2017

Chapter 3: Itō calculus

In the absence of external potential, the dynamics of our colloid in the overdamped limit is described by

$\dot{x}(t) = \sqrt{2D}\,\eta(t)$ (1) with $\eta(t)$ a Gaussian white noise

$\langle \eta(t) \rangle = 0 \quad \langle \eta(t)\eta(t') \rangle = \delta(t-t')$

I/ Is this really serious?

$\eta(t)$ is a random variable → new value at every time, uncorrelated with previous values ⇒ quite far from continuous, differentiable functions usually used in ordinary differential equations in physics.

History: → R. Brown, 1827, observation of the motion of pollen grains suspended in water. (Actually Jan Ingenhousz did the same with coal particle on the surface of alcohol in 1785)

→ Einstein, 1905, connection with atomistic theory

→ Smoluchowsky, 1906, Langevin, 1908 ⇒ birth of stochastic equations

Mathematical basis are hard to build: Wiener (1918), Itō (1944)

Why? Two important problems

① Formal solution of (1) $x(t) = \int_0^t \eta(t')\,dt' + x(0)$

$$\rightarrow \frac{x(t+\tau) - x(t)}{\tau} = \frac{1}{\tau}\int_t^{t+\tau} \eta(t')\,dt'$$

$$\left\langle \frac{x(t+\tau) - x(t)}{\tau} \right\rangle = \frac{1}{\tau}\int_t^{t+\tau} \langle \eta(t') \rangle\,dt' = 0 \qquad \text{OK} \checkmark$$

$$\left\langle \left(\frac{x(t+\tau)-x(t)}{\tau}\right)^2 \right\rangle = \frac{1}{\tau^2}\left\langle \int_t^{t+\tau} \eta(s)\,ds \int_t^{t+\tau} \eta(u)\,du \right\rangle = \frac{1}{\tau^2}\int_t^{t+\tau} ds \int_t^{t+\tau} du\, \overbrace{\langle \eta(s)\eta(u)\rangle}^{\delta(s-u)}$$

$$\forall s \in [t, t+\tau] \qquad \int_t^{t+\tau} \delta(s-u)\,du = 1$$

$$\left\langle \left(\frac{x(t+\tau)-x(t)}{\tau}\right)^2 \right\rangle = \frac{1}{\tau^2}\int_t^{t+\tau} ds = \frac{1}{\tau} \xrightarrow[\tau\to 0]{} \infty$$

$x(t)$ is not differentiable $\Rightarrow$ what does $\dot{x}(t)$ means?

Mathematicians: nothing, only $x(t) = \int_0^t \eta(s)\,ds$ means something $\rightarrow$ Wiener process

Physicists: Yeah, right, but let's still use it, because (1) is a useful notation!

② Diffusion $\quad x^2(t) = \int_0^t ds \int_0^t du\, \eta(s)\eta(u) \Rightarrow \langle x^2(t)\rangle = t$

$\rightarrow$ correct diffusive scaling

$\dot{x}(t) = \eta(t)$; $\frac{d}{dt}x^2(t) = 2x\dot{x} = 2x\eta$ (standard chain rule)

$\frac{d}{dt}\langle x^2(t)\rangle = \langle 2x\eta\rangle = 0$ since $\langle \eta = 0\rangle$ and $x(t)$ is expected to be correlated only with $\eta(t'<t)$ (causality)

so that we expect $\langle x(t)\eta(t)\rangle = \langle x(t)\rangle\langle \eta(t)\rangle$

But $\frac{d}{dt}\langle x^2(t)\rangle = 0$ incompatible with $\langle x^2(t)\rangle = t \Rightarrow$ paradox!

Comment: Not so obvious that $\langle x(t)\eta(t)\rangle = \langle x(t)\rangle\langle \eta(t)\rangle$

Indeed (1) $\Rightarrow x_1(t+dt) = x_1(t) + dt\,\eta(t)$ indeed means $\langle x_1(t+dt)\,\eta(t+dt)\rangle = \langle\rangle \cdot \underset{=0}{\langle\rangle}$

But $x_2(t+dt) = x_2(t) + dt\,\frac{\eta(t)+\eta(t+dt)}{2}$ looks also ok at order dt (semi-implicit scheme). This time $x_2(t+dt)$ and $\eta(t+dt)$ are not independent.

a) Choice of Itō $\langle x(t)\eta(t)\rangle = \langle x(t)\rangle\langle \eta(t)\rangle$ simple but we need to learn how to do calculus again : $\frac{d}{dt}x^2 \neq 2x\dot{x}$

b) Choice of Stratonovich $\Rightarrow$ standard calculus applies but computing $\langle x(t)\eta(t)\rangle$ is painful.

II Itō formula

How does $f(x(t))$ evolve when $x(t)$ is solution of $\dot{x} = F(x) + \eta$ (*)

where $\eta(t)$ is a Gaussian white noise with $\langle \eta(t)\rangle = 0$; $\langle \eta(t)\,\eta(t')\rangle = \sigma\,\delta(t-t')$

(or equivalently $\dot{x} = F(x) + \sqrt{\sigma}\,\xi(t)$ with $\langle \xi(t)\,\xi(t')\rangle = \delta(t-t')$)

Comment: Naive solution of (*) $x(t+dt) = x(t) + \underbrace{\int_t^{t+dt} F(x(s))ds}_{\simeq dt\,F(x(t)) + \mathcal{O}(dt^2)} + \underbrace{\int_t^{t+dt} \eta(s)ds}_{d\xi}$

$$\langle d\xi\rangle = 0 \quad ; \quad \langle d\xi^2\rangle = \int_t^{t+dt} ds \int_t^{t+dt} du\, \langle \eta(s)\eta(u)\rangle = \sigma\,dt$$

$d\xi \sim \sqrt{dt}$! unusual $\rightarrow$ this will alter the chain rule.

Comment: To simulate (*), use $x(t+dt) = x(t) + dt\,F(x(t)) + \sqrt{2\sigma dt}\;u$ where u is chosen from a unit-variance, zero mean Gaussian distribution $P(u) = \frac{1}{\sqrt{2\pi}}\,e^{-\frac{u^2}{2}}$

2017 | 3.4

A) Evolution of $f(x(t))$

$$x(t+dt) = x(t) + F(x(t))\,dt + d\xi(t) + \mathcal{O}(dt^2) \quad ; \quad d\xi(t) = \int_t^{t+dt} \eta(t')\,dt'$$

$t_j = j\,dt \ ; \ t = N dt$

$$f(x(t)) = f(x(0)) + \sum_{j=0}^{N-1} f(x(t_{j+1})) - f(x(t_j))$$

<u>Idea</u>: N large, dt small $\Rightarrow$ expand $f(x(t_{j+1})) - f(x(t_j)) \simeq \frac{\partial f}{\partial x}(x(t_j))dx_j + \frac{1}{2}\frac{\partial^2 f}{\partial x^2}(x(t_j))dx_j^2$

where $dx_j = x(t_{j+1}) - x(t_j) \simeq F(x(t_j))\,dt + d\xi(t_j)$ and $d\xi(t_j) = \int_{t_j}^{t_{j+1}} \eta(s)\,ds$

<u>Then</u> identify $f(x(t)) - f(x(0)) = \int_0^t \frac{df}{dt}(x(s))\,ds$

$$f(x(t)) - f(x(0)) = \sum_{j=0}^{N-1} \frac{\partial f}{\partial x} dx_j + \frac{1}{2}\frac{\partial^2 f}{\partial x^2}\left[F^2 dt^2 + 2F\,dt\,d\xi + d\xi^2\right]$$

<u>Analyse term by term</u>

$$\sum_{j=0}^{N-1} \frac{\partial f}{\partial x} dx_j = \sum_{j=0}^{N-1} \frac{\partial f}{\partial x}\frac{dx_j}{dt}dt \underset{dt\to 0}{\sim} \int_0^t ds\, \frac{\partial f(x(s))}{\partial x}\dot{x}(s)\,ds = \int_0^t ds\, \frac{\partial f(x(s))}{\partial x}\left[F(x(s)) + \eta(s)\right]$$

$$\sum_{j=0}^{N-1} \frac{\partial^2 f}{\partial x^2} F^2 dt^2 = dt \sum_{j=0}^{N-1} \frac{\partial^2 f}{\partial x^2}(x(t_j))F^2[x(t_j)]\,dt \underset{dt\to 0}{\sim} dt \int_0^t \frac{\partial^2 f}{\partial x^2}(x(s))F^2(x(s))\,ds \xrightarrow[dt\to 0]{} 0$$

$$\cancel{\sum_{j=0}^{N-1} \frac{\partial^2 f}{\partial x^2}(x(s))F(x(s))\,dt}$$

$$\sum_{j=0}^{N-1} \frac{\partial^2 f}{\partial x^2}(x(t_j))F(x(t_j))\,d\xi(t_j)\,dt = \sum_{j=0}^{N-1} \frac{\partial^2 f}{\partial x^2}(x(t_j))F(x(t_j))\,dt \int_{t_j}^{t_{j+1}} \eta(s)\,ds \equiv A \quad \text{random variable}$$

$$\langle A\rangle = \sum_{j=0}^{N-1} dt \left\langle \frac{\partial^2 f}{\partial x^2}(x(t_j))F(x(t_j)) \int_{t_j}^{t_{j+1}} \eta(s)\,ds \right\rangle$$

$$\underset{\text{Itō}}{=} \sum_{j=0}^{N-1} dt \left\langle \frac{\partial^2 f}{\partial x^2}(x(t_j))F(x(t_j))\right\rangle \underbrace{\left\langle \int_{t_j}^{t_{j+1}} \eta(s)\,ds \right\rangle}_{=0} \Rightarrow \langle A\rangle = 0$$

$$\langle A^2\rangle = \sum_{j,k=0}^{N-1} dt^2 \left\langle \frac{\partial^2 f}{\partial x^2}(x(t_j)) \frac{\partial^2 f}{\partial x^2}(x(t_k)) F(x(t_j)) F(x(t_k))\, d\xi(t_j)\, d\xi(t_k)\right\rangle$$

if $t_j < t_k$, $d\xi(t_k)$ is independent of the rest $\Rightarrow \langle \dots d\xi(t_k)\rangle = \langle\dots\rangle \underbrace{\langle d\xi(t_k)\rangle}_{=0}$

if $t_j = t_k$, $d\xi^2(t_k)$ ________________

$$\langle A^2\rangle = \sum_{j=0}^{N-1} dt^2 \left\langle \frac{\partial^2 f}{\partial x^2}(x(t_j))^2\, F(x(t_j))^2\right\rangle \underbrace{\langle d\xi(t_j)^2\rangle}_{=\sigma dt}$$

$$\sim \sigma dt^2 \int_0^t \left\langle \left(\frac{\partial^2 f}{\partial x^2}(x(s))\, F(x(s))\right)^2\right\rangle ds \xrightarrow[dt\to 0]{} 0$$

same for all the higher moments.

One term left $\frac{1}{2}\sum_{j=0}^{N-1} \frac{\partial^2 f}{\partial x^2}(x(t_j))\, d\xi^2(t_j)$

$d\xi^2(t_j)$ is a random variable such that $\langle d\xi^2\rangle = \sigma dt$. Its higher moments scale as dt^n, $n>1$. Let us show that to compute $f(x(t)) - f(x(0))$ we can simply replace $d\xi^2$ by σdt (Note the absence of $\langle\dots\rangle$).

$$\Rightarrow B \equiv \sum_j \frac{\partial^2 f}{\partial x^2}(d\xi^2 - \sigma dt)$$

$$\langle B\rangle = \sum_j \left\langle \frac{\partial^2 f}{\partial x^2}(x(t_j))\,(d\xi^2_{(t_j)} - \sigma dt)\right\rangle \underset{\text{Itô}}{=} \sum_j \left\langle\frac{\partial^2 f}{\partial x^2}(x(t_j))\right\rangle \underbrace{\langle d\xi^2(t_j) - \sigma dt\rangle}_{=0}$$

$$= 0$$

$$\langle B^2\rangle = \sum_{j,k} \left\langle \frac{\partial^2 f}{\partial x^2}(x(t_j)) \frac{\partial^2 f}{\partial x^2}(x(t_k)) (d\xi^2(t_j) - \sigma dt)(d\xi^2(t_k) - \sigma dt)\right\rangle$$

if $t_j < t_k$, then $d\xi^2(t_k) - \sigma dt$ is independent from the rest and

$\langle\dots\rangle = \langle\dots\rangle \cdot \langle d\xi^2(t_k) - \sigma dt\rangle = 0 \Rightarrow$ only $j=k$ matters.

$$\langle B^2\rangle \underset{\text{Itō}}{=} \sum_{j=0}^{N-1} \left\langle \frac{\partial^2 f}{\partial x^2}(t_j)^2 \right\rangle \cdot \left\langle d\xi^4(t_j) - 2\sigma dt\, d\xi^2(t_j) + \sigma^2 dt^2 \right\rangle$$

$\langle d\xi^4(t_j)\rangle \overset{?}{=}$ $\Rightarrow d\xi$ is a Gaussian random variable $\Rightarrow \langle d\xi^4\rangle = 3\langle d\xi^2\rangle^2$
(fourth cumulant $C_4 = \langle x^4\rangle - 3\langle x^2\rangle^2 = 0$)

<u>Proof</u>: $\displaystyle \langle x^4\rangle = \frac{1}{\sqrt{2\pi\sigma}} \int_{-\infty}^{+\infty} dx\, x^4 e^{-\frac{1}{2}\frac{x^2}{\sigma}} = \frac{\sigma}{\sqrt{2\pi\sigma}} \int_{-\infty}^{+\infty} dx\, x^3 \frac{x}{\sigma} e^{-\frac{1}{2}\frac{x^2}{\sigma}}$

$$= \frac{\sigma}{\sqrt{2\pi\sigma}} \left[-x^3 e^{-\frac{1}{2}\frac{x^2}{\sigma}} \right]_{-\infty}^{+\infty} + \sigma \cdot \frac{3}{\sqrt{2\pi\sigma}} \int dx\, x^2 e^{-\frac{1}{2}\frac{x^2}{\sigma}}$$

$$= 0 + 3\sigma^2 = 3\langle x^2\rangle^2$$

<u>Thus</u>: $\langle d\xi^4\rangle = 3\langle d\xi^2\rangle^2 = 3\sigma^2 dt^2$

$$\langle B^2\rangle = \sum_j \left\langle \frac{\partial^2 f}{\partial x^2}(x(t_j))^2 \right\rangle 2\sigma^2 dt^2 \sim 2\sigma dt \int_0^t ds \left\langle \frac{\partial^2 f}{\partial x^2}(s) \right\rangle \xrightarrow[dt\to 0]{} 0$$

Higher moments also vanish and in practice we take $B=0$ in the limit $dt\to 0$

<u>All in all</u>

$$f(x(t)) - f(x_0) = \int_0^t ds \left[\frac{\partial f}{\partial x}(x(s))\, \dot{x}(s) + \frac{\sigma}{2} \frac{\partial^2 f}{\partial x^2}(x(s)) \right]$$

Itō lemma: $\boxed{\dfrac{df}{dt} = \dfrac{\partial f}{\partial x}\dot{x} + \dfrac{\sigma}{2}\dfrac{\partial^2 f}{\partial x^2}}$

(β) Generalisation to $f(x(t), t)$

$$\boxed{\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\sigma}{2}\frac{\partial^2 f}{\partial x^2}}$$

(γ) <u>N-dimensional Itō formula</u>

$\dot{x}_i = F_i(x_1, \dots, x_N) + \eta_i$; $\langle \eta_i\rangle = 0$; $\langle \eta_i(t)\eta_j(t')\rangle = \sigma_{ij}\,\delta(t-t')$

$$\boxed{\frac{df(x_1(t), \dots, x_N(t))}{dt} = \sum_i \frac{\partial f}{\partial x_i}\dot{x}_i + \frac{1}{2}\sum_{ij} \sigma_{ij} \frac{\partial^2 f}{\partial x_i \partial x_j}}$$

Let us come back to $\langle x^2(t)\rangle$

$f(x)=x^2$; $f'(x)=2x$; $f''(x)=2$

$\dot{x}=\sqrt{2D}\,\eta(t) \iff \dot{x}=\xi(t)$

$\langle\eta(t)\rangle=0 \qquad \langle\xi(t)\rangle=0$

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

Itō: $\dfrac{df(x(t))}{dt}=\dfrac{\partial f}{\partial x}\dot{x}+D\dfrac{\partial^2 f}{\partial x^2}=2x\xi+2D \Rightarrow \dfrac{d}{dt}\langle x^2(t)\rangle=2\underbrace{\langle x\xi\rangle}_{\text{Itō}\to 2\langle x\rangle\langle\xi\rangle=0}+2D$

$\Rightarrow \langle x^2(t)\rangle=2Dt$

Comment: can now do better $\dfrac{d}{dt}x^2(t)=2D+\underbrace{2x(t)\xi(t)}$ characterizes the fluctuations of x^2.

Also works for higher moments

$\dfrac{d}{dt}\langle x^4\rangle=4\langle x^3\dot{x}\rangle+D\,12\langle x^2\rangle \underset{\text{Itō}}{=} 4\langle x^3\rangle\underbrace{\langle\dot{x}\rangle}_{=0}+24D^2t$

$\Rightarrow \langle x^4\rangle=12D^2t^2=3\cdot(2Dt)^2=3\langle x^2(t)\rangle^2$

You can now compute moments of $x(t)$ without knowing $P(x,t)$

Comment: the $\xi(t)$ form a set of correlated Gaussian variables. What is their joint probability distribution?

$$P[\xi(t)]=Z^{-1}\exp\left[-\frac{1}{2}\int_0^t\xi^2(s)ds\right]$$

$\Rightarrow$ weight in trajectory space; can be used to construct path-integral representation of a stochastic process.

Bibliography: Oksendal, "Stochastic differential equations", Springer

⚠ Remember that $\dot{x}(t)=\sqrt{2D}\,\eta(t)$ is not defined, only ~~$x(t)-x(0)=\int$~~ $x(t)-x(0)=\int_0^t\eta(s)\sqrt{2D}\,ds$ is well defined. The same holds for Itō formula, only $f(t)-f(0)=\int_0^t ds\left[\dfrac{\partial f}{\partial x}\dot{x}+\dfrac{\partial^2 f}{\partial x^2}\dfrac{\Gamma}{2}\right]$ has been proven. Do not start to play with, say, $\exp[\dot{f}(t)]$ and use Itō formulae.