

Dynamics
Reading
Group
Most likely
paths

Paul Ritchie
Advised by
Jan Sieber

Outline

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potential wells

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May 14, 2014

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- Consider a deterministic ODE:

$$\dot{x} = \mu(x(t))$$

For a given starting position, end point and time there is one solution.

- But if we were to add noise to this then suddenly there are many different paths possible and we're interested in finding the most likely path.

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- Objectives:
 - Calculate the most likely path from a known starting position to a known end position in a given time.
 - What is the probability of following this path?
 - Is there an optimum time to make the transition?
- Brownian motion of a particle is governed by the stochastic differential equation:

$$dX_t = \mu(X_t, t)dt + \sqrt{2D(X_t, t)}dW_t$$

with drift $\mu(X_t, t)$ and $D(X_t, t)$ is a diffusion coefficient.

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- Probability density function of the random variable X_t is governed by the Fokker-Planck equation:

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

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

$$\frac{dU(x, t)}{dx} = -\mu(x, t)$$

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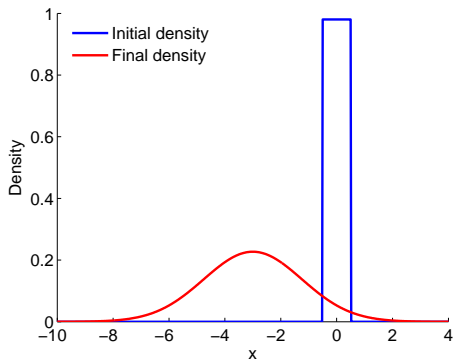


Figure : Fokker-Planck run for $\dot{x} = -1 + \eta$, $x_0 = 0$, $T = 3$

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- Case 1: Pure diffusion

$$\tilde{P} \propto \exp\left(-\frac{1}{4D} \int_{t_0}^T \left(\frac{dx}{d\tau}\right)^2 d\tau\right)$$

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- Case 1: Pure diffusion

$$\tilde{P} \propto \exp\left(-\frac{1}{4D} \int_{t_0}^T \left(\frac{dx}{d\tau}\right)^2 d\tau\right)$$

- Case 2: annihilation model

$$\tilde{P} \propto \exp\left(-\frac{1}{4D} \int_{t_0}^T \left(\frac{dx}{d\tau}\right)^2 d\tau - \int_{t_0}^T A(x(\tau), \tau) d\tau\right)$$

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- Case 3: Most likely path will maximise:

$$W(x(\tau)) = \exp\left(\frac{U(x_0) - U(x_T)}{2D}\right) \exp\left(-\int_{t_0}^T \mathbb{L}(x(\tau))d\tau\right)$$

where

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

and

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

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In order to minimise need to solve the Euler-Lagrange equation:

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

From this a 2nd order ODE is created that the most likely trajectory will satisfy:

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

Example

Consider the example:

$$dx_t = -ax_t dt + \sigma dW_t$$

Most likely path satisfies:

$$\ddot{x} - a^2 x = 0$$

In this case the solution can be obtained analytically:

$$x(t) = x_0 e^{at} + (x_T - x_0 e^{aT}) \frac{\sinh(at)}{\sinh(aT)}$$

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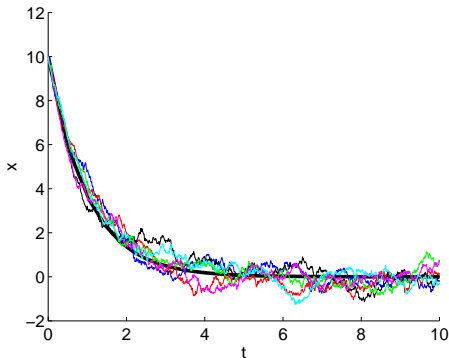


Figure : Most likely path for constant single potential well,
 $a = 1, x_0 = 10, x_T = 0, T = 10$

Time dependent potential wells

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- Time dependent potential wells of the form $U(x, t)$
- 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 ODE remains the same with just an extra term in V_s :

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

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- Suppose now a is not constant, $a(t) = a_0 - \epsilon t$, with drift speed ϵ
- The most likely path now satisfies:

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

- To be solved numerically

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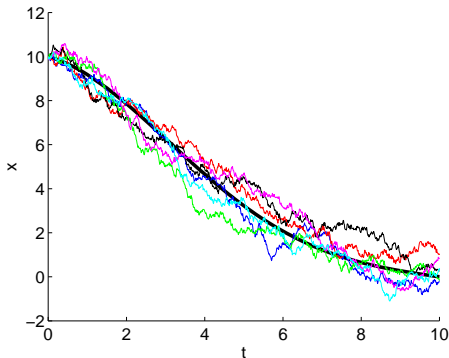


Figure : Most likely path for time dependent single potential well,
 $a_0 = 0.05, \epsilon = -0.07, x_0 = 10, x_T = 0, T = 10$

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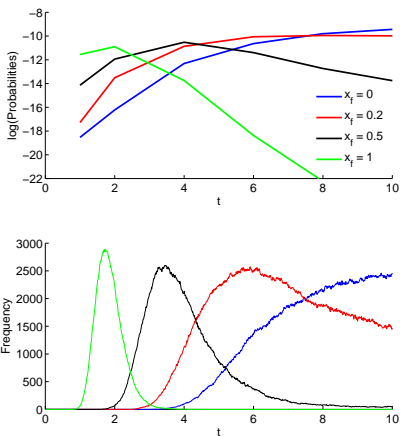


Figure : Optimal time for constant single potential well,
 $a = 0.4, D = 0.01, x_0 = 2$

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