Machine learning methods for the study of rare events in stochastic systems

REU: Modern topics in pure and applied mathematics

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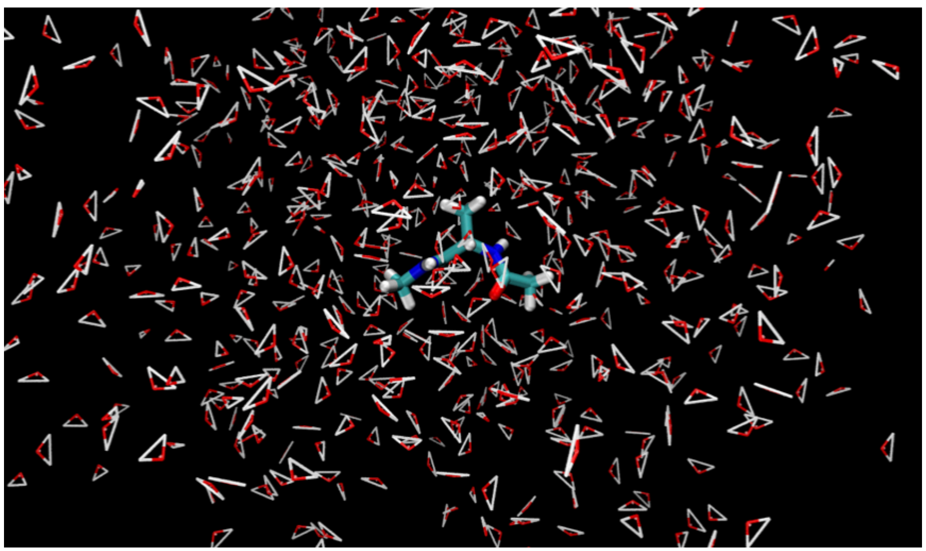
What are rare events?

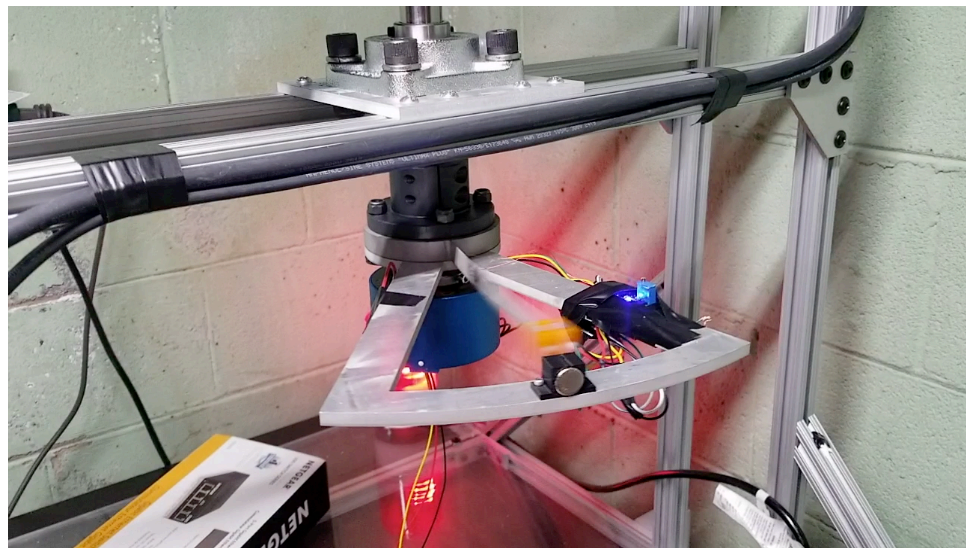
Rare events are those that occur rarely on the timescale of the system

Dynamics of
an alanine-dipeptide molecule
pushed around by water molecules



https://ambermd.org/tutorials/basic/tutorial0/index.php

A noise-driven transition from
the high- to the low-amplitude attractor
in an electromechanical
nonlinear oscillator



Lautaro Cilenti, Clark Fellow, Dept. of Mech. Eng. UMD

Stochastic differential equations

$$dX_t = \underbrace{b(X_t)dt}_{\text{Deterministic forcing}} + \underbrace{\sqrt{\epsilon}\sigma(X_t)dW_t}_{\text{Stochastic forcing}}, \qquad X_t \in \mathcal{M} \subset \mathbb{R}^d$$

Deterministic forcing: $b(X_t)dt$

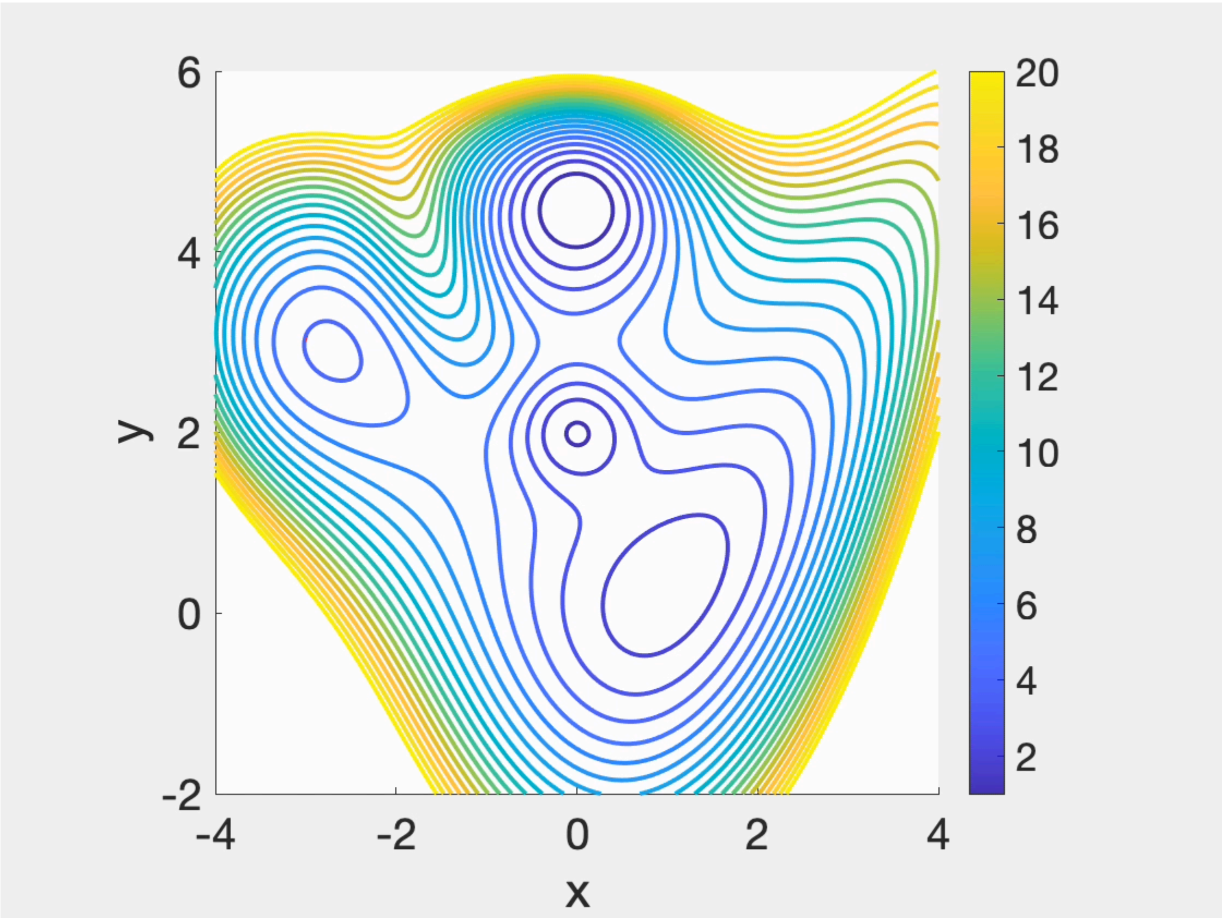
Stochastic forcing: $\sqrt{\epsilon}\sigma(X_t)dW_t$

- b: A smooth vector field
- ϵ: A small parameter
- σ: A smooth matrix function
- W_t: The standard Brownian motion

The overdamped Langevin dynamics

A simple and important model

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



Invariant pdf is
the Gibbs density:

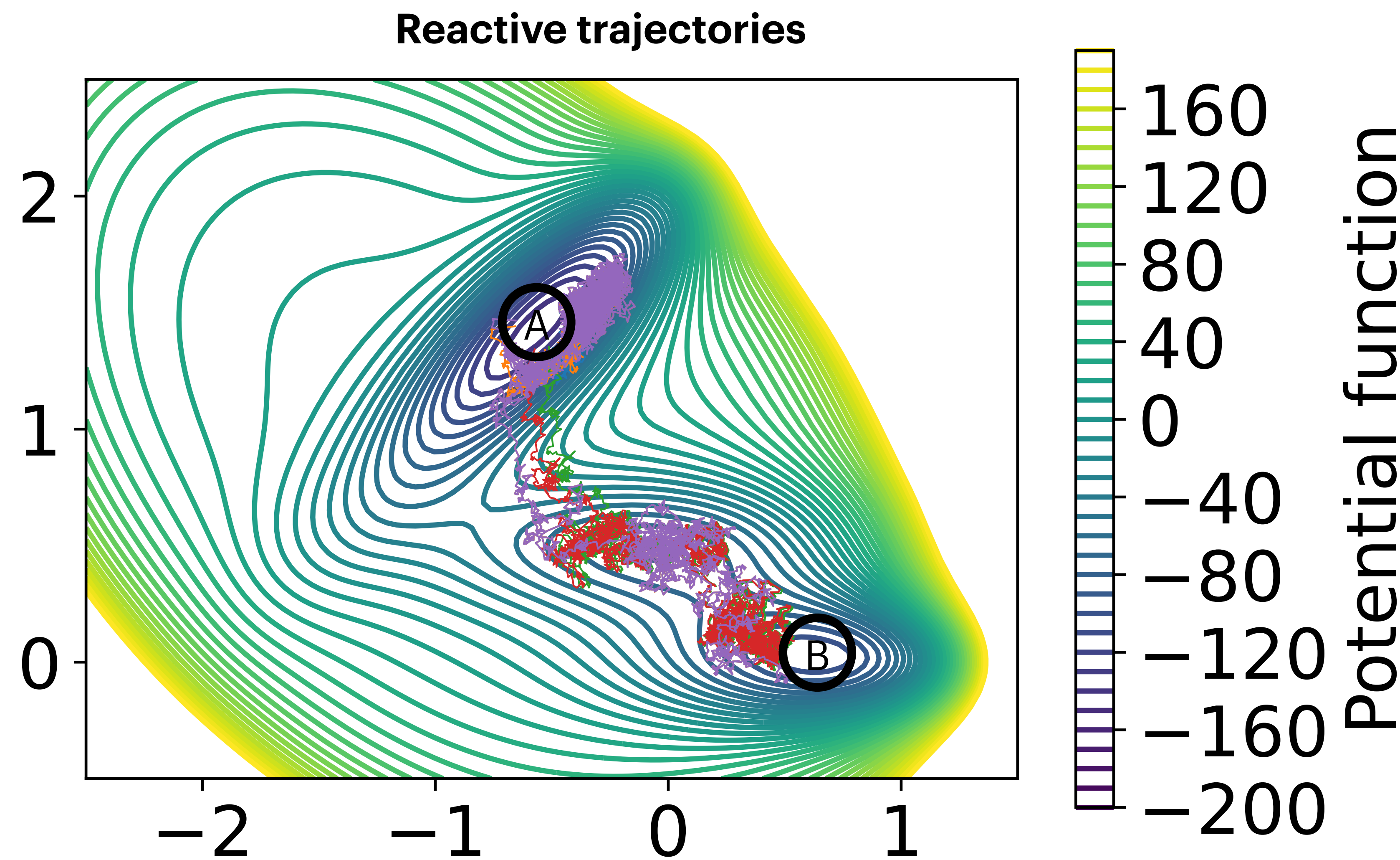
$$\mu(x) = Z^{-1}e^{-\beta V(x)}$$

Expected exit time
from the basin of $x_{\min}$:

$$\mathbb{E}[\tau_{\partial B_{x_{\min}}}] \approx Ce^{\beta(V(x_{\text{saddle}})-V(x_{\min}))}$$

Transition path theory

W. E and E. Vanden-Eijnden, 2006



The ***committor*** is the probability that the process starting at *x* will reach region *B* prior to reaching region *A*

$$q(x) := \text{Prob}_x(\tau_B < \tau_A)$$

Transition path theory

W. E and E. Vanden-Eijnden, 2006

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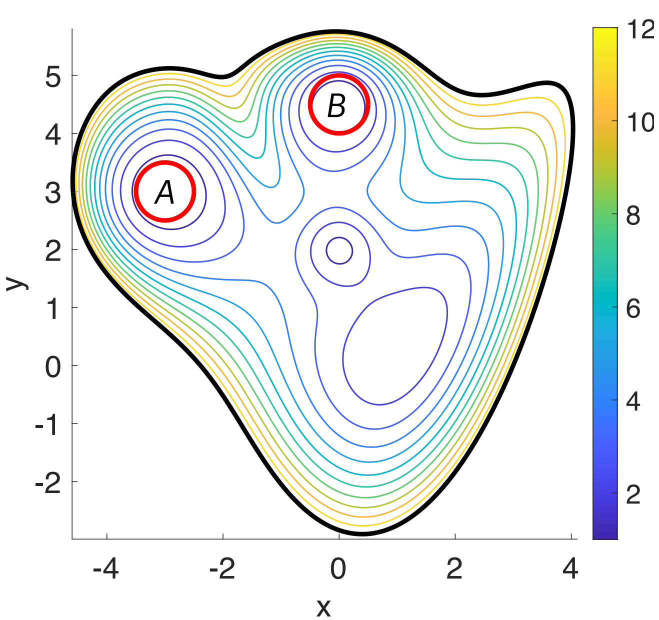
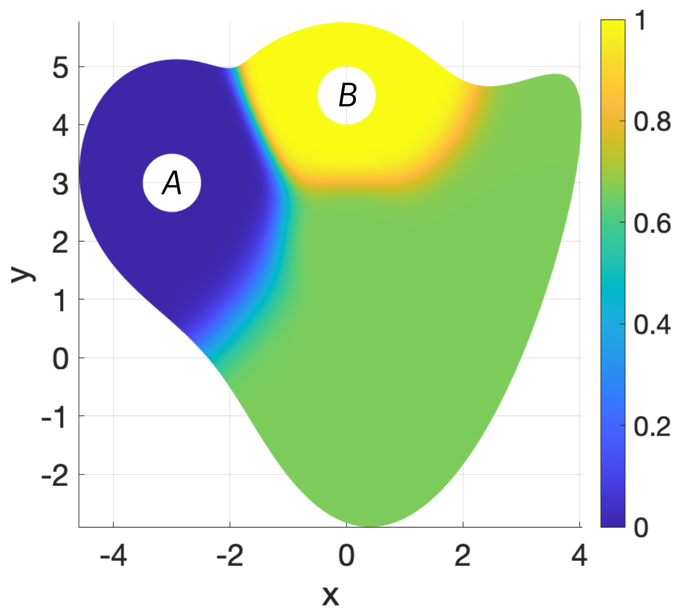
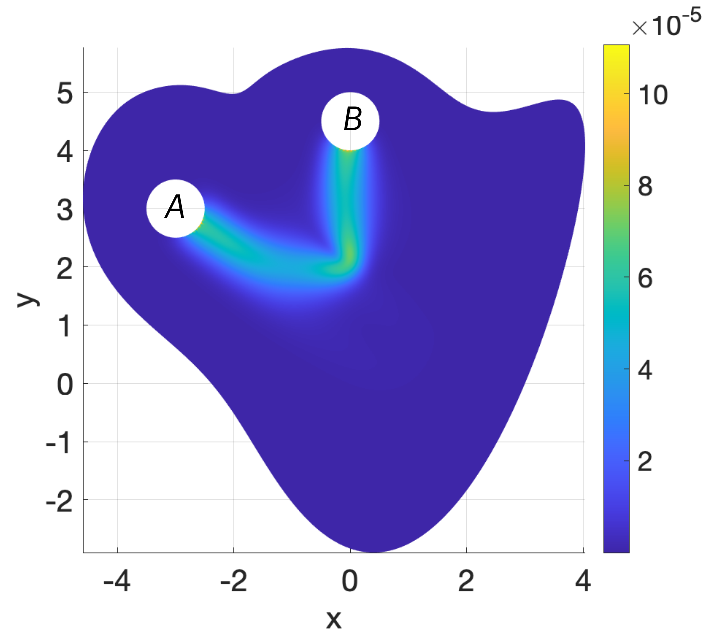
The potential function



The committor



The reactive current



$$\mu(x) = Z^{-1} e^{-\beta V(x)}$$

$$J(x) = \beta^{-1} \mu \nabla q(x)$$

The reaction rate: $$\nu_{AB} = \beta^{-1} \int_{\Omega_{AB}} \|\nabla q\|^2 \mu dx$$

Transition path theory

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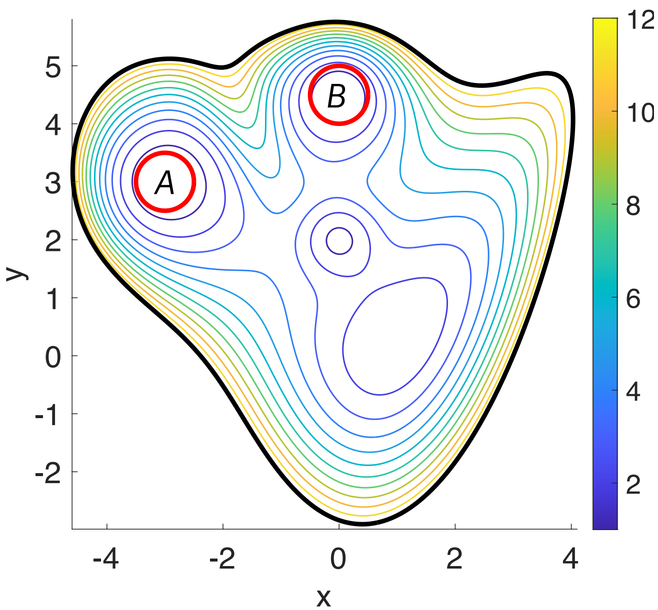
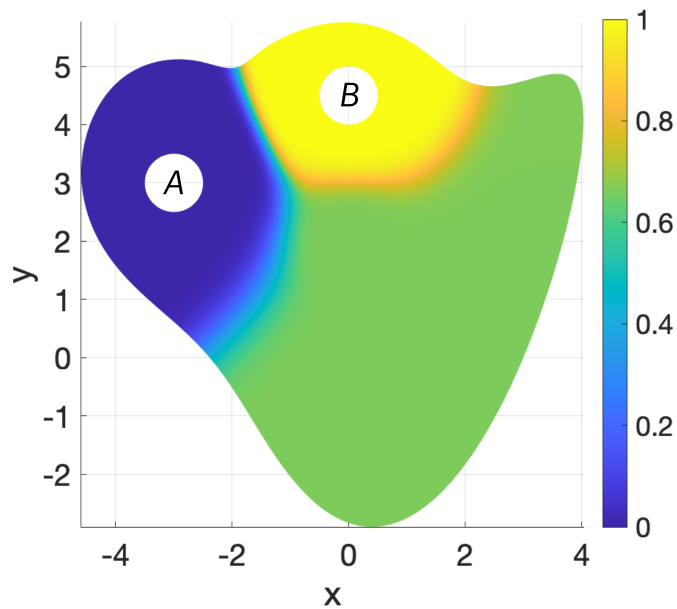
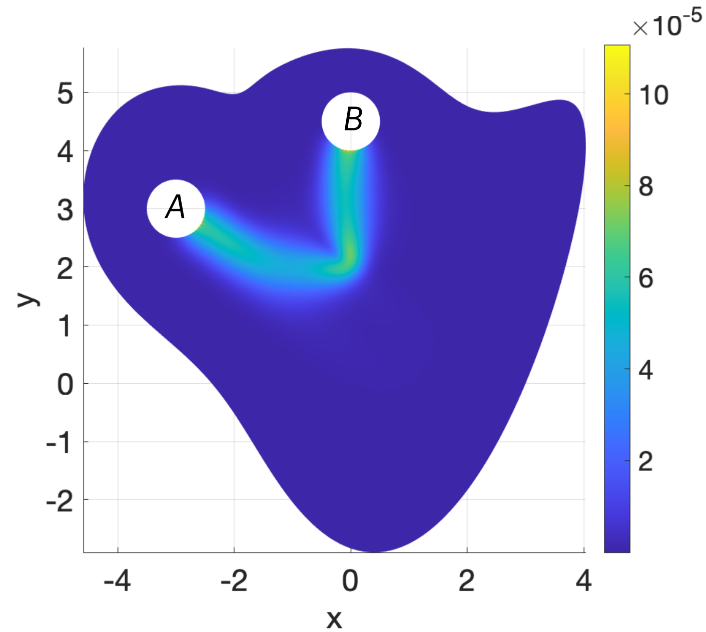


$$\mu(x) = Z^{-1} e^{-\beta V(x)}$$

The committor



The reactive current



$$J(x) = \beta^{-1} \mu \nabla q(x)$$

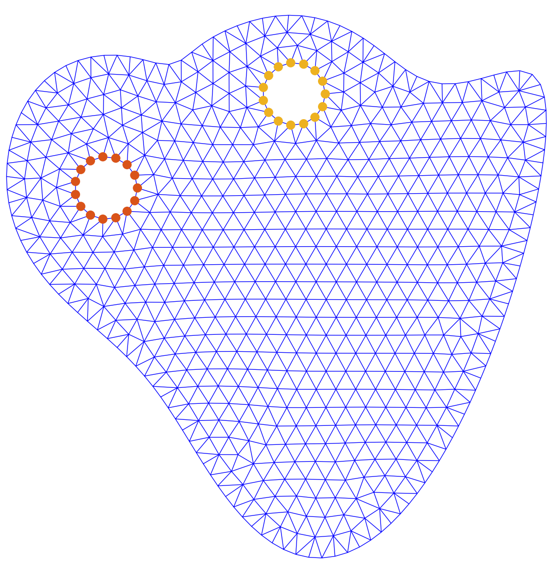
The reaction rate: $$\nu_{AB} = \beta^{-1} \int_{\Omega_{AB}} \|\nabla q\|^2 \mu dx$$

Computing the committor

To find the committor, we need to solve:

$$\mathcal{L}q = \beta^{-1} e^{\beta V} \nabla \cdot \left(e^{-\beta V} \nabla q \right) = 0$$
$$q(\partial A) = 0$$
$$q(\partial B) = 1$$

- **Approach 1:** ***finite element method***



Good only for low dimensions

d = 2: easy to use

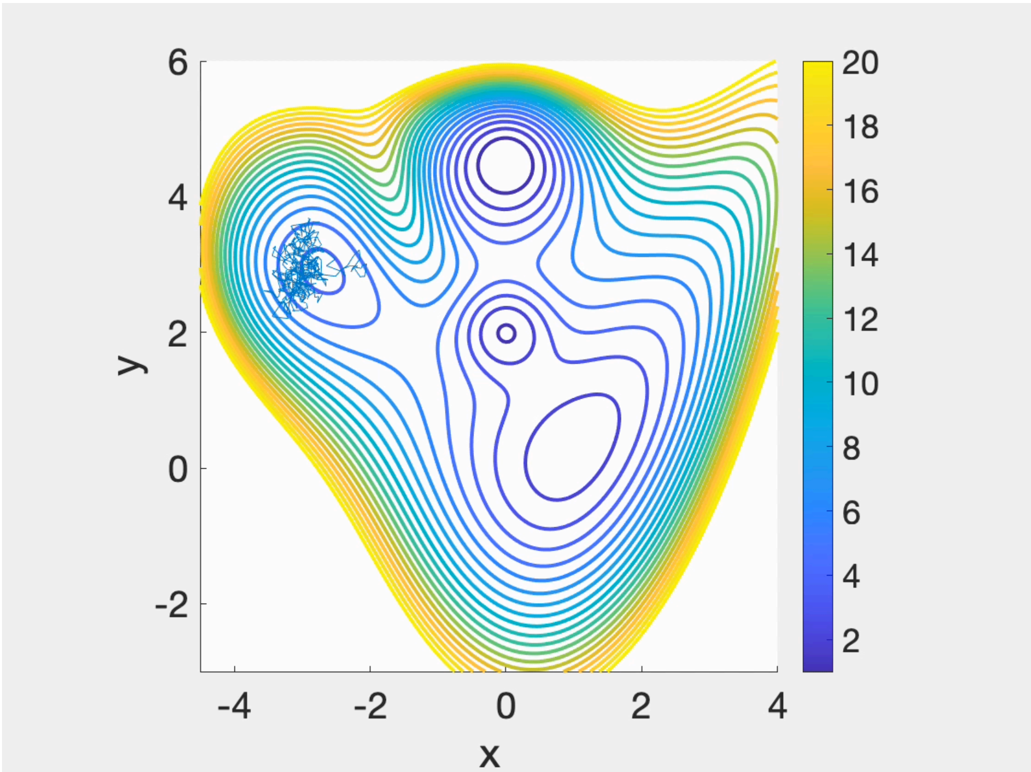
d = 3: possible but harder

Computing the committor

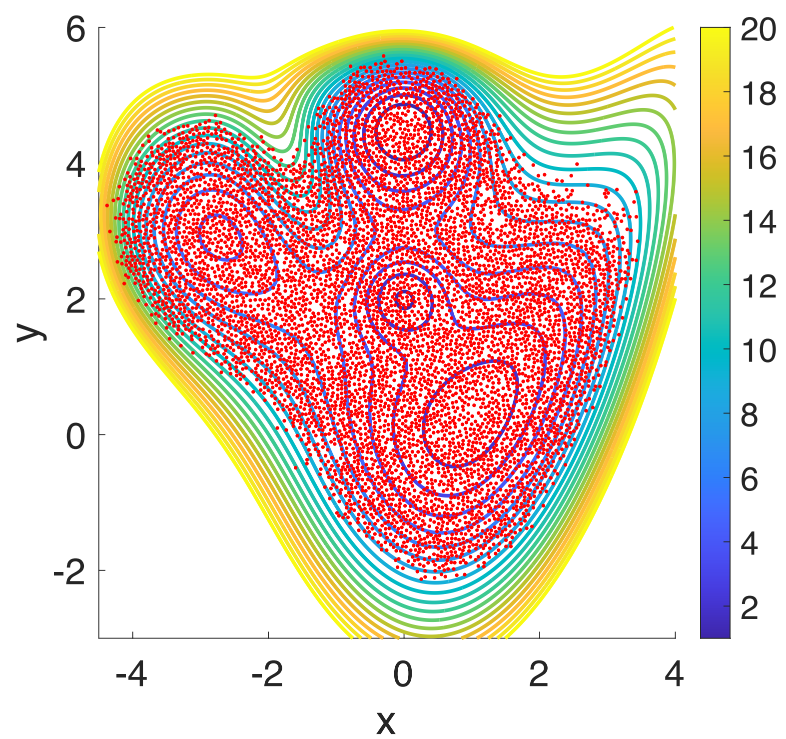
$$\mathcal{L}q = \beta^{-1} e^{\beta V} \nabla \cdot \left(e^{-\beta V} \nabla q \right) = 0, \qquad q(\partial A) = 0, \quad q(\partial B) = 1$$

- **Meshless approaches:** diffusion maps, neural networks

Enhanced sampling: ***metadynamics***



Subsample data set: ***delta-net***



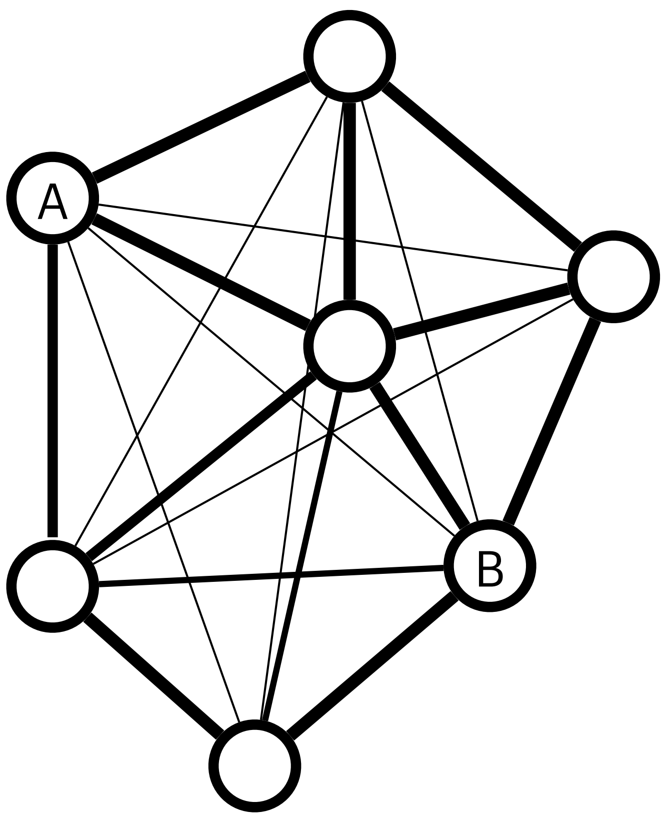
$$\delta = 0.05$$

Computing the committor

- **Approach 2:** ***diffusion map***

Ref: Coifman and Lafon (2006)

Idea: we construct a Markov chain whose dynamics approximate the dynamics of the original SDE



$$P = \{P_{ij}\}$$ Stochastic matrix

$$L = P - I$$ Generator matrix

The committor equation

$$\sum_j L_{ij} q_j = 0, \quad i \in (A \cup B)^c$$

$$q_i = 0, \quad i \in A$$
$$q_i = 1, \quad i \in B$$

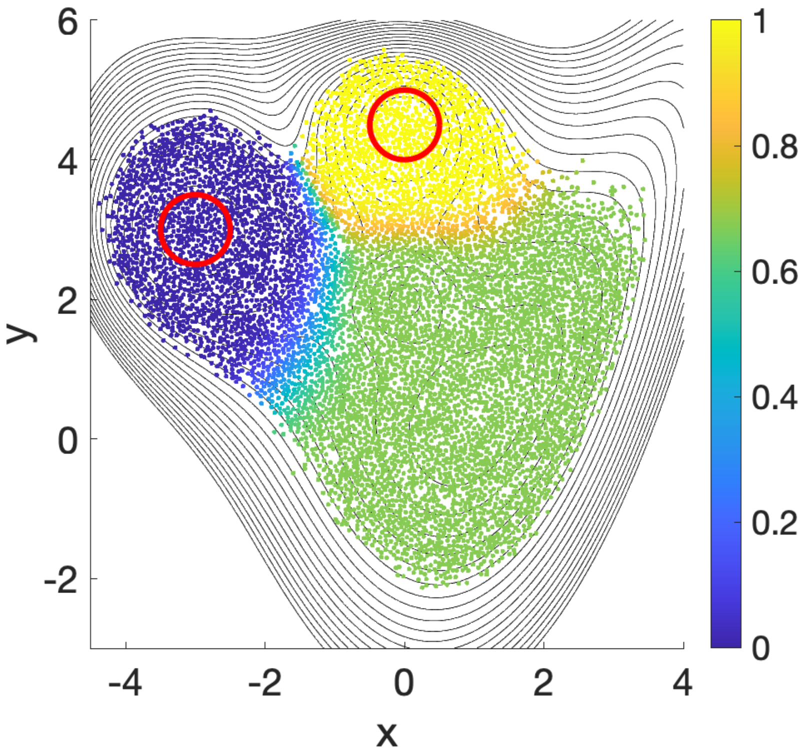
Computing the committor

- **Approach 2:** ***diffusion map***

Key refs: Coifman and Lafon (2006), Banisch, Trstanova, Bittracker, Klus, Koltai (2020)

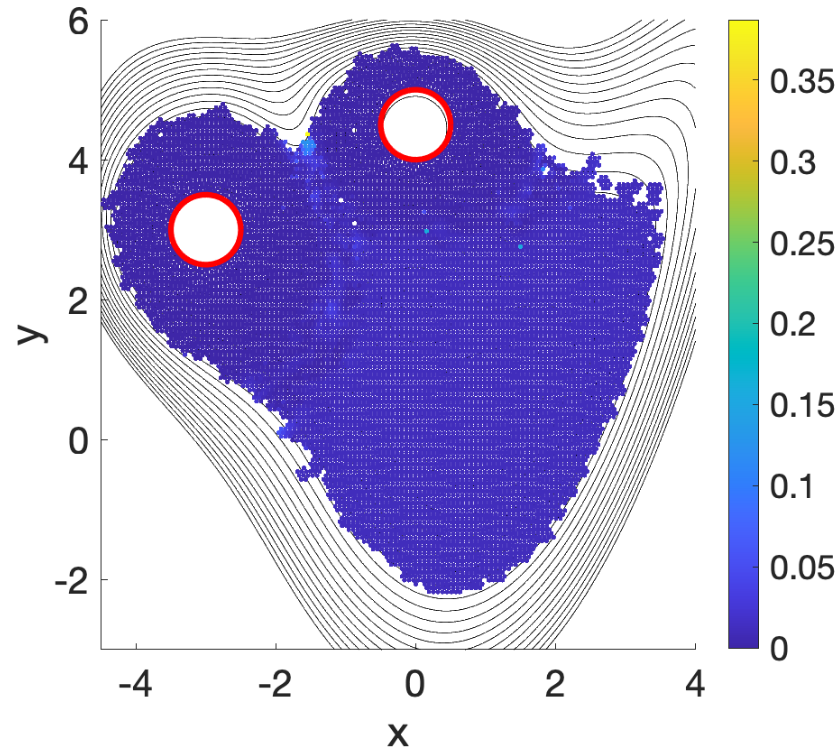
Idea: we construct a Markov chain whose dynamics approximate the dynamics of the reactive trajectories

The committor found using ***target measure diffusion map***



$\epsilon = 0.01$

Error relative to the FEM solution



$$\sum_j \mu_R(x_j)[q_{FEM}(x_j) - q_{TMDmap}(x_j)] = 1.03 \cdot 10^{-2}$$

Computing the committor

- **Approach 3:** ***neural network***

Key refs: Khoo, Lu, Ying (2018), Li, Lin, Ren (2019)

Idea: setup up an optimization problem for the committor, represent its solution as a neural network, and train the neural network

$$\mathcal{N}(x,\theta) = \sigma_1\left(A_1(\sigma_0\left(A_0 x + b_0\right) + b_1\right)$$ A neural network

$$\theta = \{A_0, b_0, A_1, b_1\}$$ The parameters to be found

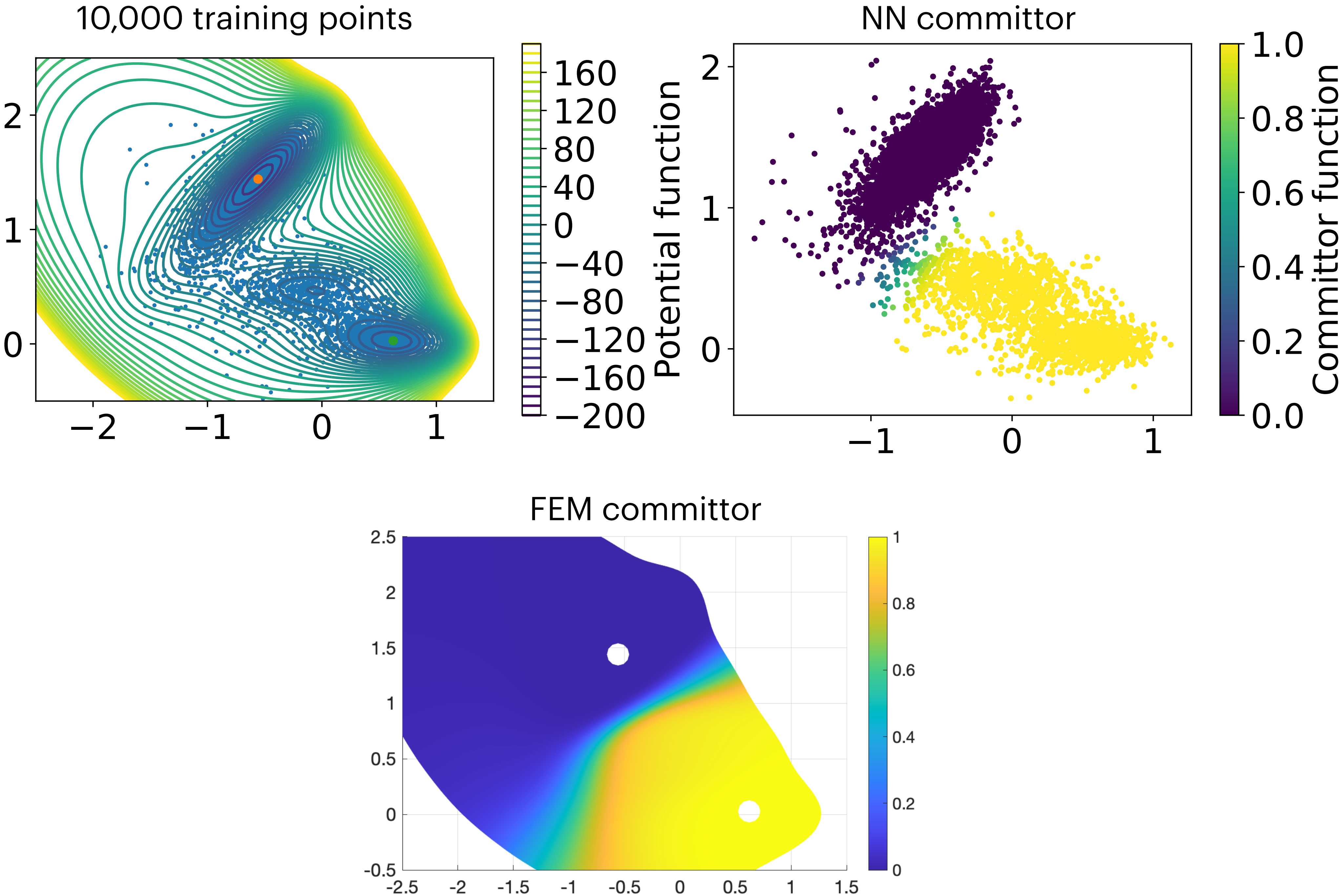
$$q(x) = f\left(\mathcal{N}(x,\theta), x\right)$$ We represent the committor as a function of the neural network

The committor is the solution to:

$$\mathcal{L}q = \beta^{-1} e^{\beta V} \nabla \cdot \left(e^{-\beta V} \nabla q\right) = 0$$
$$q(\partial A) = 0$$
$$q(\partial B) = 1$$

⇔

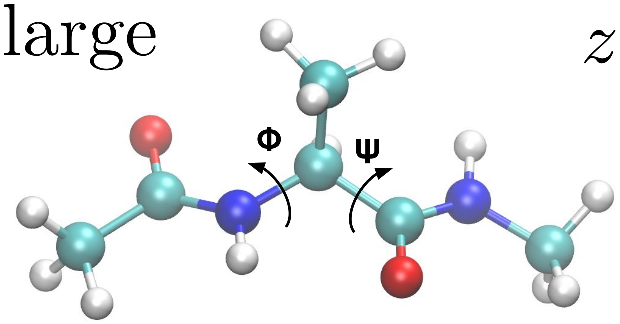
$$\int_{(A \cup B)^c} \|\nabla q\|^2 \mu(x) dx \quad \to \quad \min$$
subject to
$$q(\partial A) = 0$$
$$q(\partial B) = 1$$


10,000 training points
Potential function
NN committor
Committor function
FEM committor

The committor as an optimal controller for sampling reactive trajectories

$x \in \mathbb{R}^n, \quad n$ is very large

Full-space data



$z \in \mathbb{R}^d, \quad d$ is 2,3,4

Collective variables

- We can approximate the committor *q*(*z*) in collective variables via solving the backward Kolmogorov equation via: (1) Diffusion maps, (2) neural networks, (3) tensor trains, (4) FEM (if *d* = 2).

- Use the committor *q*(*z*(*x*)) as the ***controller*** for the stochastic process: Zhang, Sahai, Marzouk https://arxiv.org/abs/2101.07330, Gao, Li, Li, Liu https://arxiv.org/abs/2010.09988

- Sample rare events in higher-dimensional space. A good test: Alanine dipeptide: go from two to four dihedral angles.

The committor as an optimal controller for sampling reactive trajectories

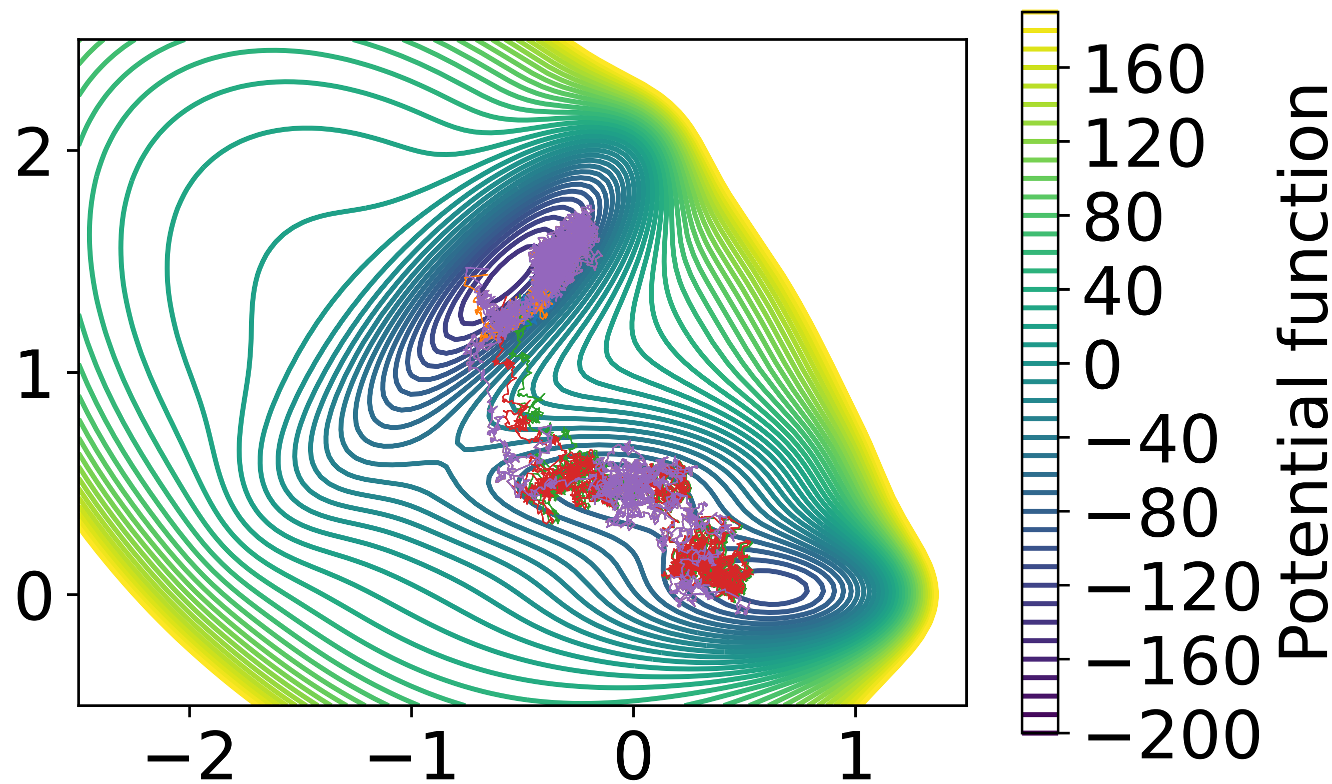
Key ref: Gao, Li, Li, Liu (2020)

The original governing SDE: $$dX_t = -\nabla V(X_t)dt + \sqrt{2\beta^{-1}}dW_t$$

Modify the drift: $$dX_t = -\left(\nabla V(X_t) - \frac{2\nabla q(X_t)}{\beta q(X_t)}\right)dt + \sqrt{2\beta^{-1}}dW_t$$

Sample reactive trajectories:

Restore the transition rate (e.g. B. Keller et al.)



Tutorials

June 14 — June 24

- Stochastic differential equations
- Markov Chains
- Transition Path Theory
- FEM
- Diffusion Maps
- Neural Networks
- Sampling reactive trajectories with the aid of an optimal controller

Tentative projects

- How does the architecture of the neural network affect the accuracy of the solution to the committor problem?
- How should we choose a training set for the neural network?
- Can a low-dimensional approximation to the committor be used to design a controller for a high-dimensional process?
- How can we restore the true transition rate if we are using an SDE with a controller for sampling transition paths?
- How does the training set affect the accuracy of the diffusion map-based solution to the committor problem?
- How can we adapt the diffusion map algorithm to compute committors for more complicated SDEs?
- A case study: alanine-dipeptide molecule described via two or four dihedral angles.
- Extension to systems with inertia: oscillators.