Theory and numerical solution of SDEs

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Motivation

Chemical Kinetics - Deterministic Version

$$\frac{dC_i}{dt} = f(C_1, C_2, \cdots, C_N)$$

This model works for reactions in test-tubes or larger sizes. For smaller systems, discreteness and randomness plays a role. An example is cellular systems in biology.

Stochastic Chemical Kinetics

- Assume N species and M reactions
- Propensity Function : $a_j(\mathbf{c})dt$ be the probability that given $\mathbf{C}(t) = \mathbf{c}$ the reaction R_j occurs in time $[t, t + dt)$
- a_j needs to be calculated from molecular physics

Stochastic Chemical Kinetics

Poisson Random Variable

$$P(X = k) = \frac{\lambda^k \exp(-\lambda)}{k}$$

- k is the number of occurances in a time interval
- The mean rate of occurance is λ
- The events are independent
- For large λ Poisson distribution approaches the Gaussian distribution with the same mean (and std. dev.)

TAU-LEAPING [Gil07]

- During $[t, t+\tau)$, propensity functions do not change value
- R_j then is a Poisson random variable with mean $a_j(\mathbf{c})\tau$
- Therefore, $\mathbf{C}(t+\tau) = \mathbf{C}(t) + \sum \mathcal{P}_j(a_j(\mathbf{c})\tau)\nu_j$

Stochastic Chemical Kinetics

TAU-LEAPING (Contd..)

- Assume that $a_j(\mathbf{c})\tau \gg 1$. Then, each $\mathcal{P}_j(a_j(\mathbf{c})\tau)$ is close to a Gaussian random variable.
- Therefore,

$$\begin{aligned}
\mathbf{C}(t+\tau) &= \mathbf{C}(t) + \sum \mathcal{P}_j(a_j(\mathbf{c})\tau)\nu_j \\
&= \mathbf{C}(t) + \sum \mathcal{N}_j(a_j(\mathbf{c})\tau, a_j(\mathbf{c})\tau)\nu_j \\
&= \mathbf{C}(t) + \sum (a_j(\mathbf{c})\tau + \sqrt{a_j(\mathbf{c})\tau}\mathcal{N}_j(0,1)\nu_j \\
&= \mathbf{C}(t) + \sum a_j(\mathbf{c})\nu_j\tau + \sum \sqrt{a_j(\mathbf{c})}\mathcal{N}_j(0,1)\nu_j\sqrt{\tau}
\end{aligned}$$

- $\mathbf{C}(t+\tau) - \mathbf{C}(t) = \sum a_j(\mathbf{c})\nu_j\tau + \sum \sqrt{a_j(\mathbf{c})}\nu_j\mathcal{N}_j(0,1)\sqrt{\tau}$

Stochastic Chemical Kinetics

TAU-LEAPING (Contd..)

$$\begin{aligned}\Delta \mathbf{C}(t) &= \sum a_j(\mathbf{C}(t))\nu_j \Delta t + \sum \sqrt{a_j(\mathbf{C}(t))}\nu_j \Gamma_j \sqrt{\Delta t} \\ &= \sum a_j(\mathbf{C}(t))\nu_j \Delta t + \sum \sqrt{a_j(\mathbf{C}(t))}\nu_j \Delta B_t\end{aligned}$$

Stochastic Differential Equation

The above is an SDE of the form

$$dX_t = b(t, X_t)dt + \sigma(t, X_t)dB_t$$

where B is called Brownian motion.

Random Variables

Random Variable

X taking real values randomly!

Gaussian Random Variable

$$P(a \leq X \leq b) = \int_a^b \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx$$

Mean and Variance

$EX := \int_{-\infty}^{\infty} x f_X(x) dx, E(X - EX)^2 := \int_{-\infty}^{\infty} (x - EX)^2 f_X(x) dx$

Random Functions / Stochastic Processes [Kal80]

Discrete Time Stochastic Process

A sequence of random variables $X_t, t = 1, 2, \cdots$ is called a discrete time stochastic process. These are random sequences!

Continuous Time Stochastic Process*

A collection of random variables indexed by a continuous parameter e.g. $X_t, t \geq 0$

[1] Measurability conditions are also required

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Random Functions! What are some unique features of CT vs DT processes?

The joint distributions (a.k.a. finite dimensional distributions) completely specify the path properties in the DT case whereas this is not true in the CT case!

[1] Measurability conditions are also required

Brownian Motion

Brownian Motion

A continuous time stochastic process $B_t, t \geq 0$ satisfying

1. $B_0 = 0$
2. $B_t - B_s \sim \mathcal{N}(0, t - s)$ for $t > s$
3. $B_s - B_r$ and $B_q - B_t$ are independent for $q > t > s > r$
4. The paths of the B_t are continuous

Construction [SP12]

Methods :

1. Wiener's Construction (based on Trignometric functions)
2. Levy-Ciesieslki (General orhto normal systems, e.g. Haar functions)
3. Kolmogorov's consistency theorem (Existence only!) - Identify a stochastic process as a probability measure on the space of all functions!

Limit of Random Walks

1. Let X_i be i.i.d. random variables taking values ± 1 with probability $\frac{1}{2}$ and $S_n = X_1 + X_2 + \cdots X_n$
2. Linear interpolation + Gaussian Scaling : $W^n(t) := \frac{1}{\sqrt{n}} \left(S_{\lfloor nt \rfloor} + (nt - \lfloor nt \rfloor) X_{\lfloor nt \rfloor + 1} \right),\ t \in [0, 1].$
3. As $n \to \infty$, the limiting process is a Brownian motion (in the weak sense)

Construction using Haar Functions [Kal80]

Haar Orthonormal System

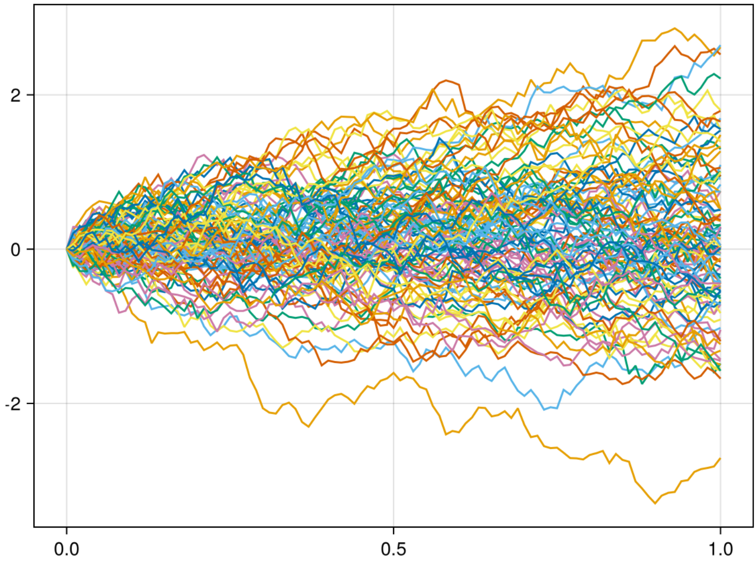
$$g_{00}(s) = 1$$

$$g_{nj}(s) = \begin{cases} 2^{(n-1)/2}, & s \in \left[\frac{j}{2^{n-1}}, \frac{j+\frac{1}{2}}{2^{n-1}}\right) \\ -2^{(n-1)/2}, & s \in \left[\frac{j+\frac{1}{2}}{2^{n-1}}, \frac{j+1}{2^{n-1}}\right) \\ 0, \text{ otherwise} \end{cases}$$

Construction

$B_t = \sum_{n=0}^{\infty} \sum_{j \in S_n} Y_{n,j} G_{n,j}$ where $S_n = \{0, 1, \cdots, 2^{n-1} - 1\}$, $G_{n,j}$ are the integrals of g and $Y_{n,j}$ are i.i.d. $N(0,1)$ random variables.

Simulation (using Haar Functions)



Properties

Properties of Brownian Motion

1. Gaussian Process - (any finite linear combination is a Gaussian Random Variable)
2. Self Similarity - $\frac{1}{\sqrt{a}} B_{at}$ is also a Brownian Motion!
3. The Brownian paths are nowhere differentiable!

Reimann-Stieltjes Integral

1. $\int_a^b fdg = \lim \sum_i f(c_i)(g(t_i) - g(t_{i-1}))$, where f and g are functions.
2. The integral exists whenever f is continuous and g is bounded variation, i.e. $\sup \sum |g(t_{i+1}) - g(t_i)| < \infty$.

1. $\int_a^b f(x)dg(x) = f(b)g(b) - f(a)g(a) - \int_a^b g(x)df(x)$
2. B_t has infinite variation! Therefore, the integral cannot defined directly!
3. Can we define $\int_a^b f_s dB_s := f_b B_b - f_a B_a - \int_a^b B_s df_s$? Yes, but it restricts the functions f that can be integrated!

Ito Integral

1. Let $0 = t_0 < t_1 < t_2 \cdots t_n = t$ be a partition of $[0, t]$ and consider $\int_0^1 B_t dB_t$
2. $L_n = \sum_{i=1}^n B_{t_{i-1}}(B_{t_i} - B_{t_{i-1}})$, $R_n = \sum_{i=1}^n B_{t_i}(B_{t_i} - B_{t_{i-1}})$

What can we say about the limits of L_n, R_n?

L^2-convergence

A sequence of random variables X_n are said to converge to another random variable X in L^2, if $E|X_n - X|^2 \to 0$ as $n \to \infty$.

End-Point matters!

1. $R_n \xrightarrow{L^2} \frac{1}{2}(B_t^2 + t)$
2. $L_n \xrightarrow{L^2} \frac{1}{2}(B_t^2 - t)$ (a Martingale)

1. Ito-Integral : Take left end-point, i.e. L_n
2. Stratonivich Integral : Take right end-point, i.e. R_n

The Ito-integral is defined in terms of convergence in probability in the general case. However, we skip this important generalization here.

Ito Formula

Integration by parts

$\int_a^b f'(g)dg(x) = \int_a^b d(f \circ g) = (f \circ g)(b) - (f \circ g)(a)$

Ito Formula

For any $f : \mathbb{R} \to \mathbb{R}$ which is twice continuously differentiable,
$\int_a^b f'(B_t)dB_t = f(B_b) - f(B_a) - \frac{1}{2}\int_a^b f''(B_s)ds$

Ito Formula - Example

1. Take $f(x) = \frac{1}{2}x^2$, $\int_0^t B_s dB_s = \frac{1}{2}(B_t^2 - t)$
2. Take $f(x) = \exp(x)$,
   $\int_0^t \exp(B_s)dB_s = \exp(B_t) - 1 - \frac{1}{2}\int_0^t \exp(B_s)ds$

Ito Formula

Ito Process

$X_t = X_a + \int_a^t f_s dB_s + \int_a^t g_s ds, a \le t \le b$

Ito Formula - General Version [Kuo06]

Let $\theta(t,x)$ be a continous function such that $\frac{\partial\theta}{\partial x}, \frac{\partial\theta}{\partial t}, \frac{\partial^2\theta}{\partial x^2}$ are continuous. Then $\theta(t, X_t)$ is also an Ito process and

$$\theta(t, X_t) = \theta(a, X_a) + \int_a^t \frac{\partial\theta}{\partial x}(s, X_s) f_s dB_s + \int_a^t \left(\frac{\partial\theta}{\partial t}(s, X_s) + \frac{\partial\theta}{\partial x}(s, X_s) g_s + \frac{1}{2}\frac{\partial^2\theta}{\partial x^2}(s, X_s) f_s^2 \right) ds$$

Shorthand notation

$d\theta = \frac{\partial\theta}{\partial x} f_t dB_t + \left(\frac{\partial\theta}{\partial t} + \frac{\partial\theta}{\partial x} g_t + \frac{1}{2}\frac{\partial^2\theta}{\partial x^2} f_t^2 \right) dt$

Ito Formula

Calculus

$dt^2 = dtdB_t = 0$ and $(dB_t)^2 = dt$

$$dX_t = f_t dB_t + g_t dt$$
$$(dX_t)^2 = f_t^2 dt$$

Simplified Representation

$$d\theta = \frac{\partial\theta}{\partial t}dt + \frac{\partial\theta}{\partial x}dX_t + \frac{1}{2}\frac{\partial^2\theta}{\partial x^2}(dX_t)^2$$

Application of Ito Formula

Example 1

$X_t = \int_0^t f_s dB_s - \frac{1}{2}\int_0^t f_s^2 ds$ and let $\theta(t, x) = e^x$.

$$de^{X_t} = e^{X_t} f_t dB_t X_t dt +$$

Langevin Equation - First SDE

$dX_t = \alpha dB_t - \beta X_t dt, X_0 = x_0$ and let $\theta(t, x) = e^{\beta t} X_t$

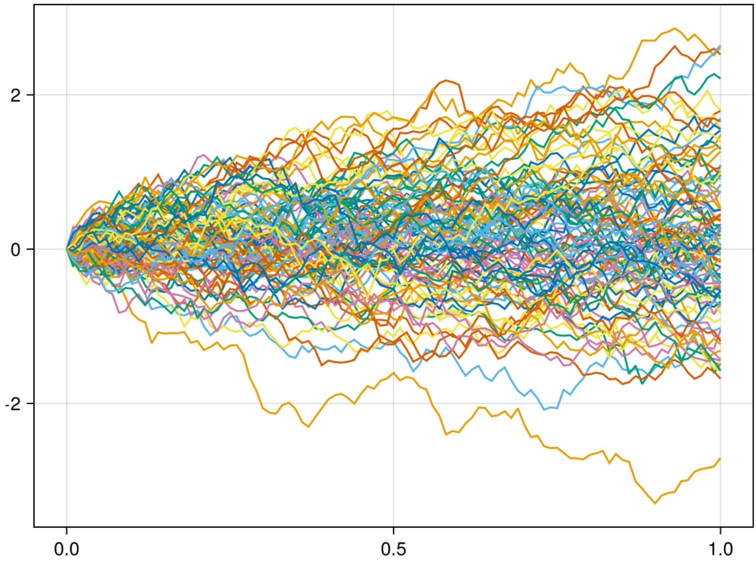
$$d(e^{\beta t} X_t) = \beta e^{\beta t} X_t dt + e^{\beta t}(\alpha dB_t - \beta X_t dt)$$

$$d(e^{\beta t} X_t) = \alpha e^{\beta t} dB_t$$

$$e^{\beta t} X_t = X_0 + \int_0^t e^{\beta t} dB_t$$

This is the Ornstein–Uhlenbeck process!

Simulation - Langevin SDE



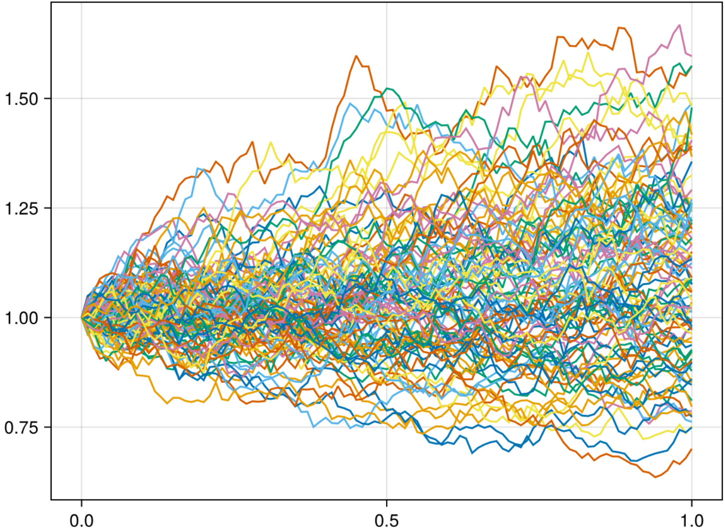
Application of Ito Formula

Stock Prices!

$$
\begin{aligned}
dX_t &= \mu X_t dt + \sigma X_t dB_t \\
d(\log X_t) &= \frac{1}{X_t} dX_t - \frac{1}{2X_t^2}(dX_t)^2 \\
&= \frac{1}{X_t} dX_t - \frac{\sigma^2}{2X_t^2}((X_t)^2 dt) \\
&= \mu dt + \sigma dB_t - \frac{\sigma^2}{2} dt \\
X_t &= X_0 \exp\left((\mu - \frac{1}{2}\sigma^2)t + \sigma B_t\right)
\end{aligned}
$$

This is Geometric Brownian Motion!

Simulation - Stock Price SDE



Stochastic Differential Equations

SDE

$dX_t = b(t, X_t)dt + \sigma(t, X_t)dB_t$

Solution to SDE

Find a stochastic process X_t which satisfies
$X_t = X_a + \int_0^t b(t, X_t)dt + \int_0^t \sigma(t, X_t)dB_t$

Important!

SDEs are not meaningful in the differential form! They have to be understood in the integral sense.

SDE - Existence and Uniqueness of solution [Øks10]

Growth and Lipschitz Conditions

1. $|b(t,x)| + |\sigma(t,x)| \leq C(1+|x|)$: Linear Growth Condition
2. $|b(t,x) - b(t,y)| + |\sigma(t,x) - \sigma(t,y)| \leq D|x-y|$: Lipschitz Condition

Strong Solution

The SDE $dX_t = b(t, X_t)dt + \sigma(t, X_t)dB_t$ has a unique continuous solution in $[0, T]$ provided the above conditions are satisfied and X_0 is independent of the Brownian motion $B_t, t \geq 0$.

Numerical Solution

Euler Approximation

Let $a = t_0 < t_1 < \cdots < t_n = b$ and $\delta = \max_j |t_{j+1} - t_j|$.
$Y^\delta_{n+1} = Y^\delta_n + b(t_n, Y^\delta_n)(t_{n+1} - t_n) + \sigma(t_n, Y^\delta_n)(B_{t_{n+1}} - B_{t_n})$

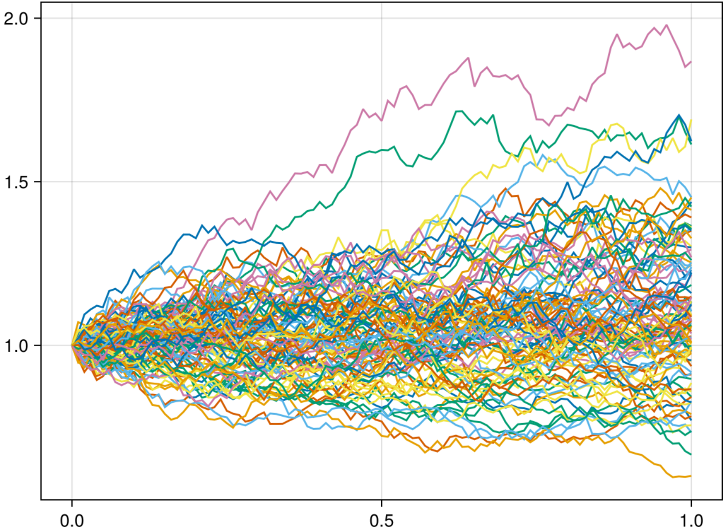
Convergence of Euler Scheme

$E\left[\sup_{a\leq t\leq b} |X_s - Y^\delta_s|^2\right] = O(\delta^{1/2})$

Milstein scheme is a higher order scheme with

$$E\left[\sup_{a\leq t\leq b} |X_s - Y^\delta_s|^2\right] = O(\delta)$$

Simulation - Stock Price SDE



Densities!

We have simulated along the time direction. How about the distribution of the solution at a given time t?

Fokker-Plank

$$\frac{\partial}{\partial t}p(x,t) = -\frac{\partial}{\partial t}[\mu(x,t)p(x,t)] + \frac{1}{2}\frac{\partial^2}{\partial t^2}[\sigma^2(x,t)p(x,t)]$$

Example

$\mu = 0$ and $\sigma = 1.0$, then $\frac{\partial}{\partial t}p(x,t) = \frac{1}{2}\frac{\partial^2}{\partial t^2}[p(x,t)]$

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