Dynamics Reading Group
Optimal paths: Revisited

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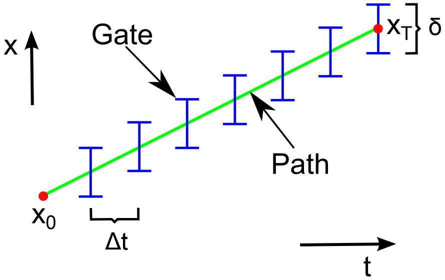
Overview

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

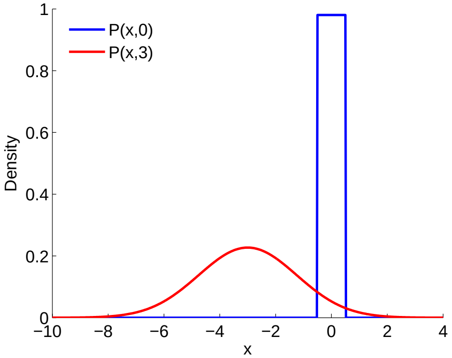
Probability density function $P(x,t)$ of the random variable $x(t)$ is governed by the Fokker-Planck equation:

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

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

$$\frac{\partial U(x,t)}{\partial x} = -f(x,t)$$

Introduction



Fokker-Planck run for $\dot{x} = -1 + \eta$, $x_0 = 0, T = 3$

Identities

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

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

Dirac delta identity

$$\int_{-\infty}^{\infty} f(x)\delta(x - x_0)\mathrm{d}x = f(x_0)$$

Inverse Fourier Transform

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

Gaussian integral

$$\int_{-\infty}^{\infty} e^{-\alpha x^2}\mathrm{d}x = \sqrt{\frac{\pi}{\alpha}}$$

Notation

- $t_k = t_{k-1} + \Delta t$, for $k = 1, .., N+1$
- $x_k = x(t_k)$: 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
- $\mathbb{P}_k^{(T)}$: Total probability of passing through first k gates
- $\mathbb{P} = \mathbb{P}_{N+1}^{(T)}$: Probability of passing through all $N+1$ gates

Key book results

- Case 1: Pure diffusion

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

Key book results

- Case 1: Pure diffusion

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

- Case 2: Absorbing medium

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

Key book results

- Case 3: Fokker-Planck equation

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

where

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

and

$$V_s(x) = \frac{1}{4D}\left(\frac{\mathrm{d}U}{\mathrm{d}x}\right)^2 - \frac{1}{2}\frac{\mathrm{d}^2U}{\mathrm{d}x^2}$$

Key book results

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

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

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

$$\ddot{x} = 2D\frac{\mathrm{d}V_s}{\mathrm{d}x}, \qquad \begin{cases} x(t_0) & = x_0 \\ x(T_{\mathrm{end}}) & = x_T \end{cases}$$

where

$$V_s = \frac{1}{4D}\left(\frac{\mathrm{d}U}{\mathrm{d}x}\right)^2 - \frac{1}{2}\frac{\mathrm{d}^2U}{\mathrm{d}x^2}$$

Ornstein-Uhlenbeck example

Consider the Ornstein-Uhlenbeck process:

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

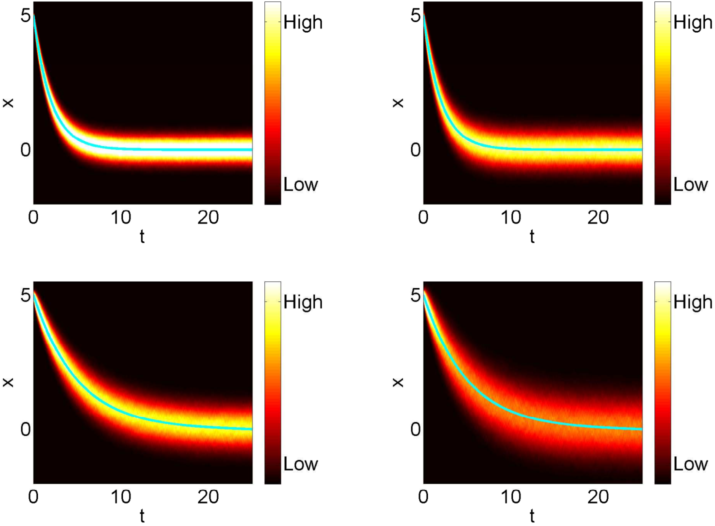
Optimal path satisfies:

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

Solution can be obtained analytically:

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

Ornstein-Uhlenbeck example



$a = 0.5$

$a = 0.2$

$D = 0.05$ $\qquad$ $D = 0.1$

Time dependent potentials $U(x,t)$

New PDE is:

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

2^{nd} order BVP remains the same:

$$\ddot{x} = 2D\frac{\mathrm{d}V_s}{\mathrm{d}x}$$

where

$$V_s = \frac{U'^2}{4D} - \frac{U''}{2} - \frac{\dot{U}}{2D}$$

Ornstein-Uhlenbeck example

Consider the Ornstein-Uhlenbeck process:

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

where a is not constant, instead

$$a(t) = a_0 - \epsilon t$$

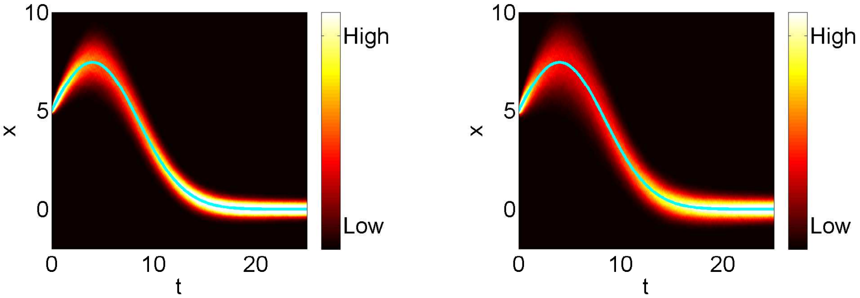
The optimal path satisfies:

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

To be solved numerically

Ornstein-Uhlenbeck example

$$a_0 = -0.2, \qquad \epsilon = -0.05$$



$D = 0.05$ $D = 0.1$

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