Optimal control for sampling the transition path process and estimating rates

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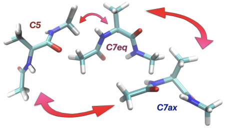
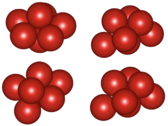
Motivation

We would like to study rare transitions in systems governed by SDEs



Conformal changes in biomolecules



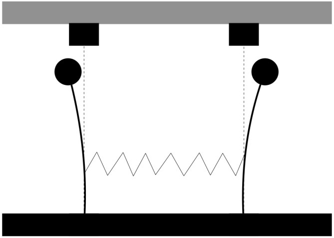
Cluster rearrangements

Langevin SDE

$$\begin{cases} dX_t = m^{-1} P_t dt \\ dP_t = -(\nabla U + \gamma P_t) dt + \sqrt{2\gamma\beta^{-1} m} dW_t^n \end{cases}$$

Overdamped Langevin SDE

$$dX_t = -\nabla U(X_t) dt + \sqrt{2\beta^{-1}} dW_t^n$$

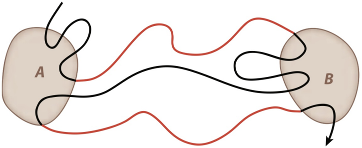


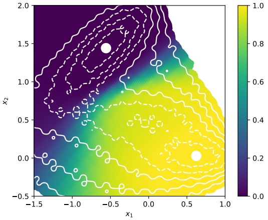
Oscillators with multiple equilibria or stable modes

Transition path theory

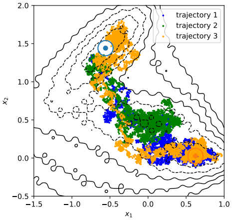
Forward and backward committor function

$$\begin{cases} q^+(y) = \mathbb{P}\{\tau_B^+(y) < \tau_A^+(y)\} \\ q^-(y) = \mathbb{P}\{\tau_A^-(y) < \tau_B^-(y)\} \end{cases}$$

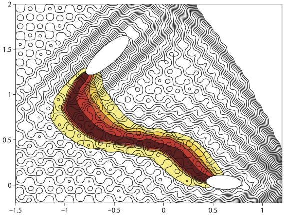




Committor function



Reactive trajectories



Probability current (E and Vanden-Eijnden, 2010)

Reactive current: $J_R(x) = \beta^{-1} Z^{-1} e^{-\beta U(x)} \nabla q(x)$

Transition rate: $\nu_R = \beta^{-1} Z^{-1} \int_{\Omega_{AB}} \|\nabla q(x)\|^2 e^{-\beta U(x)} dx$

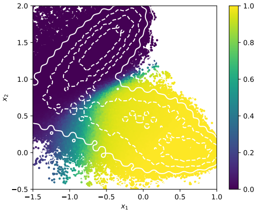
Committor function

The **forward committor function** satisfies

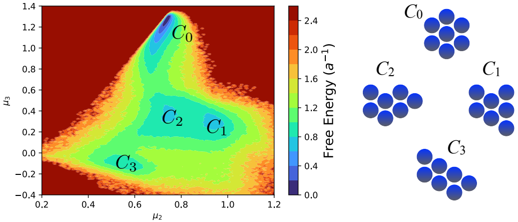
$$\begin{cases} Lq(x) = \nabla U \cdot \nabla q - \beta^{-1}\Delta q = 0, & x \in \Omega\backslash(A \cup B) \\ q(x) = 0, & x \in \partial A \\ q(x) = 1, & x \in \partial B \end{cases}$$

The **backward committor function**

$$\begin{cases} \text{Langevin Equation:} \quad q^{-}(x,p) = 1 - q(x,-p) \\ \text{Overdamped Langevin Equation:} \quad q^{-}(x) = 1 - q(x) \end{cases}$$



NN approximation



Reduced model for LJ7

Stochastic optimal control

Inexact committor $\rightarrow$ inexact transition rate.

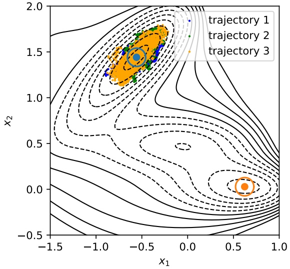
Our remedy: stochastic optimal control.

SDEs with rare transitions

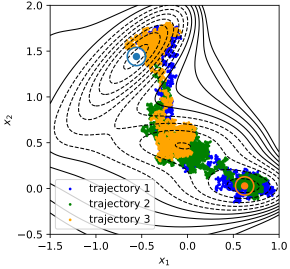
$$dX_t = -b(X_t)dt + \sigma(X_t)dW_t^n$$

SDEs with stochastic controller

$$d\tilde{X}_t = \left[-b(\tilde{X}_t) + \sigma\sigma^\top(\tilde{X}_t)v(t,\tilde{X}_t)\right]dt + \sigma(\tilde{X}_t)dW_t$$



(a) trajectories without control



(b) $\sigma\sigma^\top v = 2\beta^{-1}\nabla \log q^+$

Related work and our goal

- Lu and Nolen (2015): Doob's h-transform; transition path process for Ito's SDEs.
- Gao, Li, Li, Liu (2022): optimal control problem for sampling reactive trajectories for overdamped Langevin dynamics and a rigorous proof for the optimal controller $\frac{\beta}{2}\nabla \log q$
- Zhang, Sahai, Marzouk (2022): fixed time horizon, even a rough approximation to the backward Kolmogorov equation yields a good controller
- Zhang, Hartmann, Schuette (2016): transition rate is overestimated due to inexact committors from the reduced model

We propose:

To combine transition path theory with stochastic optimal control for a more accurate estimate of transition rates and sampling transition paths.

Theorem

(Yuan, Shah, Bentz, and Cameron, 2023)

$$d\tilde{X}_t = \left[-b(\tilde{X}_t) + \sigma\sigma^\top(\tilde{X}_t)v(t, \tilde{X}_t)\right] dt + \sigma(\tilde{X}_t)dW_t$$

Assume that $\sigma(X_t) \in \mathbb{R}^{d\times r}$*: full rank. Cost functional:*

$$C_x[v(\cdot)] = \mathbb{E}_P \left[\frac{1}{2}\int_0^{\tau_{AB}} \|\sigma^\top(Y_s)v(Y_s)\|^2 ds + g(Y_\tau) \mid X_0 = x\right],$$

$$\text{where} \quad g(x) = \begin{cases} +\infty, & x \in \overline{A} \\ 0, & x \in \overline{B} \end{cases}, \quad \tau_{AB} = \inf\{t > 0 \mid X_t \in \bar{A} \cup \bar{B}\}$$

Under non-restrictive assumptions,

$$\mathbf{c}^*(\mathbf{x}) := \inf_{\mathbf{v}\in\mathcal{V}} \mathbf{C_x}[\mathbf{v}(\cdot)] = -\log \mathbf{q}^+(\mathbf{x}). \tag{1}$$

The corresponding optimal control v^* *satisfies*

$$\sigma^\top \mathbf{v}^* = \sigma^\top \nabla \log \mathbf{q}^+. \tag{2}$$

Cases of interest

Overdamped Langevin equations in collective variables

$$dX_t = [-M(X_t)\nabla F(X_t) + \beta^{-1}\nabla \cdot M(X_t)]dt + \sqrt{2\beta^{-1}}M(X_t)^{\frac{1}{2}}dW_t.$$

$$\Rightarrow \quad dX_t = [-M(X_t)\{\nabla F(X_t) - 2\beta^{-1}\nabla \log q^+\} + \beta^{-1}\nabla \cdot M(X_t)]dt + \sqrt{2\beta^{-1}}M(X_t)^{\frac{1}{2}}dW_t.$$

Langevin equations

$$\begin{cases} dx_t = m^{-1}pdt \\ dp_t = \left(-\nabla U(x_t) - \gamma_f p\right) dt + \sqrt{2\gamma_f \beta^{-1} m}dw_t \end{cases}$$

$$\Rightarrow \quad \begin{cases} dx_t = m^{-1}pdt \\ dp_t = \left(-\nabla U(x_t) - \gamma_f p + 2\gamma_f \beta^{-1} m \nabla_p \ln q\right) dt + \sqrt{2\gamma_f \beta^{-1} m}dw_t \end{cases}$$

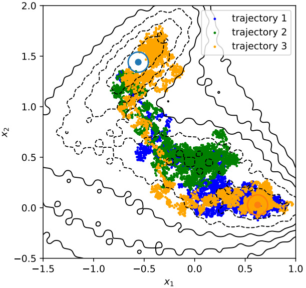
Challenges

1. Computation of the committor function in high-dimensional space

$$\begin{cases} Lq(x) = \nabla U \cdot \nabla q - \beta^{-1}\Delta q = 0, & x \in \Omega_{AB} \\ q(x) = 0, & x \in \partial A \\ q(x) = 1, & x \in \partial B \end{cases}$$

2. Rate estimation from crossover times

$$\nu_{AB} = \lim_{T\to\infty} \frac{N_{AB}}{T}$$



Solution to the committor

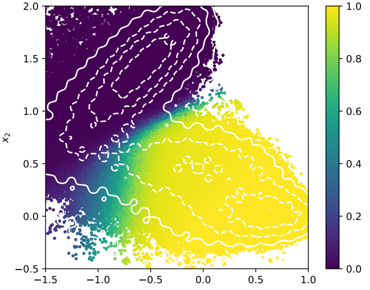
- **Overdamped Langevin equation**: scheme by Li, Lin, Ren (2019)

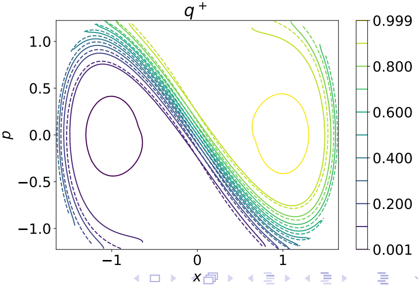
$$q(x;\theta) = (1-\chi_A(x))[(1-\chi_B(x))\mathcal{N}(x;\theta)+\chi_B(x)], \quad x\in\Omega_{AB},$$

$$\text{Loss}(\theta) = \frac{1}{K}\sum_{k=1}^{K}\left[\nabla q(x_k;\theta)^\top M(x_k)\nabla q(x_k;\theta)\frac{e^{-\beta F(x_k)}}{\rho(x_k)}\right].$$

- **Langevin equation**: PINN by Karniadakis et al. (2022)

$$\text{Loss}(\theta) = \frac{1}{K}\sum_{(x_k,p_k)\in\Omega_{AB}}|\mathcal{L}\mathcal{N}(x_k,p_k;\theta)|^2 + \frac{1}{K_{\partial A}}\sum_{(x_k,p_k)\in\partial A}|\mathcal{N}(x_k,p_k)|^2 + \frac{1}{K_{\partial B}}\sum_{(x_k,p_k)\in\partial B}|\mathcal{N}(x_k,p_k)-1|^2$$





Estimation of transition rate

Transition rate

$$\nu_{AB} = \lim_{T\to\infty} \frac{N_{AB}}{T}$$

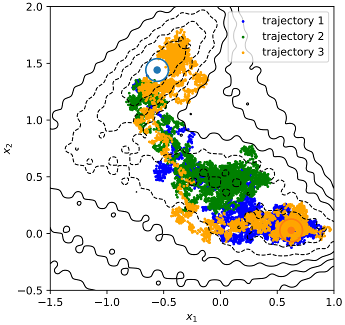
- inaccurate estimate of the committor function
- suboptimal choice set of collective variables when model reduction is used

$$\nu_{AB} = \frac{\rho_{AB}}{\mathbb{E}[\tau_{AB}]}$$

where

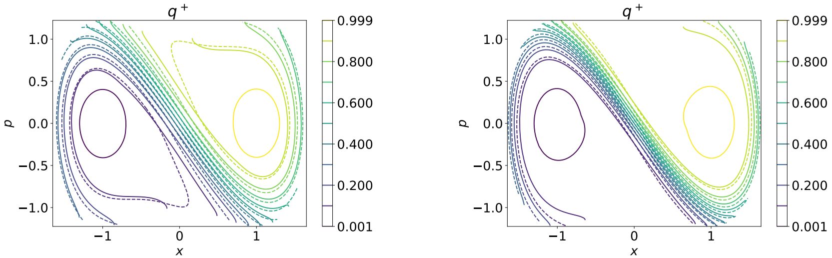
$$\rho_{AB} = \int_{\Omega_{AB}} \mu q^+ q^- dx$$

$$\nu_{AB} = \beta^{-1} Z^{-1} \int_{\Omega_{AB}} \|\nabla q(x)\|^2 e^{-\beta U(x)} dx$$



Duffing Oscillator in 1D

$$d\begin{bmatrix} X_t \\ P_t \end{bmatrix} = \begin{bmatrix} P_t \\ -X_t(X_t^2 - 1) - \frac{1}{2}P_t \end{bmatrix} dt + \sqrt{\epsilon}\begin{bmatrix} 0 \\ dW_t \end{bmatrix}.$$



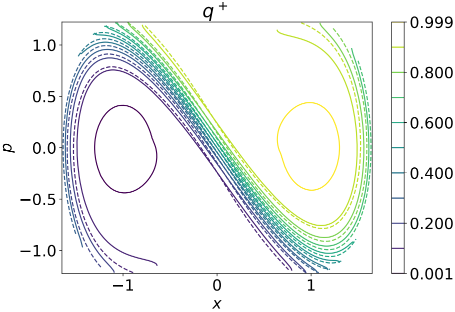
(a) $\epsilon = 0.1$ (b) $\epsilon = 0.05$

Duffing oscillator $\epsilon = 0.1$				
	Simul., o/c	Simul., w/o o/c	TPT, NN	TPT, FEM
ν_{AB}	[5.50e-3,6.07e-3]	**[5.76e-3,6.01e-3]**	4.53e-3	5.74e-3
Duffing oscillator $\epsilon = 0.05$				
ν_{AB}	[5.53e-4,6.06e-4]	**[5.49e-4,6.51e-4]**	4.72e-4	5.49e-4

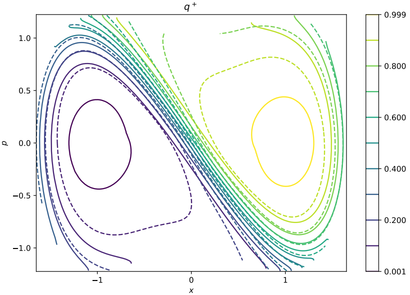
Effect of undertrained NN

	wMAE	wRMSE	$\mathbb{E}[\tau_{AB}]$
Case 0 (epoch 500)	1.3e-2	2.0e-2	7.34 ± 0.33
Case 1 (epoch 300)	4.9e-2	6.1e-2	7.88 ± 0.36
Case 2 (epoch 150)	6.0e-2	7.7e-2	8.48 ± 0.84
Case 3 (epoch 125)	7.9e-2	10.2e-2	12.18 ± 2.49
Case 4 (epoch 100)	13.6e-2	16.7e-2	48.86 ± 5.71

Ground truth $\mathbb{E}[\tau_{AB}] = \mathbf{7.48 \pm 0.49}$



case 0

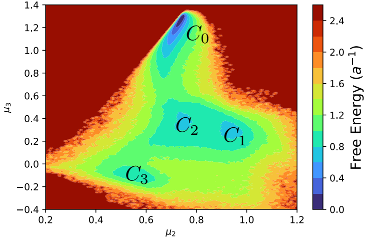


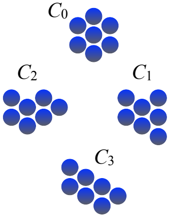
case 1

Lennard-Jones-7 in 2D

$$V_{\text{pair}}(r) = 4a\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

$$V_{\text{LJ}}(x) = \sum_{\substack{i,j=1\\ i<j}}^{7} V_{\text{pair}}(\|x_i - x_j\|)$$





Reduced model

$$c_i(x) = \sum_{i\neq j} \frac{1-\left(\frac{r_{ij}}{1.5\sigma}\right)^8}{1-\left(\frac{r_{ij}}{1.5\sigma}\right)^{16}}, \quad r_{ij} = \|x_i - x_j\|.$$

$$\mu_k(x) = \frac{1}{7}\sum_{i=1}^{7}(c_i(x) - \bar{c}(x))^k, \quad \text{where} \quad \bar{c}(x) = \frac{1}{7}\sum_{j=1}^{7} c_j(x).$$

	Simul., o/c	Simul., w/o o/c	TPT, NN	TPT, FEM
Dimension	14D	14D	2D	2D
ν_{AB}	**0.022, [0.020, 0.024]**	**0.025, [0.019, 0.033]**	0.097	0.086

Future work

Overestimation of transition rates in reduced model
(Zhang, Hartmann, and Schuette, 2016)

$$\nu_{AB} \leq \tilde{\nu}_{AB} = \nu_{AB} + \frac{1}{\beta}\int_{\Omega_{AB}} \nabla[q(x) - \tilde{q}(\xi(x))]^\top M(x)\nabla[q(x) - \tilde{q}(\xi(x))]\mu(x)dx$$

Develop a methodology for learning collective variables that represent the dynamics well.

Reference

Jiaxin Yuan, Amar Shah, Channing Bentz, and Maria Cameron. *Optimal control for sampling the transition path process and estimating rates.* Communications in Nonlinear Science and Numerical Simulation. Volume 129, February 2024, 107701. ArXiv: 2305.17112.