Optimal Control in Transition Path Theory

Amar Shah

University of California, Berkeley

GCURS, October 8th 2022

Table of Contents

Table of Contents

General Case

Ordinary Differential Equation

$$dx = \mathbf{b}(x)dt \tag{1}$$

We can solve this differential equation to understand how our system evolves in time. But what if we added randomness to our system:

Stochastic Differential Equation

$$dx = \mathbf{b}(x)dt + \sigma(\mathbf{x})d\mathbf{w} \tag{2}$$

Setting

Goal

We have two compact, connected sets $A, B \subseteq \mathbb{R}^n$ and we want to consider the paths in our evolution that start in A and end up in B.

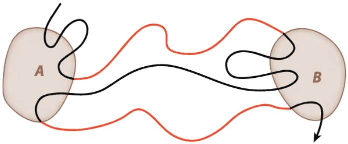


Figure: E & Vanden-Eignden(2006, 2010) [1] [2]

We call these reactive trajectories.

Committor functions

Forward Committor

We define the forward committor $q^+(x)$ as:

$$\tau_A(x) = min\{t > 0 : x(0) = x; x(t) \in \delta A\}$$
$$\tau_B(x) = min\{t > 0 : x(0) = x; x(t) \in \delta B\}$$
$$q^+(x) = \mathcal{P}_x[\tau_B(x) < \tau_A(x)]$$

Table of Contents

In a dynamic system where there is some function v that "we" can control. Our goal is to pick $v(\cdot)$ to maximize the pay off function $P[v(\cdot)]$

(a) landing a rocket (b) centering a rocket

Figure: Evans(1980) [3]

Adding a controller

Let's return to our setting at the beginning of the presentation:

Stochastic Differential Equation

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

Adding a controller

Let's return to our setting at the beginning of the presentation:

Stochastic Differential Equation

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

We want to introduce a control function $v : \mathbb{R}^n \to \mathbb{R}$ and we have the equation:

Controlled Stochastic Differential Equation

$$dx = (\mathbf{b}(x) + \mathbf{v}(x))dt + \sigma d\mathbf{w}$$

Table of Contents

Gao's Optimal Controller

Theorem

Gao et al Theorem 3.3[4]: *If we have the controlled SDE* $dx = (-\nabla U + \mathbf{v}(x))dt + \sqrt{2\epsilon}d\mathbf{w}$, *we have the optimal control* $v^* = \frac{2\epsilon\nabla q}{q}$

Gao's Optimal Controller

Theorem

Gao et al Theorem 3.3[4]: *If we have the controlled SDE* $dx = (-\nabla U + \mathbf{v}(x))dt + \sqrt{2\epsilon}d\mathbf{w}$, *we have the optimal control* $v^* = \frac{2\epsilon\nabla q}{q}$

But remember our original SDE:

Controlled SDE

$$dx = (\mathbf{b}(x) + \mathbf{v}(x))dt + \sigma d\mathbf{w}$$

Gao's Optimal Controller

Theorem

Gao et al Theorem 3.3[4]: *If we have the controlled SDE* $dx = (-\nabla U + \mathbf{v}(x))dt + \sqrt{2\epsilon}d\mathbf{w}$, *we have the optimal control* $v^* = \frac{2\epsilon \nabla q}{q}$

But remember our original SDE:

Controlled SDE

$$dx = (\mathbf{b}(x) + \mathbf{v}(x))dt + \sigma d\mathbf{w}$$

How can we apply Gao's argument to this general case?

General Case

Maybe we can't apply Gao's Argument to the full general case, but we can definitely do it for general drift $\mathbf{b}$ and invertible σ:

Controlled SDE

$$dx = (\mathbf{b}(x) + \mathbf{v}(x))dt + \sigma d\mathbf{w}$$

To solve it for the general case, we need to solve the Hamilton Jacobi Bellman equation.

Hamilton Jacobi Bellman Equation

We introduce the controlled SDE, with control $v(x)$:

$$\begin{cases} dX(s) = f(X(s), v(X_s))dt + \sigma(X_s)dW(s) \ (t \leq s \leq T) \\ X(t) = x \end{cases}$$

We have the expected payoff function:

$P_{x,t}[v(\cdot)] := E[\int_t^T r(X(s), v(X_s))ds + g(X(T))]$

The value function is $\gamma(x,t) = \sup_{v(\cdot)\in\mathcal{V}} P_{x,t}[v(\cdot)]$, i.e. the best possible payoff we can achieve.

Hamilton Jacobi Bellman Equation

We introduce the controlled SDE, with control $v(x)$:

$$\begin{cases} dX(s) = f(X(s), v(X_s))dt + \sigma(X_s)dW(s) \ (t \le s \le T) \\ X(t) = x \end{cases}$$

We have the expected payoff function:

$P_{x,t}[v(\cdot)] := E[\int_t^T r(X(s), v(X_s))ds + g(X(T))]$

The value function is $\gamma(x,t) = \sup_{v(\cdot)\in\mathcal{V}} P_{x,t}[v(\cdot)]$, i.e. the best possible payoff we can achieve.

Stochastic-Hamilton-Jacobi-Bellman equation

Then our value function γ solves this PDE:

$$\begin{cases} \gamma_t(x,t) + \frac{\sigma^2}{2}\Delta v(x,t) + \max_{v\in\mathcal{V}}\{f(x,v)\cdot\nabla_x\gamma(x,t) + r(x,a)\} = 0 \\ \gamma(x,T) = g(x) \end{cases}$$

Solution

Theorem

The optimal controller for the general SDE when σ is invertible is $v^* = \sigma\sigma^T \frac{\nabla q}{q}$

Solution

Theorem

The optimal controller for the general SDE when σ *is invertible is* $v^* = \sigma\sigma^T \frac{\nabla q}{q}$

Proof Sketch

- Solve the maximization term to get $v = -\nabla\gamma$

Solution

Theorem

The optimal controller for the general SDE when σ is invertible is $v^* = \sigma\sigma^T \frac{\nabla q}{q}$

Proof Sketch

- Solve the maximization term to get $v = -\nabla\gamma$
- Plug in for v to simplify our HJB to:

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

Solution

Theorem

The optimal controller for the general SDE when σ is invertible is $v^* = \sigma\sigma^T \frac{\nabla q}{q}$

Proof Sketch

- Solve the maximization term to get $v = -\nabla\gamma$
- Plug in for v to simplify our HJB to:

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

- Show that this is satisifed by $\gamma = -log(q)$ using properties from Transition Path Theory

Solution for full Langevin dynamics

Full Langevin is given by the equation:

$$\begin{cases} d\mathbf{x} = m^{-1}\mathbf{p}dt \\ d\mathbf{p} = -(\nabla U + \gamma\mathbf{p})dt + \sqrt{2\gamma\beta^{-1}m}d\mathbf{w} \end{cases} \tag{3}$$

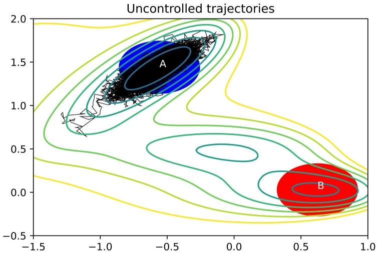
Thus, $\sigma = \sqrt{2\gamma\beta^{-1}m}\begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}$ which is not invertible.

Theorem

The optimal controller for the general SDE when σ is (symmetric) and invertible is $v^* = 2\gamma\beta^{-1}m\frac{\nabla_p q}{q}$ applied to the momentum part of the equation.

Table of Contents

Overdamped Langevin dynamics with Mueller Potential



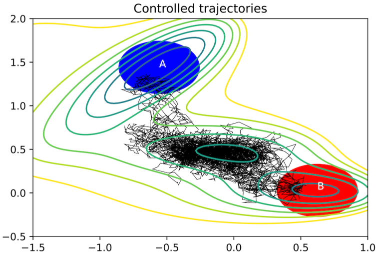


Figure: 10 Uncontrolled and Controlled trajectories until $T = 10$

Overdamped Langevin dynamics with Mueller Potential

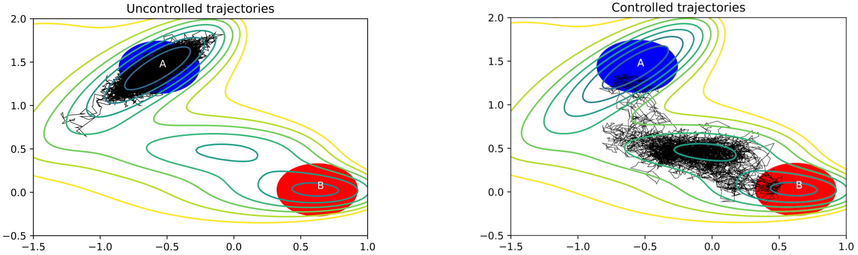


Figure: 10 Uncontrolled and Controlled trajectories until $T = 10$

This follows the overdamped equation $dx = (-\nabla U(x) + \frac{2}{\beta}\frac{\nabla q}{q})dt + \sqrt{\frac{2}{\beta}}dw$. In the uncontrolled case, we have a succes rate of 0 and in the controlled case we have a success rate of 0.932

Duffing Oscillator for $\beta = 10$

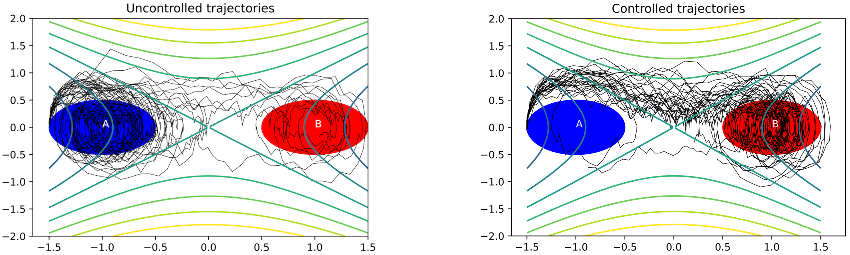


Figure: 25 Uncontrolled and Controlled trajectories until $T = 10$ for $\beta = 10$

The Duffing Oscillator is essentially Full Langevin Dynamics in two dimensions.

The uncontrolled process transitions with rate 0.313 and the controlled process transitions with rate 0.917

Results and Next Steps

Results

1. Proved an Optimal Controller result for a General SDE if the diffusion matrix σ is invertible
2. Proved an Optimal Controller result for Full Langevin dynamics, where σ is not invertible
3. Applied these results to several numerical examples

Results and Next Steps

Results

1. Proved an Optimal Controller result for a General SDE if the diffusion matrix σ is invertible
2. Proved an Optimal Controller result for Full Langevin dynamics, where σ is not invertible
3. Applied these results to several numerical examples

Further Work

1. Apply these results to more complicated systems including Full Langevin Dynamics in multiple dimensions
2. Apply these ideas to similar problems, for example to calculate escape rates.

Bibliography I

Weinan E. and Eric Vanden-Eijnden.
Towards a theory of transition paths.
2006.

Weinan E. and Eric Vanden-Eijnden.
Transition-path theory and path-finding algorithms for the study of rare events.
2010.

Lawrence C Evans.
An introduction to mathematical optimal control theory version 0.2.
https://math.berkeley.edu/~evans/control.course.pdf,
1983.

Bibliography II

Yuan Gao, Tiejun Li, Xiaoguang Li, and Jian-Guo Liu.
Transition path theory for langevin dynamics on manifold: optimal control and data-driven solver.
2021.

Acknowledgement: This work was supported by the NSF grant DMS 2149913 "REU: Modern topics in pure and applied mathematics".