p6 | Ito vs. Stratonovich

- Q: Given an ODE, e.g.

$$\dot{x} = f(x):$$

What does it mean?

A: Constructive approach:
estimate $x_i = x(i\,dt)$, numerically then let $dt \to 0$.

- Possibility no 1: explicite Euler scheme

$$x_i = x_{i-1} + f(x_{i-1}) \cdot dt.$$

- Possibility no 2: implicite

$$x_i = x_{i-1} + f(x_i)\, dt.$$

- Possibility no 3: mixed

$$x_i = x_{i-1} + \tfrac{1}{2}[f(x_{i-1}) + f(x_i)]\, dt.$$

⇒ For deterministic ODEs different schemes differ only in terms of numerical performance, stability, etc.
Not in the limit result

- What about SDEs ?

$$\dot{x} = f(x) + \sqrt{2D(x)}\,\xi$$

$$\langle \xi(t)\,\xi(t') \rangle = \delta(t-t').$$

- Explicit Euler scheme:

$$x_i = x_{i-1} + f(x_{i-1})\,dt + \sqrt{2D(x_{i-1})}\,\mathcal{N}\cdot\sqrt{dt}$$

$\mathcal{N}$ ≡ ~~normally~~ distributed ~~normal~~ variable ~~mean 0~~, variance 1

≡ Wiener increment.

⟶ Ito

- Mixed scheme:

$$x_i = x_{i-1} + \frac{1}{2}\left[f(x_{i-1}) + f(x_i)\right]dt + \frac{1}{2}\left[\sqrt{2D(x_{i-1})} + \sqrt{2D(x_i)}\right]\mathcal{N}\cdot\sqrt{dt}.$$

⟶ Stratonovich

$$x_i = x_{i-1} + f(x_{i-1})\cdot dt + O(dt^{3/2}) + g(x_{i-1})\cdot\mathcal{N}\cdot\sqrt{dt} + g'(x_{i-1})\cdot g(x_{i-1})\cdot\mathcal{N}^2\cdot dt + O(dt^{\frac{3}{2}})$$

$g(x) = \sqrt{2D(x)}$

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$\Rightarrow \langle \mathcal{N}^2 \rangle = 1 \neq 0$

$\Rightarrow$ Itô vs. Stratonovich interpretation give different drift terms.

Wrap-up

- stating a nonlinear SDE without specifying its interpretation does not make sense (it's like writing a text and not specifying in which language it was written)

  $\longrightarrow$ Many more interpretations:
  - Itô-thermal
  - alpha-calculus by Lau & Lubensky PRE

- A Stratonovich SDE (S) $\dot{x} = f(x) + g(x)\xi$ can be rewritten as Itô SDE (I) $\dot{x} = f(x) + g(x)\xi + \frac{1}{2} g' g$ and vice-versa. Use interpretation most suitable for a given task.

Stratonovich: ordinary chain rule $y(x)$: $\dot{y} = \frac{\partial y}{\partial x}\dot{x}$

Itô chain rule

$$(I) \quad \dot{x}_k = f_k + g_{kl}\xi_l .$$

$$\langle \xi_k(t_1)\xi_l(t_2)\rangle = \delta_{kl}\delta(t_1-t_2)$$

$$y = y(\underline{x}):$$

$$\dot{y} = \frac{\partial y}{\partial x_j}\dot{x}_j + \frac{1}{2}\frac{\partial^2 y}{\partial x_k \partial x_l} g_{km} g_{ml}$$

Switching between Itô & Stratonovich

$$(S) \quad \dot{x}_k = f_k + g_{kl}\xi_l .$$

$$(I) \quad \dot{x}_k = f_k + g_{kl}\xi_l + \frac{1}{2}\frac{\partial g_{kl}}{\partial x_m} g_{ml} .$$

Fokker-Planck-equation

refers to entire drift term.

$$\dot{P} = \frac{\partial}{\partial x_k}\Big[-\big(\underbrace{f_k}_{\text{det. drift}} + \underbrace{\alpha \frac{\partial g_{kl}}{\partial x_m} g_{ml}}_{\text{noise induced drift}}\big)P + \underbrace{\frac{1}{2}\frac{\partial}{\partial x_m}(g_{kl}g_{ml})P}_{\text{diffusion}}\Big].$$

$\alpha = 0$: Itô

$\alpha = 1/2$: Stratonovich

$\alpha = 1$: Iso-thermal

Lau-Lubensky PRE ( )

- finance loves Ito: not looking back into the past.

- Physics: often Stratonovich used, often Wong-Zakai-theorem applies:

Theorem (Wong-Zakai):
If $\dot{x} = f(x) + g(x)\xi$
is an SDE with colored noise of finite correlation time T, then taking the limit $T \to$ will yield a Stratonovich SDE with Gaussian white noise ξ.

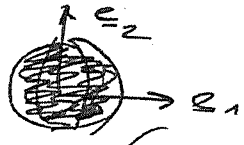
Example of colored noise (Ornstein-Uhlenbeck process)

$$T\dot{\xi} = -\xi + \eta$$

$$\langle \eta(t)\eta(t')\rangle = \delta(t-t')$$

Example: rotational diffusion in 2D.

$$\dot\varphi = \xi .$$



$$\underline{e}_1 = \begin{pmatrix}\cos\varphi\\ \sin\varphi\end{pmatrix}, \quad \underline{e}_2 = \begin{pmatrix}-\sin\varphi\\ \cos\varphi\end{pmatrix}.$$

$SO(2)$: $\frac{d}{dt}[\underline{e}_1, \underline{e}_2] = [\underline{e}_1, \underline{e}_2]\cdot \xi \cdot \begin{pmatrix}0 & -1\\ +1 & 0\end{pmatrix}$

$$(S)\quad \begin{cases} \dot{\underline{e}}_1 = \xi\, \underline{e}_2 \\ \dot{\underline{e}}_2 = -\xi\, \underline{e}_1 \end{cases}$$

$$\Downarrow$$

$\underline{e}_1 = \begin{pmatrix}x_1\\ x_2\end{pmatrix}$, $\underline{e}_2 = \begin{pmatrix}x_3\\ x_4\end{pmatrix}$, $g = \sqrt{2D}\begin{pmatrix}x_3\\ x_4\\ -x_1\\ -x_2\end{pmatrix}$ $\Rightarrow \sum_m \frac{\partial g_k}{\partial x_m} g_m = 2D\begin{pmatrix}-x_1\\ -x_2\\ -x_3\\ -x_4\end{pmatrix}$

correct, but not needed.

$$(I)\quad \begin{cases} \dot{\underline{e}}_1 = \cancel{\xi\, \underline{e}_2 + \tfrac12 \underbrace{\langle \xi \tfrac{\partial \underline{e}_2}{\partial \underline{e}_1}\cdot \dot{\underline{e}}_1\rangle}_{0} + \tfrac12 \underbrace{\langle \xi \tfrac{\partial \underline{e}_2}{\partial \underline{e}_2}\cdot \dot{\underline{e}}_2\rangle}_{\tfrac12 (2D_{rot})\cdot(-\underline{e}_1)}} \\ \quad = \xi\, \underline{e}_2 - D_{rot}\, \underline{e}_1 \\ \dot{\underline{e}}_2 = -\xi\, \underline{e}_1 - D_{rot}\, \underline{e}_2 . \end{cases}$$

Exercise:

Run simulations for

(I) $\dot{\underline{e}}_1 = \xi\, \underline{e}_2 - D_{rot}\, \underline{e}_1$
$\quad\ \dot{\underline{e}}_2 = -\xi\, \underline{e}_1 - D_{rot}\, \underline{e}_2$

and:

(I) $\dot{\underline{e}}_1 = \xi\, \underline{e}_2$
$\quad\ \dot{\underline{e}}_2 = -\xi\, \underline{e}_1 .$

Toy example I (Geometric Brownian motion)

$$(S) \quad \mathring{x} = x\xi - Dx \quad \equiv \quad (I) \quad \mathring{x} = x\xi .$$

$$\langle \xi(t)\,\xi(t') \rangle = 2D\,\delta(t-t')$$

$$m(t) = \langle x(t) \rangle .$$

$$\frac{d}{dt} m = \langle \dot{x} \rangle = \langle (x\xi)_{Itô} \rangle$$

$$= \langle x \rangle \cdot \underbrace{\langle \xi \rangle}_{=0} = 0 .$$

$\Rightarrow \quad m(t) = m_0 .$ (but variance grows exponentially)

Note: $y = \ln x \Rightarrow \dot{y} = \xi - D \Rightarrow y \sim \mathcal{N}(-Dt, Dt)$.

Toy example II

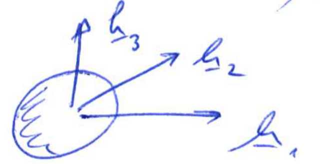
$$(S) \quad \mathring{x} = x\xi \quad \equiv \quad (I) \quad \mathring{x} = x\xi + Dx .$$

$$\frac{d}{dt} m = \langle \mathring{x} \rangle = \langle (x\xi + Dx)_{Itô} \rangle = 0 + Dm$$

$\Rightarrow m = m_0 \exp(Dt)$

$\longrightarrow$ tutorial 7 .

Rotational diffusion in 3D



$$D_{rot} = \frac{k_B T}{8\pi\eta r^3}.$$

Spherical coordinates

$$\underline{h}_3 = (\cos\varphi,\ \sin\varphi\cos\theta,\ \sin\varphi\sin\theta)$$

$$-\frac{\partial \underline{h}_3}{\partial\varphi} = g_1 = (+\sin\varphi,\ -\cos\varphi\cos\theta,\ -\cos\varphi\sin\theta)$$

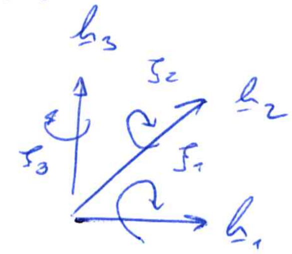
$$g_2 = (0,\ -\sin\theta,\ \cos\theta) = \underline{h}_3 \times g_1$$

$$\underline{h}_1 = \cos\varphi\, g_1 + \sin\varphi\, g_2$$

$$\underline{h}_2 = \underline{h}_3 \times \underline{h}_1.$$

Frenet Serret equations

$$(S)\quad \begin{cases} \dot{\underline{h}}_3 = \xi_2 \underline{h}_1 - \xi_1 \underline{h}_2 \\ \dot{\underline{h}}_1 = -\xi_2 \underline{h}_3 + \xi_3 \underline{h}_2 \\ \dot{\underline{h}}_2 = -\xi_1 \underline{h}_3 - \xi_3 \underline{h}_1 \end{cases}$$



$\Rightarrow$

$$(S)\quad \dot\varphi = \sin\varphi\,\xi_1 + \cos\varphi\,\xi_2$$

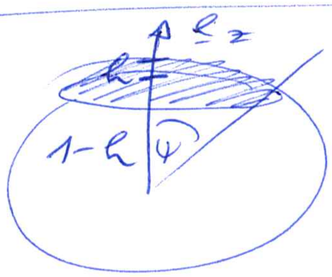
$\Rightarrow$

$$(I)\quad \dot\varphi = \underbrace{\sin\varphi\,\xi_1 + \cos\varphi\,\xi_2}_{} + D_{rot}\cot\varphi$$

equivalent to Gaussian white noise $\xi(t)$ with $\langle \xi(t_1)\xi(t_2)\rangle = 2D_{rot}\,\delta(t_1 - t_2)$

$$\boxed{\dot\varphi = D_{rot}\cot\varphi + \xi}$$

Steady state distribution must be isotropic ⇒ let's check.



- What is $P^*(\varphi)$?

$h = 1 - \cos\varphi$.

$A = 2\pi \cdot r h, \quad r = 1$

$dA = 2\pi \, dh$

$\Rightarrow P^*(h) = \frac{1}{2}$

$P^*(h)\,dh = P^*(\varphi)\,d\varphi$

$dh = \sin\varphi \, d\varphi$

$\Rightarrow P^*(\varphi) = \frac{1}{2}\sin\varphi$.

- $\dot{\varphi} = D_{rot} \cot\varphi + \xi$.

$= -\frac{1}{\gamma}\frac{\partial}{\partial\varphi}U + \xi, \quad U = -\underbrace{D_{rot}\gamma}_{k_B T} \ln\sin\varphi$

$\Rightarrow P^*(\varphi) \sim \exp\left(-\frac{U/\gamma}{D_{rot}}\right)$

$\sim \exp(\ln(\sin\varphi)) \sim \sin\varphi$.

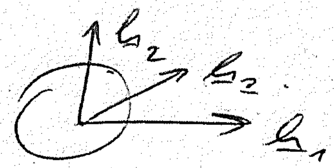
$[\xi]$ 1/s, $[k_B T]$ Nm, $[D_{rot}]$ 1/s, $[\gamma]$ Nms

- <u>Interpretation</u> of $U(\varphi)$
  - entropy $S = k_B \ln\sin\varphi$.
  - free energy $F = -TS$

$= -D_{rot}\gamma \ln\sin\varphi$

$= U!$

Rotational diffusion in 3D



$$D_{rot} = \frac{k_B T}{8\pi \eta r^3}.$$

spherical coordinates

$$\underline{h}_3 = (\cos\psi, \sin\psi\cos\theta, \sin\psi\sin\theta).$$

$$\underline{h}_1 = (\cos\varphi, \sin\varphi, 0)$$

$$\underline{h}_2 = \underline{h}_3 \times \underline{h}_1.$$

Frenet-Serret equations

$$(S)\begin{cases} \dot{\underline{h}}_3 = \xi_2 \underline{h}_1 - \xi_1 \underline{h}_2 \\ \dot{\underline{h}}_1 = -\xi_2 \underline{h}_3 + \xi_3 \underline{h}_2 \\ \dot{\underline{h}}_2 = -\xi_1 \underline{h}_3 - \xi_3 \underline{h}_1. \end{cases}$$

$\Rightarrow$

(S) $\quad \dot{\psi} = +\sin\varphi\,\xi_1 + \cos\varphi\,\xi_2.$

$\Rightarrow$ (I)

$$\dot{\psi} = \underbrace{\sin\varphi\,\xi_1 + \cos\varphi\,\xi_2}_{} + D_{rot}\cot\psi.$$

equivalent to $\xi(t)$ gaussian white noise with $\langle \xi(t_1)\xi(t_2)\rangle = 2D_{rot}\,\delta(t_1 - t_2)$

$$\boxed{\dot{\psi} = D_{rot}\cot\psi + \xi}$$

Extended example:

Persistent random walk (2D).

$$\dot{\underline{r}} = v_0 \, \underline{e}_1$$

$$\underline{e}_1 = \begin{pmatrix} \cos\varphi \\ \sin\varphi \end{pmatrix}, \quad \dot{\varphi} = \xi, \quad \langle \xi(t_1)\, \xi(t_2) \rangle = 2 D_{rot}\, \delta(t_1 - t_2)$$

Proposition

$$C(t) = \langle \underline{e}_1(0) \cdot \underline{e}_1(t) \rangle = \exp(-D_{rot}\, t)$$

$$t_p = \frac{1}{D_{rot}} \equiv \text{persistence time}$$

$$l_p = v_0 t_p \equiv \text{persistence length}$$

Proof:

$$\frac{d}{dt} C(t) = \langle \underline{e}_1(0)\, \dot{\underline{e}}_1(t) \rangle$$

+ add intermediate step.

$$= \langle [\underline{e}_1(0) \cdot \underline{e}_1(t)][\underline{e}_1(t) \cdot \dot{\underline{e}}_1(t)] \rangle$$
$$+ \langle [\underline{e}_1(0) \cdot \underline{e}_2(t)][\underline{e}_2(t) \cdot \dot{\underline{e}}_1(t)] \rangle.$$

Ito Calculus: factors independent

$$= \langle \underline{e}_1(0) \cdot \underline{e}_1(t) \rangle \cdot \langle \underline{e}_1(t) \cdot \dot{\underline{e}}_1(t) \rangle$$
$$+ \langle \underline{e}_1(0) \cdot \underline{e}_2(t) \rangle \underbrace{\langle \underline{e}_2(t) \cdot \dot{\underline{e}}_1(t) \rangle}_{0}$$

$$= C(t) \cdot (-D_{rot}) + 0$$

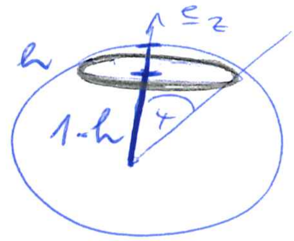
$$\cancel{\sqrt{1-C^2}} \cdot \underbrace{\cancel{\langle \xi \rangle}}_{=0}.$$

$$= -D_{rot}\, C(t).$$

q.e.d. 18B

Steady-state distribution must be isotropic

$A = 2\pi r h$



$P(h) = \frac{1}{2}$ $\qquad h = 1 - \cos\varphi.$

$P(\varphi) = \frac{1}{2}\sin\varphi.$

$P(h)\,dh = P(\varphi)\,d\varphi.$

$dh = \sin\varphi\, d\varphi.$

$\dot{\varphi} = D_{rot}\cot\varphi + \xi$

$\dot{\varphi} = -\frac{1}{\gamma}\frac{\partial}{\partial\varphi} U + \xi, \qquad U = -D_{rot}\,\gamma \ln \sin\varphi.$

$p^*(\varphi) \sim \exp\left(-\frac{U/\gamma}{D_{rot}}\right) \qquad \gamma = \frac{k_BT}{D} = 8\pi\eta r^3.$

$\sim \exp(\ln(\sin\varphi)) \sim \sin\varphi.$

<u>Interpretation</u> $U(\varphi)$

$[k_BT] = \mathrm{Nm} \qquad [\xi]\ 1/s.$
$[D_{rot}]\ 1/s$
$[\gamma]\ \mathrm{Nms}$

- entropy $S = k_B \ln \sin\varphi.$
- free energy

$F = -TS$
$= -D_{rot}\,\gamma \ln \sin\varphi$
$= U\ !$

Outlook: + ext. Field.

How to derive a correct Langevin eqn.?

- limit case of colored noise
  - Wong-Zakai-theorem
- small-number fluctuations (e.g. N particles $1 \underset{r_1}{\overset{r_2}{\rightleftarrows}} 2$)
  - Continuum limit of master equation
- only thermal fluctuations, $T = \text{const.}$
  - use $P^* \sim \exp(-\beta u)$

Master equation for two-state system

$$1 \underset{w_1}{\overset{w_2}{\rightleftarrows}} 2 \qquad N \text{ entities.}$$

state

$P(n) \equiv$ prob. n entities in state 2.

- $\dot{P}(n,t) = w_1 (n+1) P(n+1,t) - w_1 n P(n,t) + w_2 (n-1) P(n-1,t) - w_2 n P(n,t)$

more fancy.

$$\dot{P}(n,t) = w_1 (E^+ - 1) n P + w_2 (E^- - 1)(N-n) P$$

$n+1$
n
$n-1$

$E^{\pm} \equiv$ step operators (shift operator)

$$(E^+ f)(n) = f(n+1)$$

$$(E^- f)(n) = f(n-1).$$

- Let $x = n/N$, treat x as continuous variable
- Taylor expansion

$$(E^{\pm} f)(x) = f(x) \pm f'(x)\cdot\frac{1}{N} + \frac{1}{2} f''(x)\cdot\frac{1}{N^2} + \dots$$

$\Rightarrow$

$$\dot{P}(x,t) = w_1 \frac{\partial}{\partial x}(xP) + \frac{w_1}{2N}\frac{\partial^2}{\partial x^2}(xP) - w_2 \frac{\partial}{\partial x}[(1-x)P] + \frac{w_2}{2N}\frac{\partial^2}{\partial x^2}[(1-x)P]$$

$$= (w_1 + w_2)\frac{\partial}{\partial x}[(x - x^*)P] + \frac{1}{2N}\frac{\partial^2}{\partial x^2}[(w_2 + (w_1 - w_2)x)P]$$

- Steady state? $\quad x^* = \dfrac{w_2}{w_1 + w_2}$

Special case $\quad w_1 = w_2 = w_0$

Conservation equation $\quad \dot{P} = -\nabla J.$

$\Rightarrow$ at equilibrium $J = 0$

$\Rightarrow P^*(x) \sim \exp\left(-\dfrac{(x - 1/2)^2}{2\sigma^2}\right), \quad \sigma^2 = \dfrac{1}{4N}$

Langevin equation

(I) $\dot{x} = (\varphi_1 + \varphi_2)(x^* - x) + \underbrace{\sqrt{\frac{\varphi_1 x + \varphi_2 (1-x)}{2N}}}_{g(x)}\,\xi$

(S) $\dot{x} = (\varphi_1 + \varphi_2)(x^* - x) + g(x)\xi \underbrace{- \frac{1}{2}\,\frac{\varphi_1 - \varphi_2}{4N}}_{-\frac{1}{2}\frac{\partial g}{\partial x} g}$

$N \gg 1 \Rightarrow x \approx x^* \Rightarrow g(x) \approx g(x^*)$

$\Rightarrow P^*(x) = N(x^*, \sigma^2), \quad \sigma^2 = \frac{1}{N}\,\frac{\varphi_1 \varphi_2}{(\varphi_1 + \varphi_2)^2}$

Applications

- chemical reaction kinetics
- Small number fluctuations (e.g. binding/unbinding of molecular motors)

- Euler scheme for Ito SDEs.

(I) $$\dot{x} = f(x) + g(x)\,\xi(t).$$

$$\langle \xi(t)\,\xi(t') \rangle = \delta(t-t').$$

$$x_{t+\Delta t} = x_t + f(x_t)\,\Delta t + g(x_t)\,N_t.$$

$$N_t \sim \mathcal{N}(0, \Delta t).$$

- Euler-Heun scheme for Stratonovich SDEs

(S) $$\dot{x} = f(x) + g(x)\,\xi(t)$$

$$\langle \xi(t)\,\xi(t') \rangle = \delta(t-t').$$

$$x_{t+\Delta t} = x_t + f(x_t)\,\Delta t + \frac{1}{2}[g(x_t) + g(\bar{x}_t)]N_t$$

$$N_t \sim \mathcal{N}(0, \Delta t).$$

$$\bar{x}_t = x_t + g(x_t)\,N_t.$$