Optimal Design for Stochastic Differential Equations

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The Basic Setup

Consider a parametrized SDE:

$$dX = U(x, \alpha(x,t); \theta)\,\mathrm{d}t + \sqrt{2D}dW$$

$$\theta \sim \text{Unknown parameters (in the drift)}$$

$$\alpha \sim \text{External perturbation}$$

For example the 'double-well potential':

$$dX = \underbrace{-\left(4x^3 - 4x - A\frac{x}{c}e^{-(x/c)^2/2}\right) + \alpha(x,t)}_{U(x,\alpha;\theta)}\,\mathrm{d}t + \sqrt{2D}dW$$

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ASSUMPTION: 'continuous' observations of the trajectories X_t.

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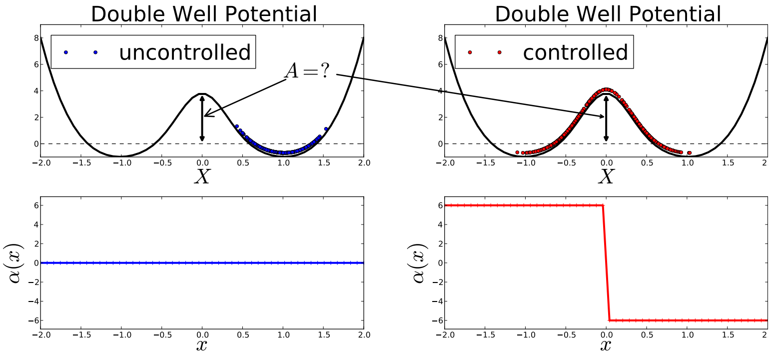
Our Goal

Choose $\alpha(x,t)$ so as to facilitate the estimation of the unknown parameters, θ.



FORMALIZING THE GOAL

Key Concepts:

- Mutual Information between two Random Variables, $I(\theta, X)$
- Belief Distribution (prior) on the parameters, $\rho(\theta)$
- The transition density of the state, $f(x, t|\theta)$

Mutual Information - Definition

For a given control, $\alpha(x,t)$, the Mutual Information, I between the R.V.s X,θ is:

$$\begin{aligned} I(X,\theta) &= \int_\Theta \int_X p(x,\theta)\cdot \log\left(\frac{p(x,\theta)}{p(x)p(\theta)}\right) \mathrm{d}x\,\mathrm{d}\theta \\ &= \int_\Theta \int_X \log\left(\frac{L(x|\theta)}{\int_\Theta L(x|\theta)\rho(\theta)\,\mathrm{d}\theta}\right)\cdot \underbrace{L(x|\theta)}_{\text{likelihood}}\,\underbrace{\rho(\theta)}_{\text{prior}}\,\mathrm{d}x\,\mathrm{d}\theta \end{aligned}$$

But

$$L(x,\theta) = \quad \prod_k f(x_k|x_{k-1})$$

and

$$dx = \prod dx_k$$

(My) conclusion: With multi-observations, $I(X,\theta)$ is intractable.

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SINGLE SLICE MUTUAL INFORMATION

For a single observation, however, the Mutual Information is tractable

$$I(X_t, \theta) = \int_\Theta \int_{\Omega_X} \log\left(\frac{f(x,t|x_0;\theta;\alpha(\cdot))}{\int_\Theta f(x,t|x_0;\theta;\alpha(\cdot)) \cdot \rho(\theta)\,\mathrm{d}\theta} \right) \cdot f(x,t|x_0;\theta;\alpha(\cdot))\rho(\theta)\,\mathrm{d}x\,\mathrm{d}\theta$$

Time out!

$$\underbrace{f}_{\text{Prob. that}} (\underbrace{x,t}_{X_t=x} \underbrace{|}_{\text{given}} \underbrace{x_0}_{X_0=x_0}; \underbrace{\theta}_{\text{params}}; \underbrace{\alpha(\cdot)}_{\text{applied control}})$$

Natural next step, integrate I over time to form the objective J:

$$J[\alpha(\cdot)] = \int_0^T I(X_t, \theta)\,\mathrm{d}t$$

$$\alpha^*(x,t) = \underset{\alpha(\cdot)}{\arg\max}\, J[\alpha(\cdot)]$$

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Integrated Single-Slice Mutual Information as the Objective

Formal Problem Statement

Given, $\rho(\theta)$, T, find

$$\alpha(x,t) = \underset{\alpha(x,t)}{\arg\max} \left\{ J[\alpha] = \int_\Theta \int_0^T \int_{\Omega_X} \log\left(\frac{f(x,t|\theta)}{\int_\Theta f(x,t|\theta) \cdot \rho(\theta)\,\mathrm{d}\theta} \right) \cdot f(x,t|\theta)\rho(\theta)\,\mathrm{d}x\,\mathrm{d}t\,\mathrm{d}\theta \right\}$$

You can also write the objective J as

$$
\begin{aligned}
J[\alpha] &= \int_{\Theta} \int_0^T \int_{\Omega_X} \log\left(\frac{f(x,t|\theta)}{\int_{\Theta} f(x,t|\theta)\cdot\rho(\theta)\,\mathrm{d}\theta} \right) \cdot f(x,t|\theta)\rho(\theta)\,\mathrm{d}x\,\mathrm{d}t\,\mathrm{d}\theta \\
&= \mathbb{E}_{\theta}\left[\mathbb{E}_{X_t|\theta;\alpha(\cdot)} \left[\int_0^T \log\left(\frac{f(X_t,t|\theta;\alpha(\cdot))}{\int_{\theta} f(X_t,t|\theta;\alpha(\cdot))\rho(\theta)\,\mathrm{d}\theta} \right) \mathrm{d}t \right] \right]
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Maximum Principle Solution

Treat the maximization of J as an Optimization Problem over Partial Differential Equations (PDEs)

Recall that the transition density, $f(x,t|)$ satisfies a Fokker-Planck (Forward Kolmogorov) PDE:

$$\begin{aligned} \partial_t f &= D \cdot \partial_x^2[f] - \partial_x[U(x,\alpha(x,t);\theta) \cdot f] \\ &= \mathscr{L}_{\theta,\alpha(\cdot)}[f] \end{aligned}$$

MAXIMUM PRINCIPLE SOLUTION

ROUGH, HAND-WAVY EXPLANATION OF WHAT THE MAXIMUM PRINCIPLE (ADJOINT METHOD) DOES

$$J[\alpha] = \mathbb{E}_\theta \left[\int_0^T \int_{\Omega_X} \log \left(\frac{f(x,t|\theta)}{\int_\Theta f(x,t|\theta) \cdot \rho(\theta)\,\mathrm{d}\theta} \right) \cdot f(x,t|\theta)\,\mathrm{d}x\,\mathrm{d}t \right]$$

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\begin{aligned}
\partial_t f_\theta &= \mathscr{L}_{\theta,\alpha(\cdot)}[f_\theta] \\
-\partial_t p_\theta &= \mathscr{L}^*{}_{\theta;\alpha}[p_\theta] + 1 - \frac{w_\theta f_\theta}{\sum_\theta w_\theta f_\theta} + \log\left(\frac{f_\theta}{\sum_\theta w_\theta f_\theta}\right)
\end{aligned}
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And once p_θ, f_θ are solved for, the differential wrt. α comes out to:

$$
\frac{\delta J}{\delta \alpha}\Big|_{x,t} = \sum_\theta w_\theta \left[\partial_x p_\theta(x,t) \cdot f_\theta(x,t)\right]
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where, for simplicity, the parameters' belief distribution, $\rho(\theta)$ has been discretized:

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\mathbb{E}_\theta[\cdot] = \int_\Theta [\cdot]\rho(\theta)\,\mathrm{d}\theta \approx \sum_\theta w_\theta[\cdot]
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Back to the Double-Well Potential

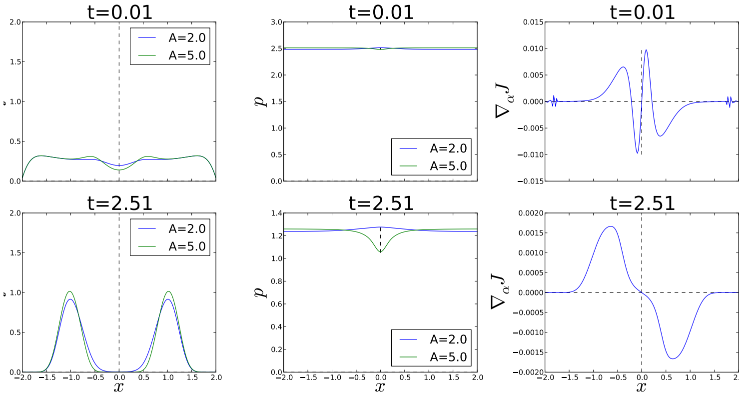
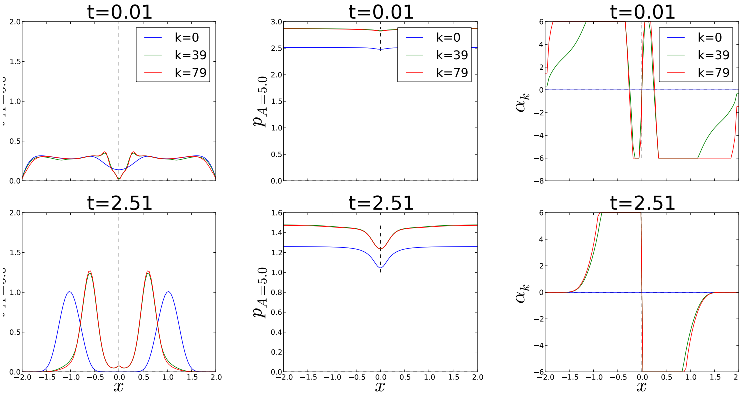


FIGURE: Solution to the test Double Well potential problem using $\alpha \equiv 0$.

Gradient Ascent (Kinda) Works



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Summary

SDE Optimal Design via the Mutual Information

- Determine the maximally informative perturbation of an SDE using the criterion of Mutual Information between a belief distribution of the parameters and the forward density of the state trajectories
- Use the Adjoint Method + a gradient ascent to obtain the optimal feedback-form perturbation
- Numerics of gradient-based optimization remain to be 'finessed'

To be addressed:

- More complex systems
- Higher dimensions
- Obviate the need for PDE numerics (Stochastic Solution?)

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