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SDES AND GENERATORS

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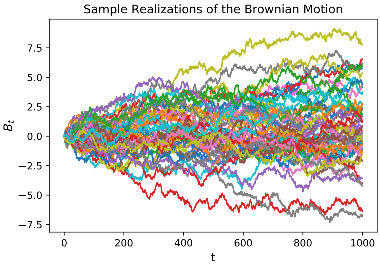
Motivation

SDE Theory

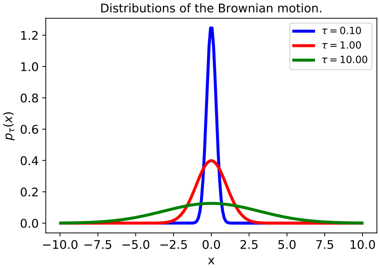
The Koopman Generator

Brownian Motion Revisited

Brownian motion with transition kernel $p_\tau(x, \cdot) \sim \mathcal{N}(x, \sqrt{\tau})$:



Paths of the Brownian motion started at $X_0 = 0$.



Distributions at times $\tau \in \{0.1, 1.0, 10.0\}$.

Brownian Motion

Definition

A stochastic process $B_t \in \mathbb{R}$ is a *Brownian motion* started at $a \in \mathbb{R}$ if
(i) $B_0 = a$ almost surely.
(ii) The paths $B_t, \ t \geq 0$ are almost surely continuous.
(iii) The process possesses independent increments: For all $t \geq s \geq 0$, $B_t - B_s$ is independent of B_s, and the distribution of $B_t - B_s$ is a normal distribution with mean zero and spread $\sqrt{t-s}$.

A Brownian Motion in $\mathbb{R}^d$ is just a vector of d independent one-dim. Brownian motions.

Motivation for SDEs

Consider a deterministic ODE $\dot{X}_t = b(x_t)$:

$$(X_{t+\mathrm{d}t} - X_t) = \mathrm{d}X_t \approx b(X_t)\mathrm{d}t.$$

Let us add some noise by means of an increment of the Brownian motion:

$$\begin{aligned}(X_{t+\mathrm{d}t} - X_t) &\approx b(X_t)\mathrm{d}t + \sigma(X_t)(B_{t+\mathrm{d}t} - B_t) \\ &= b(X_t)\mathrm{d}t + \sigma(X_t)\mathrm{d}B_t.,\end{aligned}$$

where $\sigma(\cdot)$ is a matrix field. Brownian Motion is used to generate normally distributed noise.

Formal Definition

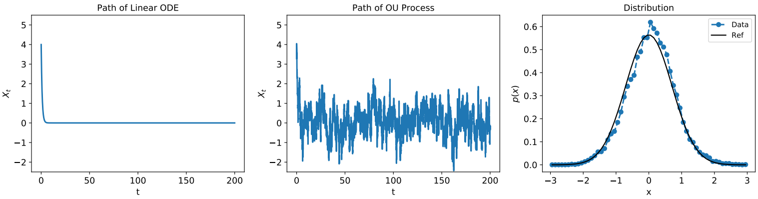
The above reasoning can be made precise in integral form: X_t is the solution of an *SDE* if

$$X_t = X_0 + \int_0^t b(X_s)\,\mathrm{d}s + \int_0^t \sigma(X_s)\,\mathrm{d}B_s.$$

- The second integral is the *Ito stochastic integral*, which can be defined similarly to a Riemann-Stieltjes Integral.
- Given typical Lipschitz-type conditions, local existence and uniqueness can be shown.
- b is called the *drift* field, and σ is the *diffusion* field.

Examples

1. Brownian Motion itself: just set $b \equiv 0$, $\sigma \equiv \mathrm{Id}$.
2. *Ornstein-Uhlenbeck Process* on the real line: set $b(x) = -x$, $\sigma = \sqrt{2\beta^{-1}}\mathrm{Id}$:



Stationary measure is $\mu \sim \mathcal{N}(0, \sqrt{\beta})$.

Examples

- More generally, consider the *overdamped Langevin dynamics*

$$\mathrm{d}X_t = -\nabla V(X_t)\mathrm{d}t + \sqrt{2\beta^{-1}}\mathrm{d}B_t.$$

The scalar function V is called *potential*. The invariant measure is $\mu \sim \exp(-\beta V(x))$, called the *Boltzmann distribution*. In physics, β is related to temperature via $\beta^{-1} = k_B T$.

How to Simulate an SDE

We can simply adapt the Euler Scheme to the SDE world:

Algorithm 1 Euler-Maruyama Scheme

1: **procedure** EULER-MARUYAMA(x_0, Δ_t, m)
2: **for** $k = 0, \ldots, m-1$ **do**
3: $x_{k+1} = x_k + b(x_k)\Delta_t + \sigma(x_k)\mathcal{N}^d(0, \sqrt{\Delta_t})$.
4: **end for**
5: **end procedure**

Ito's Formula

The chain rule for SDEs: Ito's Formula

Theorem (Ito's Lemma)

Let $X_t \in \mathbb{R}^d$ solve the stochastic differential equation $dX_t = b(X_t)dt + \sigma(X_t)dB_t$, and let $f \in C^2(\mathbb{R}^d)$. Then $Y_t := f(X_t)$ solves the SDE

$$dY_t = \left[\nabla f^T(X_t)b(X_t) + \frac{1}{2}\nabla^2 f(X_t) : a(X_t)\right] dt + \nabla f^T(X_t)\sigma(X_t)dB_t,$$

where $\nabla f \in \mathbb{R}^d$ is the gradient of f, $\nabla^2 f \in \mathbb{R}^{d\times d}$ is the Hessian matrix, $a := \sigma\sigma^T$ is the covariance matrix of the diffusion, and the colon denotes the Frobenius inner product between matrices: $A : B = \sum_{i,j} A_{ij}B_{ij}$.

Motivation

SDE Theory

The Koopman Generator

Semigroup

From the Chapman-Kolmogorov equation, we know that the Koopman operators form a semigroup:

Definition

A familiy of bounded linear operators $\mathcal{T}^\tau,\ \tau \geq 0$ on a Banach space X is called a **strongly continuous semigroup** if:
(i) $\mathcal{T}^0 = \mathrm{Id}$.
(ii) $\mathcal{T}^{\tau_1+\tau_2} = \mathcal{T}^{\tau_1}\mathcal{T}^{\tau_2}$ for all $0 \leq \tau_1 \leq \tau_2$.
(iii) $\lim_{\tau\to 0} \mathcal{T}^\tau x = x$ for all $x \in X$.

The Generator

Definition

Consider the strongly continuous semigroup of Koopman operators $\mathcal{K}^\tau$ on $L^2_\mu(\mathbb{X})$. The generator $\mathcal{L}$ is a linear operator acting on a function f by

$$\mathcal{L}f := \lim_{\tau \to 0} \frac{1}{\tau}(\mathcal{K}^\tau - \mathrm{Id})f,$$

whenever this limit exists. The domain of of the generator, that is the set of all f where the above limit exists, is denoted $\mathcal{D}(\mathcal{L})$.

Generator and Time Evolution

Theorem

The generator $\mathcal{L}$ is defined on a dense subspace $\mathcal{D}(\mathcal{L})$. Moreover, we have the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\mathcal{K}^\tau f = \mathcal{L}\mathcal{K}^\tau f = \mathcal{K}^\tau \mathcal{L} f, \quad f \in \mathcal{D}(\mathcal{L}).$$

The Generator of an SDE

Proposition

Let $f \in C_0^\infty(\mathbb{R}^d)$ and X_t solve an SDE with drift b and diffusion σ. Then $f \in \mathcal{D}(\mathcal{L})$ and the action of the generator is given by

$$\mathcal{L}f(x) = b(x) \cdot \nabla f(x) + \frac{1}{2}a(x) : \nabla^2 f(x).$$

Proof

Proof.

$$
\begin{aligned}
\mathcal{L}f(x) &= \lim_{\tau\to 0}\frac{1}{\tau}\mathbb{E}^x(f(X_\tau) - f(X_0)) \\
&= \lim_{\tau\to 0}\frac{1}{\tau}\mathbb{E}^x\left[\int_0^\tau \nabla f^T(X_s)b(X_s) + \frac{1}{2}a(X_s) : \nabla^2 f(X_s)\,\mathrm{d}s\right] \\
&\quad + \mathbb{E}^x\left[\int_0^\tau \nabla f^T(X_s)\sigma(X_s)\,\mathrm{d}B_s\right] \\
&= \lim_{\tau\to 0}\frac{1}{\tau}\mathbb{E}^x\left[\int_0^\tau \nabla f^T(X_s)b(X_s) + \frac{1}{2}a(X_s) : \nabla^2 f(X_s)\,\mathrm{d}s\right] \\
&= \nabla f^T(x)b(x) + \frac{1}{2}a(x) : \nabla^2 f(x).
\end{aligned}
$$

More about Generators

Corollary

Let $f \in C_0^\infty(\mathbb{R}^d)$ and consider the function $v(\tau, x) = \mathbb{E}^x[f(X_\tau)]$, with X_τ solution of an SDE. Then v solves the PDE

$$\frac{\partial}{\partial \tau} v(\tau, x) = \mathcal{L} v(\tau, x) = b(x) \cdot \nabla_x v(\tau, x) + \frac{1}{2} a(x) : \nabla_x^2 v(\tau, x).$$

References

Oksendal, *Stochastic Differential Equations* (2013)

Pazy, *Semigroups of linear operators and applications to partial differential equations* (2012)

Bakry, Gentil, Ledoux, *Analysis and Geometry of Markov Diffusion Operators* (2014)