Control of nonequilibrium complex physical systems:
a stochastic control approach

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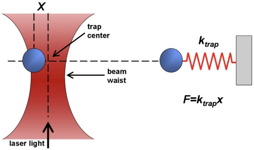
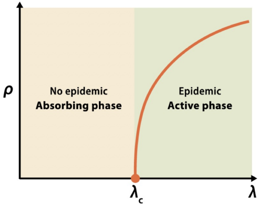
Control in complex systems

1. Diffusion processes
   - microscopic heat engine, fluid dynamics
   - optical traps
   - improve the efficiency or power of molecular engines
2. Jump processes
   - epidemic processes on social network
   - allocation of medical resources
   - restrain uncontrolled epidemic





λ = infection rate/cure rate

Dynamical description of complex systems

Let's focus on diffusion processes but results can be simply generalized to jump processes.

- Original dynamics is characterized by a stochastic differential equation, which is hard for rare events to happen, namely, with **HIGH energy barrier** $\gg k_B T$.

$$X_t = x_0 + \int_0^t b(s, X_s)\mathrm{d}s + \int_0^t \sigma(s, X_s)\mathrm{d}B_s \quad (1)$$

- What do experimentalists do? Altering potential energy profile by **introducing interactions** (forces). Controlled dynamics

$$X_t^u = x_0 + \int_0^t b(s, X_s^u) + (\sigma u)(s, X_s^u)\,\mathrm{d}s + \int_0^t \sigma(s, X_s^u)\mathrm{d}B_s \quad (2)$$

- A finite stopping time τ_D associating with measurable subset D reflects when we would like to finish control. deterministic or random

Quantitative description of control target

- The goal of control can be characterized by a measurable subset $E \subset \mathbb{R}^d$. How good a control is is judged by **target function** $g(x)$ such that $g(x) \geq 0, \; = \iff \; x \in E$.

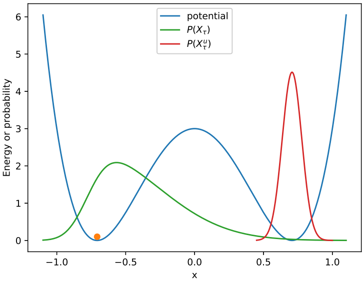
$$g(x) \begin{cases} = 0 & , x \in E \text{ ,i.e. control target is attained} \\ > 0 & \text{, otherwise} \end{cases} \tag{3}$$

- For spatial barrier crossing from x_- to x_+, the target function can be

$$g(x) = \inf_{y \in B_\epsilon(x_+)} |x - y|^2$$

where $B_\epsilon(x_+)$ is the $\epsilon-$neighbor of x_+. The target function aims to centralize particles around x_+.

P.D.F. $\textcolor{green}{green} \xrightarrow{\text{control}} \textcolor{red}{red}$



Cost functional

- Minimize the target function $\rightarrow$ May lead to a diverging policy
- Avoid divergence $\rightarrow$ constraint to the control force!
- Entropy production of control policy (KL divergence associating with controlled/uncontrolled processes)

$$D_{KL}(\mathbb{P}^u||\mathbb{P}) = \mathbb{E}^{x_0}_{\mathbb{P}^u}\left[\ln \frac{\mathrm{d}\mathbb{P}^u}{\mathrm{d}\mathbb{P}}\bigg|_{\mathcal{F}_{\tau_D}}\right] = \mathbb{E}^{x_0}\left[\frac{1}{2}\int_0^{\tau_D} u(s, X_s^u)|^2 \mathrm{d}s\right] = \frac{1}{2}\|u\|^2 \tag{4}$$

The norm of control policy has physical meaning, entropy production!

- The optimal control minimize the following **cost functional**.

$$J[u] = \mathbb{E}^{x_0}\left[\frac{\lambda}{2}\int_0^{\tau_D}|u(s, X_s^u)|^2\mathrm{d}s + g(X^u_{\tau_D})\right] \tag{5}$$

λ stands for a balance between price and utility.

Physical intuition behind

- For optimal control policy u^* s.t. $\mathbb{E}^{x_0}\left[g(X^{u^*}_{\tau_D})\right] = 0$, cost functional is entropy production averaging over paths connecting two fixed regions, which is action.
- **value function** $V = J[u^*] = \inf_{u \in \mathbb{U}} J[u]$. Hamilton-Jacobi-Bellman equation

$$V(t,x) = -\lambda \ln \mathbb{E}\left[\exp\left(-\frac{g(X_{\tau_D})}{\lambda}\right) \middle| X_t = x\right] \tag{6}$$

$$u^*(t,x) = -\frac{1}{\lambda}\sigma(t,x)^T \nabla V(t,x) \tag{7}$$

Value function is actually free energy for energy g and temperature λ. Thus, such cost functional possesses **thermodynamic meaning.** Control policy is generated by free energy gradient.

Parameterization

- Free energy interpretation of value function, experimentally introduced interactions $\rightarrow$ expand it by a class of linear independent potentials.

$$u(t,x) = -\sigma(t,x)^T \sum_k \nabla \phi_k(t,x,\alpha_k) \tag{8}$$

where $\{\phi_k(t,x;\alpha_k) : k = 1,2,\cdots,N\}$ are physically realizable potentials in experiments with parameters α_k.

- Gradients can be evaluated by Girsanov theorem. Optimization is proceeded by gradient-based methods, specifically, BFGS algorithm is used in this talk.

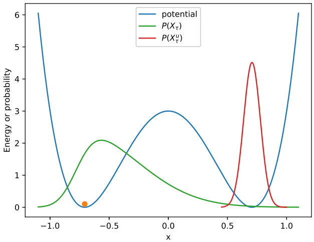
$$\alpha_{n+1} \leftarrow \alpha_n - c^{(n)} \frac{\partial}{\partial \alpha} J(\alpha_n) \tag{9}$$

Setting

- Two laser traps centralize at $x_\pm = \pm 1/\sqrt{2}$ resulting in a locally approximate potential $U(x) = 12x^4 - 12x^2$ with barrier height $\Delta = 4k_B T$.
- A Brownian particle initially sits at x_- and is expected to cross the barrier at a determinstic time.

- Target function $g(x) = \inf_{y \in B_\epsilon(x_+)} |x - y|^2$
- External potentials: laser array equally spaces between $x_\pm$ with tunable amplitude.

$$\phi_k(t, x; \alpha_k) = \alpha_k \left(-\frac{1}{\tau - t + 0.1} \exp\left(-\frac{(x - x_k)^2}{2} \right) \right)$$



Optimal policies with different λ

- Optimal control raises the initial site to gain the crossing.
- The smaller λ is, the larger an optimal control policy will be generated. Higher control utility but with higher price.
- $\lambda = 1$ results in nearly no control.

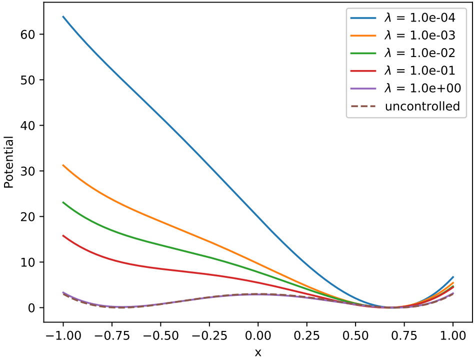


Figure: Potential energy profile under optimal policy with different λ's.

Algorithmic efficiency

- BFGS optimizer converges fast.
- Fluctuation after converge due to Monte Carlo estimation.
- Hard for small λ to find a quick descent direction $\rightarrow$ structure of cost functional, small λ means small feedback from control target.

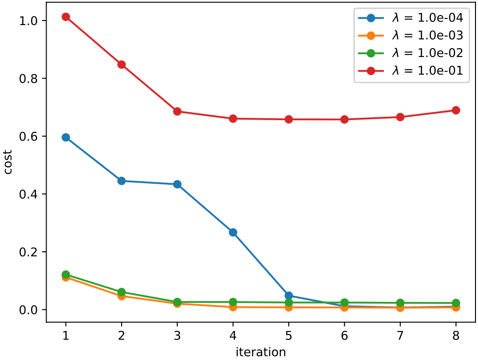


Figure: Optimization process for different λ's.

Algorithmic efficiency

- Quick convergence of BFGS optimizer in few steps.

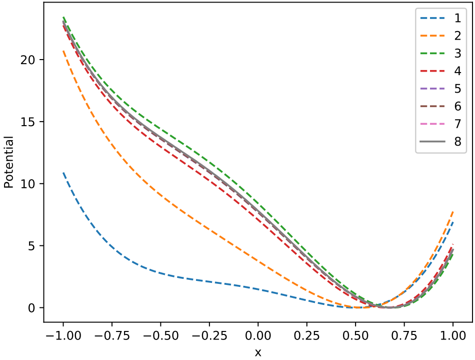


Figure: Changing of potential in each optimization steps. $\lambda = 0.01$

Thanks for your attendance!