

Most probably transition pathway of biology-modelling SDEs

Stanley Nicholson

Illinois Institute of Technology

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Why Stochastics?

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- ▶ Noise: think of Brownian motion

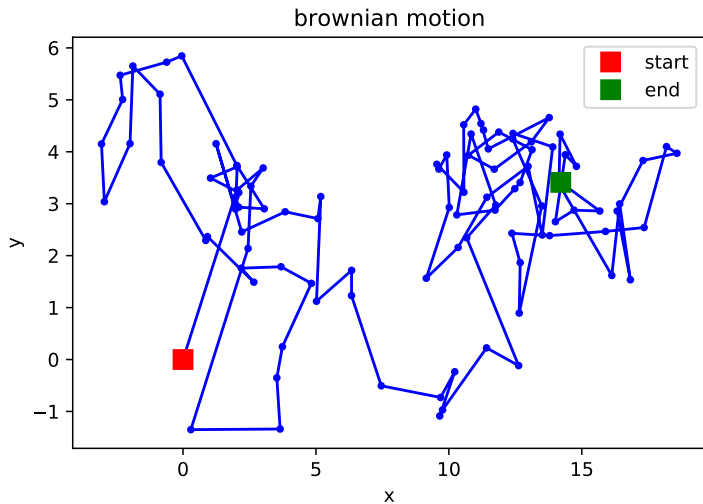
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Why Stochastics?

- ▶ All physical systems are "noisy"
- ▶ Noise: think of Brownian motion
- ▶ Accounts for sudden changes in system
- ▶ Many biological processes are stochastic: mutation, gene regulation, etc.

Brownian Motion



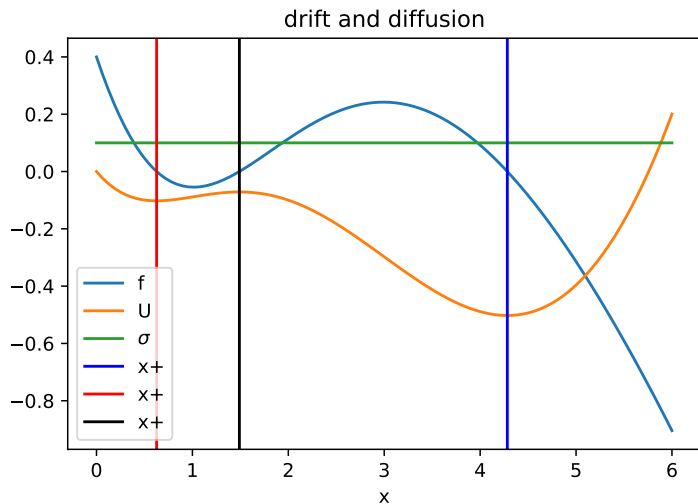
What's an SDE?

The definition of a *stochastic differential equation* given a stochastic process X_t , drift function $f(X_t, t)$, and diffusion function $\sigma(X_t, t)$:

$$dX_t = f(X_t, t)dt + \sigma(X_t, t)dB_t \quad (1)$$

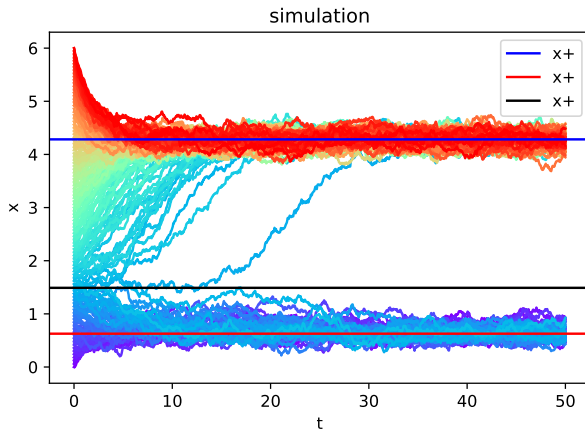
Think: f determines direction, σ denotes noise intensity

Our Model



Simulation

Given f and σ , we simulate the SDE with the Euler-Maruyama method.



Learn our Model

Given this simulated data, we wish to find learn the underlying drift and diffusion

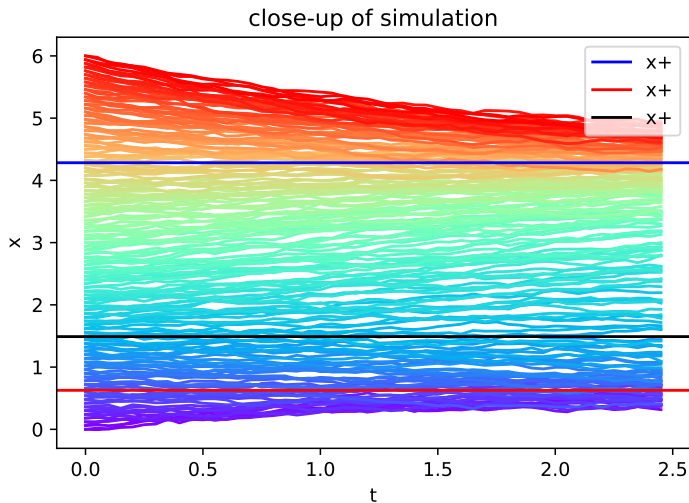
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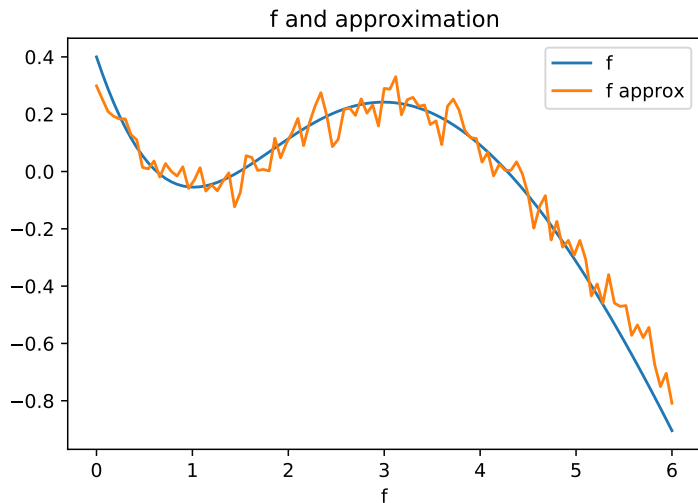
$$f(x) = \lim_{\Delta t \rightarrow 0} \mathbb{E} \left(\frac{X_{\Delta t} - X_0}{\Delta t} \middle| X_0 = x \right) \quad (2)$$

$$\sigma^2(x) = \lim_{\Delta t \rightarrow 0} \mathbb{E} \left(\frac{(X_{\Delta t} - X_0)^2}{\Delta t} \middle| X_0 = x \right) \quad (3)$$

Simulation Zoom-In



Learned f



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$$\ddot{z} = \frac{\sigma(z)^2}{2} f''(z) + f'(z)f(z). \quad (4)$$

with the condition that $z(t_0) = x_-$ and $z(t_f) = x_+$.

Most Probable Pathway

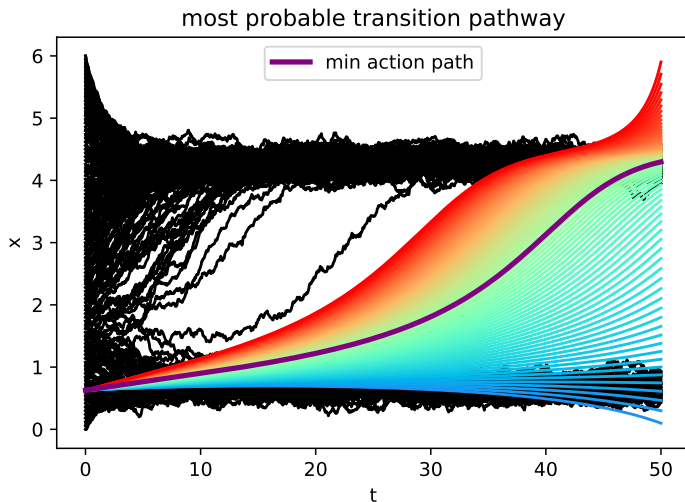
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- ▶ Solving analytically is very difficult
- ▶ The shooting method lets us find the "velocity" that minimizes the "loss"

Learned Probable Pathway



Future Work

- ▶ Fine tune/optimize specific data extraction
- ▶ Applying machine learning techniques to pathway distribution