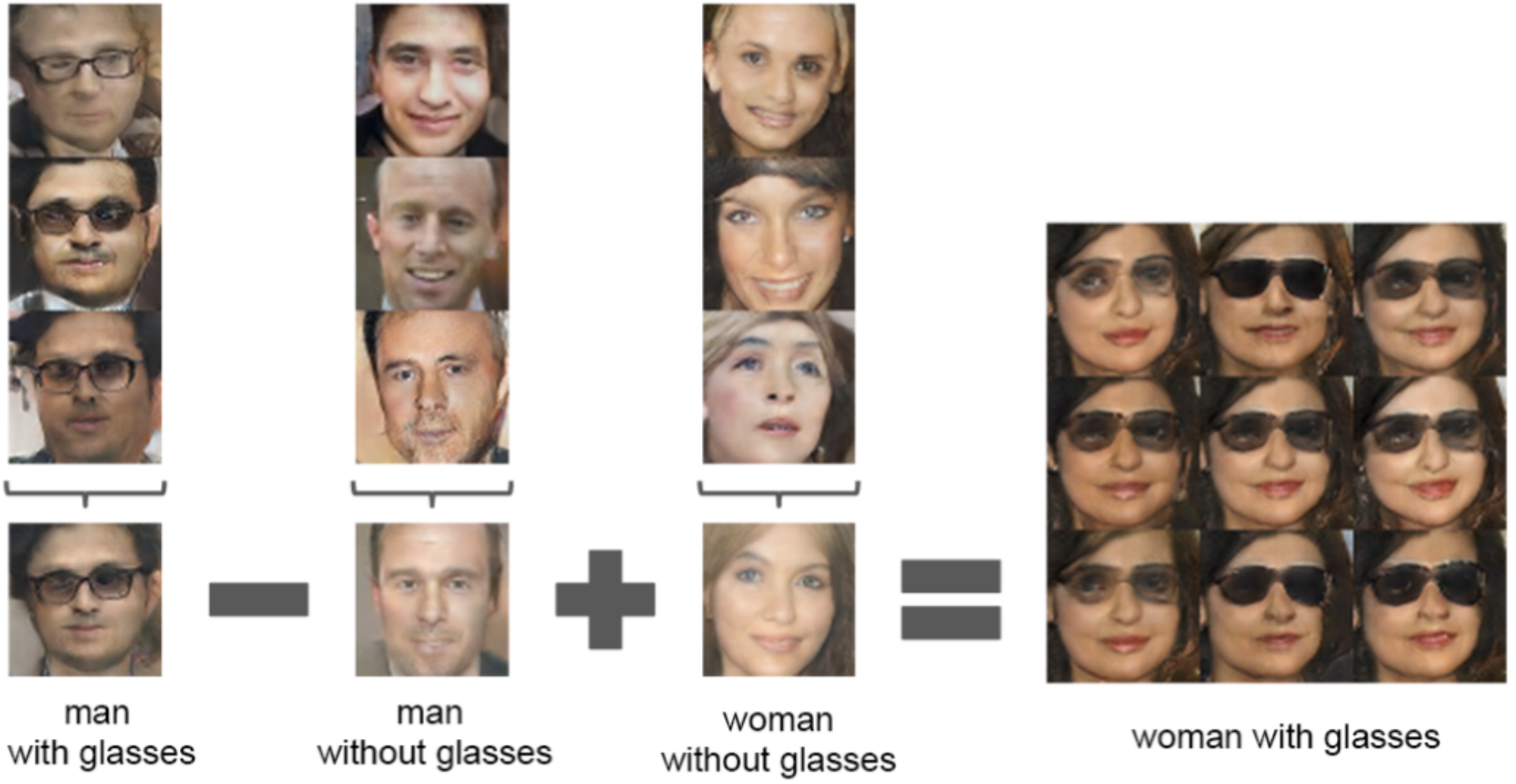


"Latent" variables
(states, kinetics, properties…)

Example:
Generative Adversarial Network

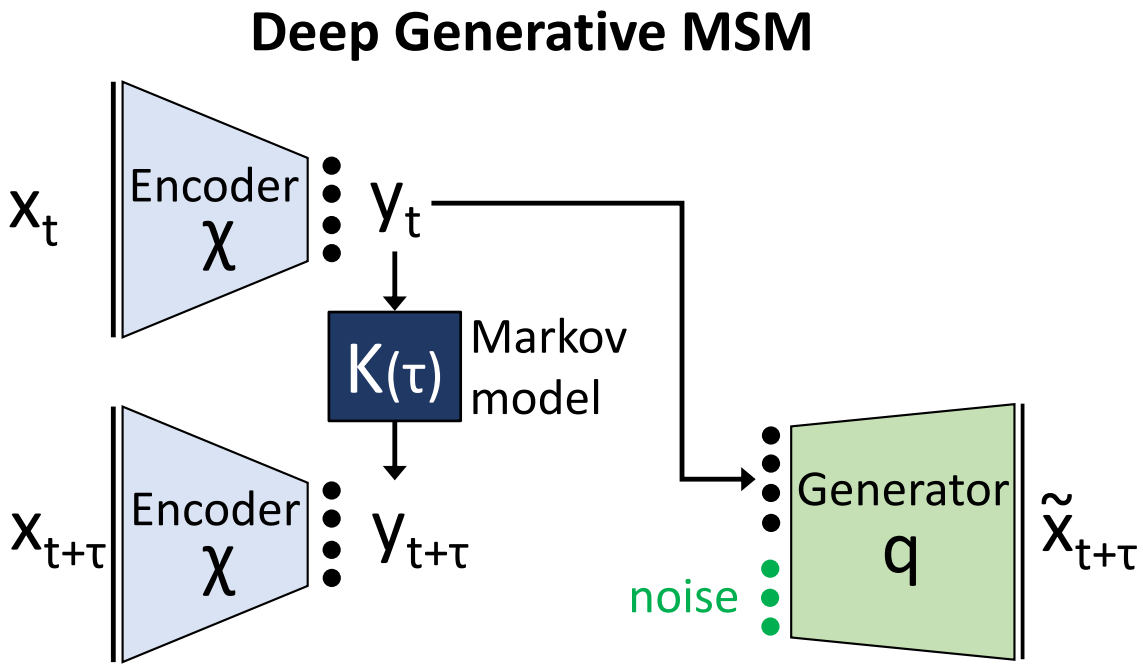


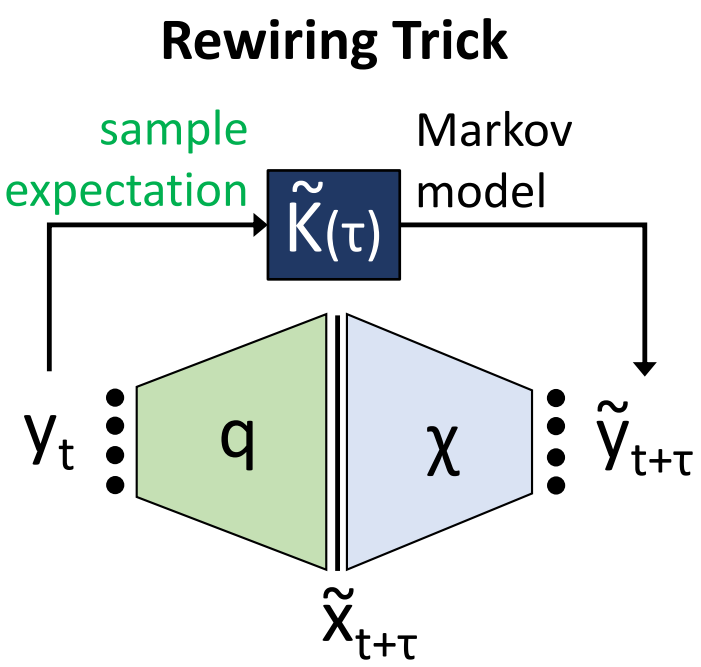
Generative Adversarial Network



Radford et al: Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks arXiv:1511.06434 (2015)

Deep Generative Markov State Models



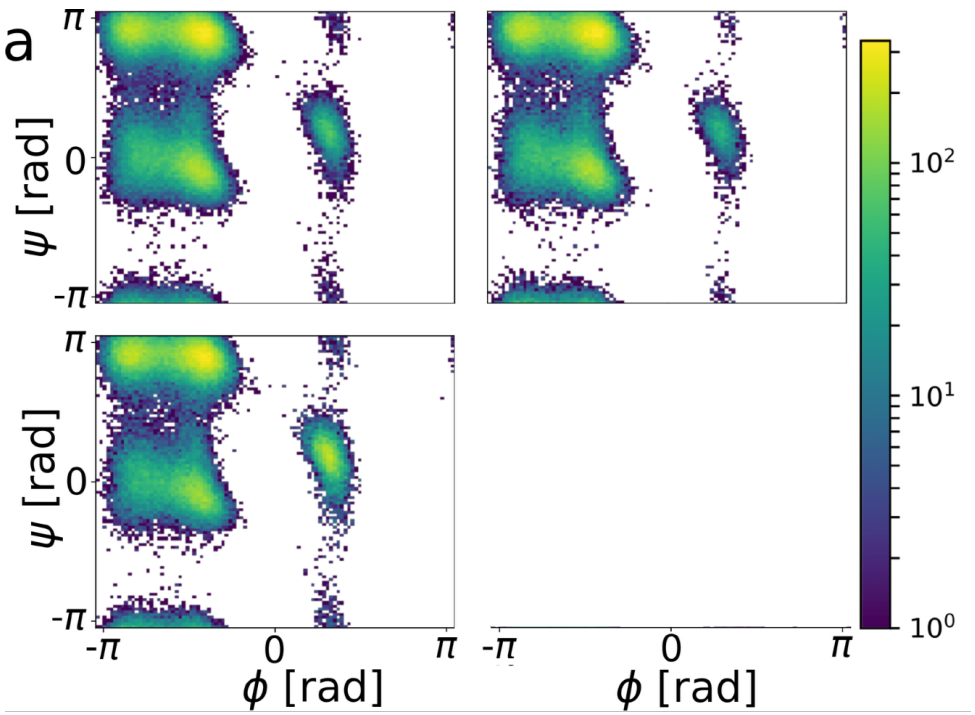


Wu, Mardt, Pasquali, Noé **NIPS** 2018 — arXiv:1805.07601

Deep Generative Markov State Models

Data

Deep MSM, resampled



"good" classical MSM

Wu, Mardt, Pasquali, Noé **NIPS** 2018 — arXiv:1805.07601

Deep Generative Markov State Models

Energy distance between distributions:

$$D_E\left(\mathbb{P}(x), \mathbb{P}(y)\right) = \mathbb{E}\left[2\left\|x-y\right\| - \left\|x-x'\right\| - \left\|y-y'\right\|\right]$$

with

$$x, x' \sim \mathbb{P}(x)$$

$$y, y' \sim \mathbb{P}(y)$$

D_E = 0 only if distributions are equal

—> Train Generator Network by minimizing Energy Distance

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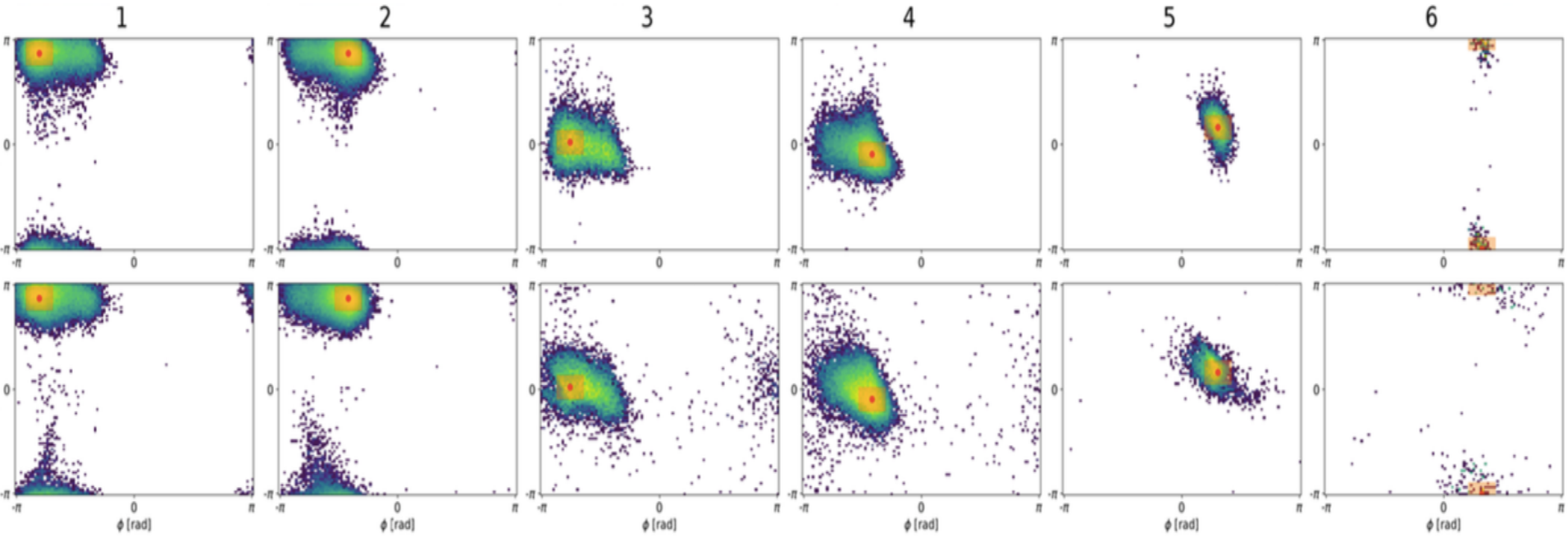
Deep Generative Markov State Models

Learning transition densities

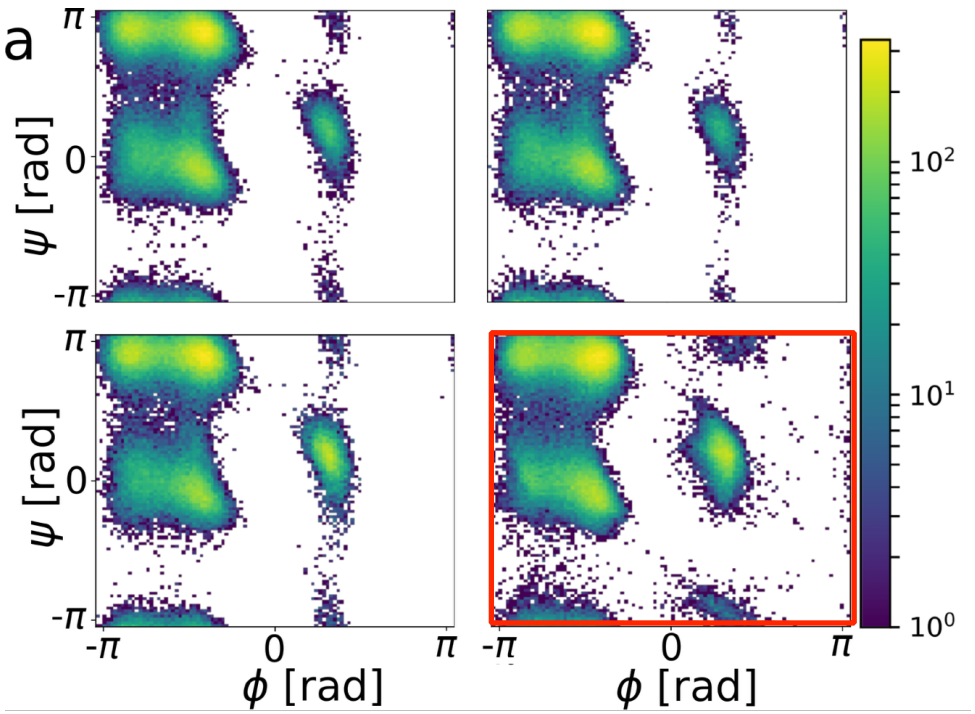


Wu, Mardt, Pasquali, Noé **NIPS** 2018 — arXiv:1805.07601

Deep Generative Markov State Models

Data

Deep MSM, resampled

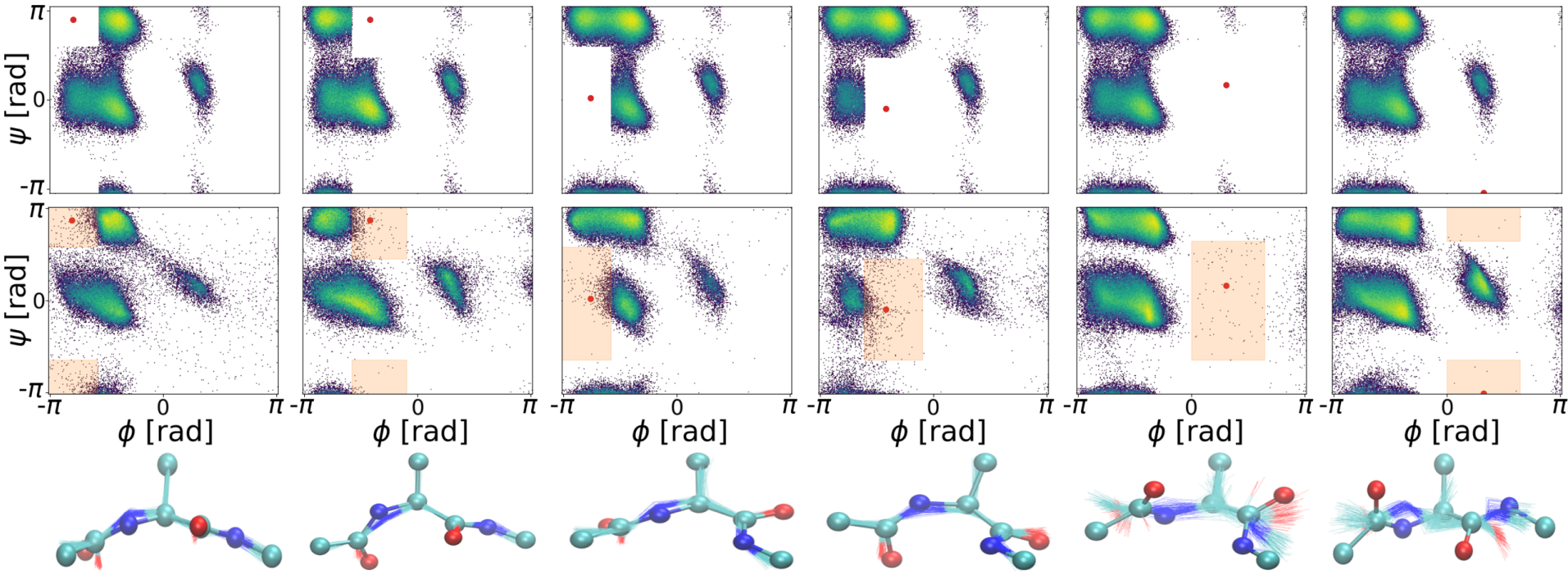


"good" classical MSM

Deep generative MSM

Wu, Mardt, Pasquali, Noé **NIPS** 2018 — arXiv:1805.07601

Deep Generative Markov State Models



Wu, Mardt, Pasquali, Noé **NIPS** 2018 — arXiv:1805.07601

Acknowledgements

Collaborations

Cecilia Clementi (Rice University)
Christof Schütte (FU Berlin)
Eric Vanden-Eijnden (Courant Institut NY)
Thomas Weikl (MPI Potsdam)
Edina Rosta (King's College London)

Vijay Pande (Stanford)
Volker Haucke (FMP Berlin)
Stephan Sigrist (FU Berlin)
Katja, Faelber, Oliver Daumke (MDC)
John Chodera (MSKCC NY)
Gianni de Fabritiis (Barcelona)

Funding

erc
EINSTEIN Foundation.de
DFG Deutsche Forschungsgemeinschaft
Freie Universität Berlin