Dynamics Reading Group
Optimal paths: Revisited

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Overview

Stochastic differential equation:

\[ \dot{x} = f(x(t), t) + \sqrt{2D}\eta(t) \]

The optimal path is the most probable path for the transition between a given starting point \( x_0 \) at time \( t_0 \) to a given end position \( x_T \) at time \( T_{end} \).

**Limit:** \( \delta \ll \Delta t \ll 1 \)

**Optimisation problem:** Optimal path derived from optimising a functional of the probability for passing through gates along a path.
Introduction

Probability density function $P(x, t)$ of the random variable $x(t)$ is governed by the Fokker-Planck equation:

$$\frac{\partial P(x, t)}{\partial t} = D \frac{\partial^2 P(x, t)}{\partial x^2} - \frac{\partial}{\partial x} (f(x, t) P(x, t))$$

where a potential $U(x, t)$ satisfies:

$$\frac{\partial U(x, t)}{\partial x} = -f(x, t)$$
Fokker-Planck run for $\dot{x} = -1 + \eta$, $x_0 = 0$, $T = 3$
Identities

Fourier Transform $\hat{P}(k, t)$ of $P(x, t)$

$$\hat{P}(k, t) = \int_{-\infty}^{\infty} P(x, t)e^{-ikx} \, dx$$

Dirac delta identity

$$\int_{-\infty}^{\infty} f(x) \delta(x - x_0) \, dx = f(x_0)$$

Inverse Fourier Transform

$$P(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{P}(k, t)e^{ikx} \, dk$$

Gaussian integral

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} \, dx = \sqrt{\frac{\pi}{\alpha}}$$
Notation

- $t_k = t_{k-1} + \Delta t$, for $k = 1, \ldots, N + 1$
- $x_k = x(t_k)$: Realisation of random variable $x$ at time $t_k$ conditioned on having passed through gates 1, ..., $k - 1$
- $\tilde{x}_k$: Location of path and represents centre of gate $k$ at time $t_k$
- $P_k(x_k)$: Probability density function for being at $x_k$ assuming passed through gates 1, ..., $k - 1$ at time $t_k$
- $\mathbb{P}_k$: Probability of passing through gate $k$ conditioned on having passed through gates 1, ..., $k - 1$
- $\tilde{P}_k(x_k)$: Probability density function for being at $x_k$ assuming passed through gates 1, ..., $k$ at time $t_k$
- $\mathbb{P}_{(T)}$: Total probability of passing through first $k$ gates
- $\mathbb{P} = \mathbb{P}_{(T)}^{N+1}$: Probability of passing through all $N + 1$ gates
Case 1: Pure diffusion

\[ P(\tilde{x}, \delta, \Delta t) = \left( \frac{\delta}{\sqrt{4\pi D\Delta t}} \right)^{N+1} \exp \left( - \frac{1}{4D} \int_{t_0}^{T_{\text{end}}} \left( \frac{d\tilde{x}}{d\tau} \right)^2 d\tau \right) \]
Key book results

- **Case 1**: Pure diffusion

  \[ P(\tilde{x}, \delta, \Delta t) = \left( \frac{\delta}{\sqrt{4\pi D \Delta t}} \right)^{N+1} \exp \left( - \frac{1}{4D} \int_{t_0}^{T_{\text{end}}} \left( \frac{d\tilde{x}}{d\tau} \right)^2 d\tau \right) \]

- **Case 2**: Absorbing medium

  \[ P(\tilde{x}, \delta, \Delta t) = \left( \frac{\delta}{\sqrt{4\pi D \Delta t}} \right)^{N+1} \exp \left( - \int_{t_0}^{T_{\text{end}}} \frac{1}{4D} \left( \frac{d\tilde{x}}{d\tau} \right)^2 + A(\tilde{x}(\tau)) d\tau \right) \]
Key book results

- Case 3: Fokker-Planck equation

\[ \mathbb{P} = \left( \frac{\delta}{\sqrt{4\pi D \Delta t}} \right)^{N+1} \exp \left( \frac{U(x_0) - U(x_T)}{2D} - \int_{t_0}^{T_{\text{end}}} \mathbb{L}(\tilde{x}(\tau))d\tau \right) \]

where

\[ \mathbb{L}(x) = \frac{1}{4D} \left( \frac{dx}{d\tau} \right)^2 + V_s(x) \]

and

\[ V_s(x) = \frac{1}{4D} \left( \frac{dU}{dx} \right)^2 - \frac{1}{2} \frac{d^2U}{dx^2} \]
Key book results

To minimise $\mathcal{L}$, solve the Euler-Lagrange equation:

$$\frac{\partial \mathcal{L}}{\partial x} - \frac{d}{d\tau} \frac{\partial \mathcal{L}}{\partial \dot{x}} = 0$$

A 2nd order BVP is derived that the most likely trajectory will satisfy:

$$\ddot{x} = 2D \frac{dV_s}{dx}, \quad \left\{ \begin{array}{l} x(t_0) = x_0 \\ x(T_{\text{end}}) = x_T \end{array} \right.$$ 

where

$$V_s = \frac{1}{4D} \left( \frac{dU}{dx} \right)^2 - \frac{1}{2} \frac{d^2U}{dx^2}$$
Ornstein-Uhlenbeck example

Consider the Ornstein-Uhlenbeck process:

$$\dot{x} = -ax(t) + \sqrt{2D} \eta(t)$$

Optimal path satisfies:

$$\ddot{x} = a^2 x, \quad \begin{cases} x(t_0) = x_0 \\ x(T_{end}) = x_T \end{cases}$$

Solution can be obtained analytically:

$$x(t) = \frac{x_0 \sinh(a(T_{end} - t)) + x_T \sinh(a(t - t_0))}{\sinh(a(T_{end} - t_0))}$$
Ornstein-Uhlenbeck example

\( D = 0.05 \)

\( a = 0.5 \)

\( a = 0.2 \)

\( D = 0.1 \)
Time dependent potentials $U(x, t)$

New PDE is:

$$\frac{\partial P_s}{\partial t} = D \frac{\partial^2 P_s}{\partial x^2} + \left( \frac{U''}{2} - \frac{U'^2}{4D} + \frac{\dot{U}}{2D} \right) P_s$$

2nd order BVP remains the same:

$$\ddot{x} = 2D \frac{dV_s}{dx}$$

where

$$V_s = \frac{U'^2}{4D} - \frac{U''}{2} - \frac{\dot{U}}{2D}$$
Consider the Ornstein-Uhlenbeck process:

\[ \dot{x} = -a(t)x(t) + \sqrt{2D}\eta(t) \]

where \( a \) is not constant, instead

\[ a(t) = a_0 - \epsilon t \]

The optimal path satisfies:

\[ \ddot{x} = a(t)^2 x + \epsilon x \]

To be solved numerically
Ornstein-Uhlenbeck example

\[ a_0 = -0.2, \quad \epsilon = -0.05 \]

\[ D = 0.05 \quad D = 0.1 \]
References