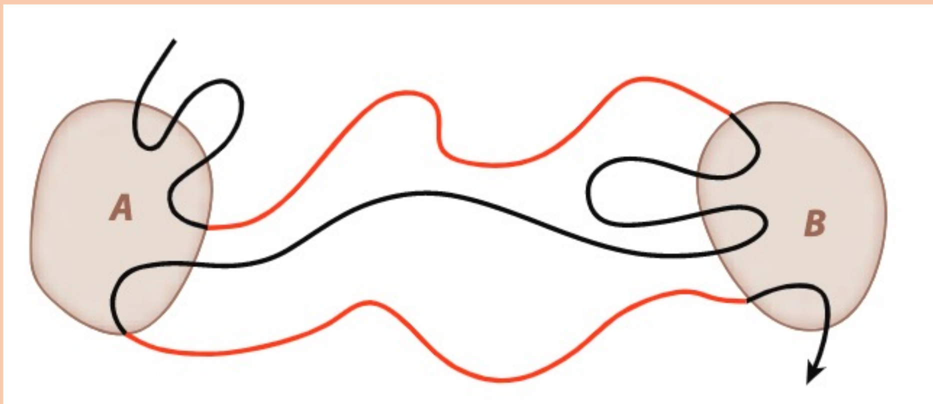
Optimal Controllers in Transition Path Theory

Amar Shah(amarshah1000@berkeley.edu)

Introduction

We consider motion in $\mathbb{R}^n$ governed by the equation:

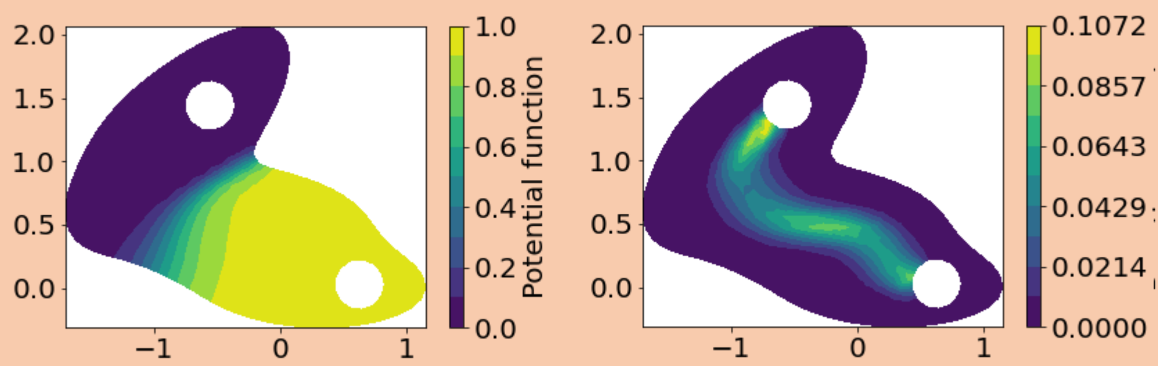
$$d\boldsymbol{x} = \boldsymbol{b}(\boldsymbol{x})dt + \boldsymbol{\sigma}(\boldsymbol{x})d\boldsymbol{w}$$



$\boldsymbol{b}(\boldsymbol{x})$ is the drift vector and $\boldsymbol{\sigma}(\boldsymbol{x})$ is the diffusion matrix

Take the reactive trajectories, i.e. transitions from set A to set B. A useful tool is the committor function:

$$q = P[\tau_B < \tau_A]$$
$$q(\delta A) = 0$$
$$q(\delta B) = 1$$



When our temperature is low, these transitions are rare, but they happen almost surely when we think of our process as a controlled process.

TPT as a controlled process

Controller $v(x)$ is such that as $x \to \delta A$, $v(x) \to \infty$ and $x \to \delta B$, $v(x) \to 0$, i.e. it drives our process from A to B. Thus, we have the controlled trajectory:

$$dX_t = [b(X_t) + \sigma(X_t)\sigma^T(X_t)v(X_t)]dt + \sigma(X_t)dW_t$$

A problem to consider is what is the optimal controller, i.e. the control that takes our trajectory on the most efficient path, minimizing $C_x[v(\cdot)] = \mathbb{E}[\frac{1}{2}\int_0^\tau |\sigma^T(X_s)v(X_s)|^2 ds + g(X_\tau)]$

with penalty $g(x) = \begin{cases} \infty \text{ on } \overline{A} \\ 0 \text{ on } \overline{B} \end{cases}$. The minimum cost is:

$$\gamma(x) = \inf_{v(\cdot)} C_x[v(\cdot)] \text{ with } v = -\nabla\gamma$$

We can simplify the Hamilton Jacobi Bellman equation to get:

$$\frac{1}{2}\sigma\sigma^T : \nabla\nabla\gamma + b\cdot\nabla\gamma - \frac{1}{2}(\nabla\gamma)^T\sigma\sigma^T\nabla\gamma = 0$$

This is solved: $\gamma = -ln(q)$ and $v = \frac{\nabla q}{q}$ assuming σ is invertible

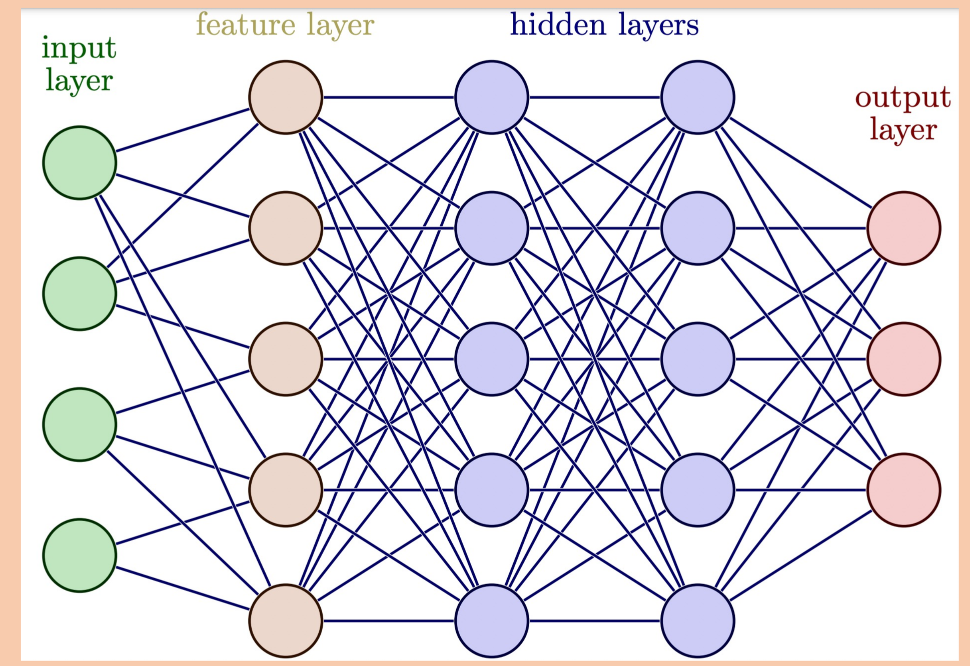
Estimation of the committor q(x)

In the overdamped Langevin equation, the committor is a solution to:

$$q(x) = \arg\min_f \frac{1}{Z}\int_{\Omega\setminus(A\cup B)} |\nabla f(x)|^2 e^{-\beta U(x)}dx$$

with boundary condition q(x) = 0 for x in $\boldsymbol{\delta}$A and q(x) = 1 for x in $\boldsymbol{\delta}$B

To impose the boundary condition [2] proposed this expression of a committor function as the output of a feed-forward Neural Network with L hidden layers:



Feed-forward Neural Network with Feature Layer

$$q_\theta(x) = (1-\chi_A(x))[(1-\chi_B(x))\tilde{q}_\theta(x) + \chi_B(x)], \quad x \in \Omega\setminus(A\cup B)$$

$\tilde{q}_\theta(x) = F_{L+1}\circ F_L \circ \ldots \circ F_2 \circ F_1(x)$ where $F_i(x) = \Phi_i(W_i x + b_i)$

The objective function to be minimized is:

$$\frac{1}{Z}\int_{\Omega\setminus(A\cup B)} |\nabla_x q_\theta(x)|^2 e^{-\beta U(x)}dx = \mathbb{E}_{X\sim\mu(x)}\left[|\nabla q_\theta(X)|^2\right] \approx \frac{1}{N}\sum_{i=1}^N |\nabla q_\theta(X^{(i)})|^2$$

Where we are sampling from $\mu(x) = \frac{1}{Z}e^{-\beta U(x)}$.

To sample more data points where the transition happens, a metadynamics sampling method can be utilized.

For Full Langevin dynamics, there is no similar variational formula, so we must use a Physics Informed Neural Network(PINN) to solve q(x) using:

$$\begin{cases} Lq = m^{-1}p\cdot\nabla_x q - \nabla U\cdot\nabla_p q - \gamma_f p\cdot\nabla_p q + \gamma_f\beta^{-1}m : \nabla\nabla q = 0 & x \in \Omega\setminus(A\cup B) \\ q(x,p) = 0 & x \in \partial A \\ q(x,p) = 1 & x \in \partial B \end{cases}$$

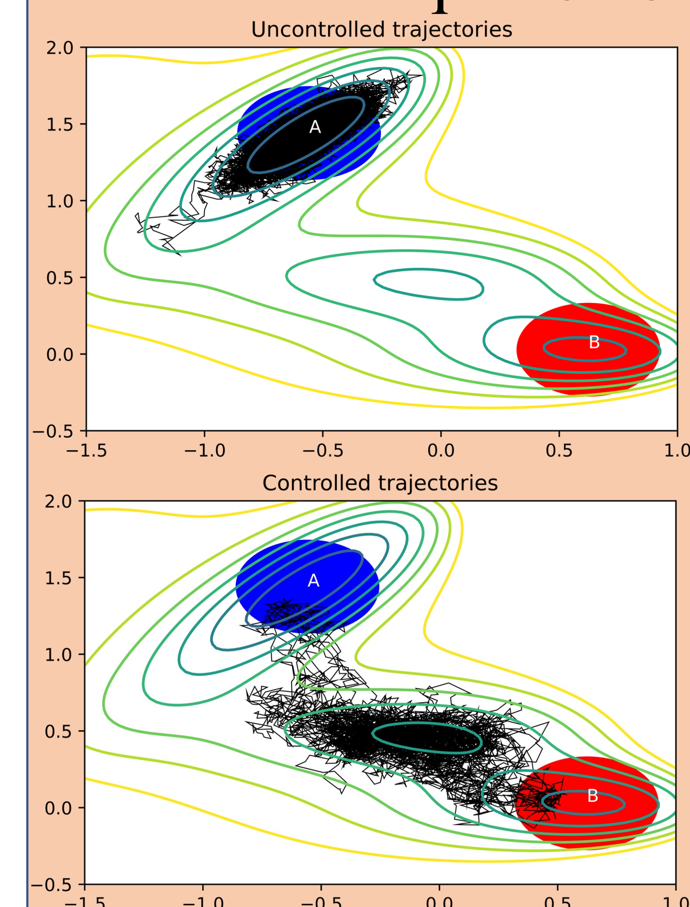
Future Work

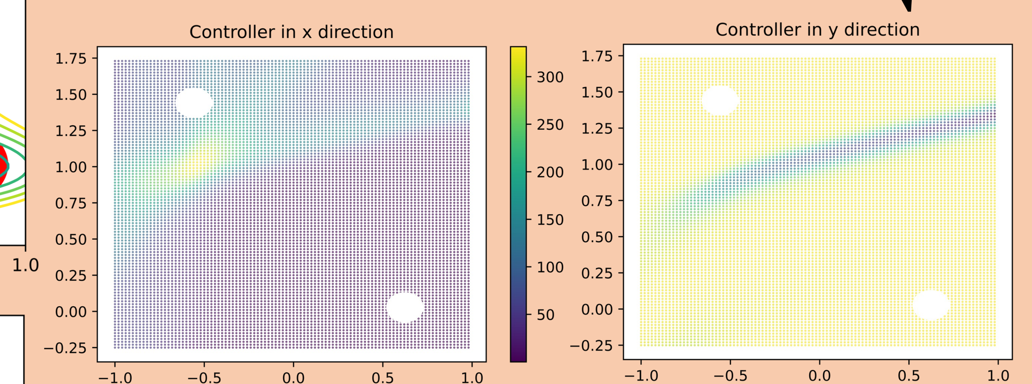
- Improve estimate of the committor for Full Langevin Dynamics
- Estimate a controlled trajectory for higher dimensional examples
- Use optimal control to help estimate the transition rate

Numerical Examples

<u>Overdamped Langevin dynamics:</u> We have the controlled differential equation of the form:

$$d\boldsymbol{x} = (-\nabla U(x) + \frac{2}{\beta}\frac{\nabla q}{q})dt + \sqrt{\frac{2}{\beta}}d\boldsymbol{w}$$



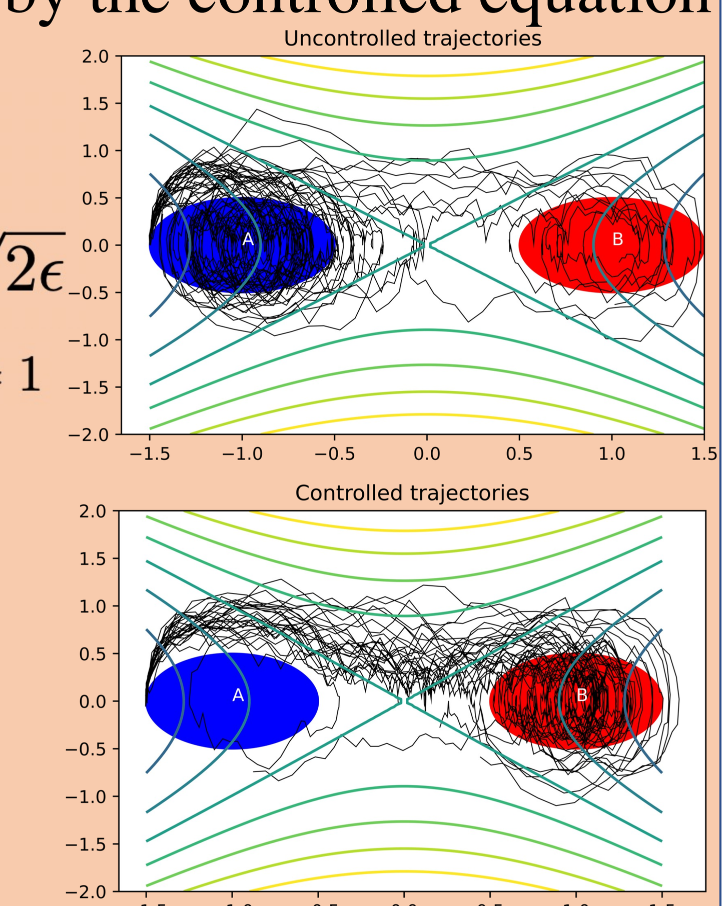


Running trajectories for 10,000 time steps 10e-5, we get that the controlled process transitions with rate 0.932 and uncontrolled with 0

<u>Duffing Oscillator:</u> This is when we consider full Langevin dynamics in two dimensions, given by the controlled equation

$$\begin{cases} dx = \frac{1}{m}pdt \\ dp = (-\delta p - x(\beta + \alpha x^2))dt + \sqrt{2\epsilon} \end{cases}$$

where $\alpha = 1, \beta = -1, \delta = 0.5, \epsilon = 0.05, m = 1$



Running trajectories for time step 0.01 until T = 10, we get that the controlled process transitions with rate 0.977 and uncontrolled with 0.313.

(Selected) Work Cited

[1] Yuan Gao, Tiejun Li, Xiaoguang Li, and Jian-Guo Liu. "Transition path theory for Langevin dynamics on manifold: optimal control and data-driven solver"

[2] Qianxiao Li, Bo Lin, and Weiqing Ren. "Computing committor functions for the study of rare events using deep learning". In: (2019).

[3] Youssef M. Marzouk Benjamin J. Zhang Tuhin Sahai. "A Koopman framework for rare event simulation in stochastic differential equations".

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