IV The Langevin equation : mathematical & computational aspects

Goal : question the meaning of Langevin framework
Introduce tools of stochastic calculus :

Computational

Stochastic processes raise subtle mathematical pbs. Most of math community did not consider probability theory to be part of mathematics, until XXth century. Processes started to be studied then, with pionners such as Bachelier, Wiener, until it gained more momentum with Kolmogorov, Khinchin, Pearson, Doeblin, Frechet, Doob, Levy, Itô, … It still is a thriving branch of mathematics, see eg the Fields Medals of W. Werner (2006) M. Hairer (2014)

1° Properties of the noise (the Langevin force)

We start with $\dot{x} = \frac{1}{m\gamma} R(t)$ and note that $\frac{1}{m^2\gamma^2}\langle R(t) R(t+\tau)\rangle = \frac{2m^2\Gamma}{\gamma}\delta(\tau) = \frac{2kT}{m\gamma}\delta(\tau)$
$= 2D\,\delta(\tau)$

hence we can write : $\dot{x} = \sqrt{2D}\,\eta(t)$ with $\langle \eta(t)\rangle = 0$

$\langle \eta(t)\,\eta(t+\tau)\rangle = \delta(\tau)$; Wiener process

We have argued that the CLT endows $x(t)$ with gaussian statistics (for Brownian motion of colloids, the statistics of $R(t)$ ie $\eta(t)$ does not matter, as long as τ_c is small enough). For convenience, it is customary to take $\eta(t)$ as gaussian itself : this process is fully characterized by $\langle \eta\rangle$ and $\langle \eta(t)\eta(t+\tau)\rangle = \delta(\tau)$. The noise $\eta(t)$ is stationary and said to be white noise. Why? Because of the $\delta(\tau)$, and of

Wiener-Khintchine theorem

Let $X(t)$ be a stationary process. We define a Fourier transform with a special prefactor

$$\tilde{X}(\omega) = \frac{1}{\sqrt{T_2-T_1}}\int_{T_1}^{T_2} X(t)\, e^{i\omega t}\,dt$$

$$\int_{-\infty}^{+\infty} |\tilde{X}(\omega)|^2 \frac{d\omega}{2\pi} = \frac{1}{T_2-T_1}\int_{T_1}^{T_2} X^2(t)\,dt \quad : \text{Parseval theorem}$$

Take $T_1 \to -\infty$, $T_2 \to \infty$: $\langle P\rangle = \lim_{T_1,T_2} \frac{1}{T_2-T_1}\int_{T_1}^{T_2}\langle X^2(t)\rangle dt = \int_{-\infty}^{+\infty} S(\omega)\frac{d\omega}{2\pi}$

$\langle P\rangle$ is the mean power,

$S(\omega) \equiv \langle |\tilde{X}(\omega)|^2\rangle$ is the power spectral density

$$\langle |\tilde{X}(\omega)|^2 \rangle = \frac{1}{T_2-T_1} \int_{T_1}^{T_2}\int_{T_1}^{T_2} \underbrace{\langle X(t_1) X(t_2)\rangle}_{\mathcal{C}(t_1-t_2)} e^{i\omega(t_1-t_2)} \, dt_1\, dt_2$$

from stationarity (autocorrelation function)

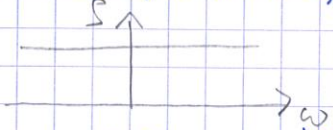
Take $(t_1, t_2) \to (\tau = t_1 - t_2, t_2)$, jacobian 1

$$= \frac{1}{T_2-T_1} \int_{T_1}^{T_2} dt_2 \underbrace{\int_{T_1-t_2}^{T_2-t_2} \mathcal{C}(\tau) e^{i\omega\tau} d\tau}_{\simeq \int_{-\infty}^{+\infty} \mathcal{C}(\tau) e^{i\omega\tau} d\tau \text{ for } |T_1|, T_2 \text{ big enough}}$$

$$\xrightarrow[\substack{T_1 \to +\infty \\ T_2 \to -\infty}]{} \int_{-\infty}^{+\infty} \mathcal{C}(\tau) e^{i\omega\tau} d\tau \equiv \hat{\mathcal{C}}(\omega)$$

$$S(\omega) = \hat{\mathcal{C}}(\omega)$$; Fourier transform of autocorrelation function.

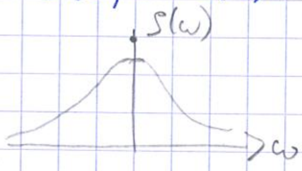
Illustrations : (i) $\mathcal{C}(\tau) = A\,\delta(\tau) \Rightarrow \hat{\mathcal{C}}(\omega) = A = S(\omega)$; Wiener-Khintchine



Flat $\Rightarrow$ white noise

(ii) $\mathcal{C}(\tau) = e^{-a|\tau|}$

$$S(\omega) = \hat{\mathcal{C}}(\omega) = \int_{-\infty}^{+\infty} e^{-a|\tau|} e^{i\omega\tau} d\tau = \frac{1}{a-i\omega} + \frac{1}{a+i\omega} = \frac{2a}{a^2+\omega^2}$$



Lorentzian power spectrum $\Leftrightarrow$ exp autocorrelation

See link : Cauchy distrib $\Leftrightarrow$ charact. function

Variant formulation of Wiener-Khintchine :

We work with usual F.T. : $\hat{X}(\omega) = \int dt\, e^{i\omega t} X(t)$

$$\Rightarrow \langle \hat{X}(\omega)\hat{X}(\omega')\rangle = \int dt\, dt' \langle X(t) X(t')\rangle e^{i\omega t} e^{i\omega' t'} \quad ; \ \tau = t - t'$$
$$= \int dt'\, d\tau\, \mathcal{C}(\tau) e^{i\omega\tau} e^{i\omega t'} e^{i\omega' t'} \quad t = \tau + t'$$
$$= \int \mathcal{C}(\tau) e^{i\omega\tau} d\tau \; 2\pi\,\delta(\omega+\omega')$$

$$\langle \hat{X}(\omega)\hat{X}(\omega')\rangle = \hat{\mathcal{C}}(\omega)\, 2\pi\,\delta(\omega+\omega')$$

Here $X(t)$ is real ; the mode $\hat{X}(\omega)$ is coupled only to mode $\hat{X}(-\omega) = \hat{X}^*(\omega)$

Transition : because the noise is white, we have $\langle \eta^2(t)\rangle = +\infty$,

Hence $\dot{x} = \sqrt{2D}\,\eta(t)$ yields a singular derivative... what are we doing ?

2° Be wise... discretize !

For the mathematicians, equation $\dot{x} = \sqrt{2D}\,\eta(t)$ is meaningless... only its differential form makes sense ("discretized"). Integrate $\int_t^{t+dt}$

$$x(t+dt) - x(t) = \sqrt{2D} \underbrace{\int_t^{t+dt} \eta(t')\,dt'}_{B_{dt}}$$

B_{dt} , increment ;

B_{dt} is a random variable, well characterized : $\langle B_{dt} \rangle = 0$; $\langle B_{dt}^2 \rangle = dt$ 44
and it has gaussian stat $\rightsquigarrow \mathcal{G}(0, \sqrt{dt})$. The singular nature of the equation appears in fact that B_{dt} is of order $\sqrt{dt}$. Yet, dt can be taken arbitrarily small*, which allows to compute the whole trajectory $x(t)$, for the present Wiener process. Let us denote this process $W(t)$. In presence of an external force F_{ext}, mathematicians write

$$dx = \mu F_{ext}\, dt + \sqrt{2D}\, dW(t) \quad ; \quad \mu \equiv \text{mobility}$$

while physicists write

$$\dot{x} = \mu F_{ext} + \sqrt{2D}\, \eta(t) \quad : \text{it is a convenient notation.}$$

Discretization and path integral

The proba of a trajectory $x(t)$ can be found from the discretization of $[0, t]$ into N steps, before taking $N \to \infty$. Back to $F_{ext} = 0$; $x(0)$ known

$$x(t+dt) = x(t) + \sqrt{2D}\, B_{dt}^{(t)}$$

So the proba of $x(dt), x(2dt), x(3dt) \dots x(t)$ is the proba of $\{B_{dt}^{(1)}; B_{dt}^{(2)}, \dots B_{dt}^{(N)}\}$

$$P(B_{dt}^{(1)}, B_{dt}^{(2)}, \dots B_{dt}^{(N)}) \prod_{i=1}^{N} dB_{dt}^{(i)} = \frac{1}{\sqrt{2\pi dt}^{\,N}} \exp\left(-\sum_{i=1}^{N} \frac{(B_{dt}^{(i)})^2}{2\,dt}\right) \prod dB^{(i)}$$

B_{dt} "=" $\eta(t)\, dt$

$$= \left(\frac{1}{\sqrt{2\pi dt}}\right)^N \exp\left[-\frac{1}{2}\sum_{i=1}^{N} \eta^2\, dt\right] \prod_i dB^{(i)}$$

$$\xrightarrow[N\to\infty]{} \exp\left[-\frac{1}{2}\int_0^t \eta^2(t')\, dt'\right] \mathcal{D}\eta(t)$$

this ∞ dimensional measure hides many subtleties

This leads to the path integral representation of the proba of the Brownian motion $x(t)$

$$P[\{x(t')\}, 0 \leq t' \leq t] = \mathcal{N} \exp\left(-\int_0^t \frac{\eta^2(t')}{2}\, dt'\right)$$

$\mathcal{N}$ is an appropriate normalization, finite only when N is finite.
The meaning of this is : discretize as above, N finite, and take N large.
We can also write :

$$P[\{x(t')\}, 0 \leq t' \leq t] = \mathcal{N} \exp\left(-\int_0^t \frac{\dot{x}(t')^2}{4D}\, dt'\right).$$

If there is a constant drift force : $F_{ext}(x,t) = F$, then

$$\dot{x} = \mu F + \sqrt{2D}\, \eta(t)$$

$$P[\{x(t')\}, 0 \leq t' \leq t] = \mathcal{N} \exp\left(-\int_0^t \frac{1}{4D}\left[\dot{x}(t') - \mu F\right]^2 dt'\right)$$

But when F depends on x : more tricky, there is a jacobian pb in going from noise $\eta \to$ position x : $\mathcal{D}x \Leftrightarrow \mathcal{D}\eta$?

This opens a fruitful analogy with Feynman integrals in quantum mechanics.

3°) Stochastic calculus

We have seen, for the Wiener process, that $\langle x^2(t)\rangle = 2D\,t$.

$$\Rightarrow \frac{d}{dt}\langle x^2\rangle = 2D = \left\langle \frac{dx^2}{dt}\right\rangle \overset{?}{=} 2\,\langle x(t)\,\dot{x}(t)\rangle = 2\int_0^t \langle \eta(t')\,\eta(t)\rangle\,dt' \cdot 2D$$

In the context of Brownian motion of colloids, we could compute this integral, remembering that $\tau_c \neq 0 \to$ gave consistent result $\int_0^t \langle \eta(t')\eta(t)\rangle dt = \frac{1}{2}$ for $t \gg \tau_c$. This corresponds to the discretization rule

$$\langle x\,\dot{x}\rangle \longrightarrow \left\langle \frac{x(t+\Delta t)+x(t)}{2}\;\underbrace{\frac{x(t+\Delta t)-x(t)}{\Delta t}}_{\sqrt{2D}\,B_{\Delta t}/\Delta t}\right\rangle \quad \text{and then, } \Delta t \to 0$$

$$x(t+\Delta t) = x(t) + \sqrt{2D}\,B_{\Delta t} \quad ; \quad \langle x(t)\,B_{\Delta t}\rangle = 0$$

$$\longrightarrow \frac{1}{\Delta t}\left\langle \left(x(t) + \frac{1}{2}\sqrt{2D}\,B_{\Delta t}\right)\sqrt{2D}\,B_{\Delta t}\right\rangle = 0 + \frac{1}{2}\,2D\,\langle B_{\Delta t}^2\rangle$$

$$\longrightarrow D \qquad \text{which is correct}$$

This is called the Stratonovich discretization. It allows dt, or Δt here, to be smaller than τ_c. Yet, mathematicians like to take $\tau_c = 0$, which also is relevant in some physical situation. Then, we have difficulty to compute $\langle x\dot{x}\rangle$. We will adopt here the so-called Itô discretization rule

$$\langle x\,\dot{x}\rangle \longrightarrow \left\langle x(t)\,\frac{x(t+\Delta t)-x(t)}{\Delta t}\right\rangle = \frac{1}{\Delta t}\langle x(t)\,B_{\Delta t}\rangle$$
$$= 0 \neq D \;;\; \text{PROBLEM}$$

What went wrong is the chain rule, ie the fact that

$$\frac{d}{dt}\langle x^2\rangle = 2\,\langle x\,\dot{x}\rangle$$

This is true at Stratonovich level, since it assumes τ_c finite but small $\to \eta(t)$ is not a singular process. With Itô and $\tau_c = 0$, we have that $\langle x(t)\,\eta(t)\rangle = 0$. Indeed, the fact that $\langle \eta(t)\,x(t)\rangle \neq 0$ for Stratonovich is due to $\tau_c \neq 0$, which correlates $\eta(t)$ to $\eta(t')$ for $t-t' = \mathcal{O}(\tau_c)$, and thus correlates $\eta(t)$ to $x(t)$.

As announced, let us pay more attention to chain rule. Take $f(x)$

$$df = f'(x)\,dx \qquad \text{in which } dx \text{ is } \mathcal{O}(\sqrt{\Delta t})$$

Thus, push expansion one order higher

$$df = f'(x)\,dx + \frac{1}{2}f''(x)\,(dx)^2$$

Thus $\langle df \rangle = \langle f'(x)\, dx \rangle + \frac{1}{2} \underbrace{\langle f''(x)\, (dx)^2 \rangle}_{\langle f''(x)\rangle \langle (dx)^2\rangle}$ since at t, $x(t)$ known

$= \langle f'(x)\, dx \rangle + \frac{1}{2}\, 2D\, \langle f''(x) \rangle$ and $dx = \sqrt{2D}\, B_{dt}$ drawn

$$\left\langle \frac{df}{dt} \right\rangle = \langle f'(x)\, \dot{x} \rangle + D \langle f''(x) \rangle \qquad (\text{Itô})$$

and with an explicit t-dependence in $f(x,t)$ $\rightarrow$ extra term $\left\langle \frac{\partial f}{\partial t} \right\rangle$

This allows us to perform a consistent calculation à la Itô of

$$\left\langle \frac{dx^2}{dt} \right\rangle = \overbrace{\langle 2x\dot{x} \rangle}^{0} + D \langle 2 \rangle = 2D \quad \Rightarrow \text{fine !}$$

We see that Itô has simple equal time correlation $\langle x\dot{x} \rangle = 0$, or more precisely $\langle x(t)\, \eta(t) \rangle = 0$, but a complicated chain rule. On the other hand, Stratonovich has a simple chain rule, but a complicated equal time correlator $\langle x \sqrt{2D}\, \eta \rangle = D$

Let us generalize this rule to $f(x)$ arbitrary

$$\langle f(x) \sqrt{2D}\, \eta(t) \rangle \overset{\text{Strato}}{=} \frac{1}{\Delta t} \left\langle \frac{1}{2}\left[f(x(t+\Delta t)) + f(x(t))\right] \underbrace{\left[x(t+\Delta t) - x(t)\right]}_{\sqrt{2D}\, B_{\Delta t}} \right\rangle$$

$$x(t+\Delta t) = x(t) + \sqrt{2D}\, B_{\Delta t}$$

$$f\left[x(t+\Delta t)\right] = f(x(t)) + \sqrt{2D}\, B_{\Delta t}\, f'(x(t))$$

$$\Rightarrow \langle f(x) \sqrt{2D}\, \eta(t) \rangle = \frac{1}{\Delta t} \left\langle \left[f(x(t)) + \frac{\sqrt{2D}}{2} B_{\Delta t}\, f'(x(t)) \right] B_{\Delta t} \right\rangle \sqrt{2D}$$

$$= 0 + \frac{1}{2\Delta t}\, 2D\, \langle B_{\Delta t}^2 \rangle \langle f'(x) \rangle$$

$$\langle f(x) \sqrt{2D}\, \eta(t) \rangle = D \langle f'(x) \rangle \qquad (\text{Stratonovich})$$

SUMMARY : we saw 2 prescriptions / views

$\longrightarrow$ Stratonovich, where $dt < \tau_c$ possible. Thus $\eta(t)$, the noise, is correlated to $\eta(t')$ in recent past (window τ_c), that defines $x(t)$, hence $x(t)$ and $\eta(t)$ are correlated. This yields the Stratonovich rule

$$\langle f(x(t)) \sqrt{2D}\, \eta(t) \rangle = D \langle f'(x) \rangle$$

This follows from the mid-point recipe

$$\langle f(x(t))\, \eta(t) \rangle \longrightarrow \left\langle \frac{f(x(t)) + f(x(t+\Delta t))}{2} \frac{1}{\Delta t} \int_t^{t+\Delta t} \eta(t')\, dt' \right\rangle$$

and then $\Delta t \to 0$

This is a bit complicated, but the finiteness of τ_c makes that noise $\eta(t)$ is actually not singular, and standard rules of calculus apply, in particular, the chain rule

$$\left\langle \frac{df}{dt} \right\rangle = \left\langle f'(x(t))\,\dot{x}(t) \right\rangle$$

$\longrightarrow$ Itô, where $\tau_c = 0$ and thus $dt > \tau_c$ always.

The Langevin equ is discretized the same way as for Strato:

$$\dot{x} = \sqrt{2D}\,\eta(t) \Rightarrow x(t+\Delta t) = x(t) + \sqrt{2D}\int_t^{t+\Delta t} \eta(t')\,dt'$$

and we consider, at variance with Strato

$$\langle f(x)\,\eta(t) \rangle = 0$$

The corresponding rule for discretizing $\langle f(x)\eta(t)\rangle$ is

$$\langle f(x)\,\eta(t) \rangle \longrightarrow \left\langle f(x(t))\,\frac{1}{\Delta t}\int_t^{t+\Delta t} \eta(t')\,dt' \right\rangle = 0$$

Simple, but comes at the expense of a new type of calculus $\rightarrow$ Itô calculus. In particular, the chain rule becomes

$$\left\langle \frac{df}{dt} \right\rangle = \left\langle \frac{\partial f}{\partial t} \right\rangle + \left\langle f'(x)\,\dot{x} \right\rangle + D\left\langle f''(x) \right\rangle \text{ ; Itô Formula}$$

Exercise: show the consistency of the 2 routes, ie that for $\dot{x} = \mu F(x) + \sqrt{2D}\,\eta(t)$

$$\left\langle \frac{d\varphi}{dt} \right\rangle = \left\langle \varphi'(x)\,F(x) \right\rangle + D\left\langle \varphi''(x) \right\rangle$$

Here, the 2 prescriptions are equivalent because the discretized Langevin eq is the same in both cases (noise is additive). For a Langevin eq of the form $\dot{x} = C(x)\,\eta(t)$ and $C(x)$ not a constant, the term in $\langle C(x)\,\eta(t)\rangle$ is treated differently in the 2 approaches, and thus the discretized Langevin eqs are not the same. In this case, noise is said to be multiplicative.

Remarks ① Strato perhaps more physical, correct view for colloids, but calculus a bit cumbersome

Itô preferred in math. Applies to some φ situations, and finance

Yet for non multiplicative noise: they are 2 equivalent techniques

② When an integral is performed in Stratonovich sense, we use a $\circ$

$$\int b(x) \circ dx \rightarrow \sum_{i=1}^{N} \frac{b(x_i) + b(x_{i+1})}{2}\,(x_{i+1} - x_i)$$

Same as $b\left[\frac{x_i + x_{i+1}}{2}\right]$ when $N \to \infty$

In the Itô sense, no $\circ$

$$\int b(x)\,dx \rightarrow \sum_{i=1}^{N} b(x_i)\,(x_{i+1} - x_i)$$

(3) Itô's lemma shows a stronger result than $\left\langle \frac{df}{dt} \right\rangle = \langle f'(x)\,\dot{x} \rangle + D \langle f''(x) \rangle$ (48)

$\Rightarrow \quad \frac{df}{dt} = f'(x)\,\dot{x} + D\, f''(x)$: can get rid of $\langle \ \rangle$

(4) Much ado about Itô / Strato ... but with underdamped dynamics (ie $m\dot{v} = -\gamma m v + F + R$ rather than $0 = -\gamma m \dot{x} + F + R$)

$\rightarrow$ the difficulties with multiplicative noise disappear! No problem with equal time correlations like $\langle x(t)\, \eta(t) \rangle$ (or $\langle x(t) R(t) \rangle$).

Hence, for colloids, the Itô/Strato discussion is not only irrelevant because $\tau_c \neq 0$ in reality, but even when taking $\tau_c = 0$, the overdamped description is an approximation, and inertia is always present.

We have to remember this when working out Fokker-Planck equations.

4°) The tragic life and ignored legacy of Wolfgang Döblin

W. Döblin (1915 - 1940), was German, and jew. Escaped the nazis in 1933 to France and became French citizen (his father was a well known novelist, who wrote Berlin Alexanderplatz in 1929). He studied under Fréchet, got his PhD at 23 (1938) in probability theory, and made a name for himself as a gifted mathematician.

Döblin, who chose the name Vincent Doblin when he became French, could have joined the army (he had to...) as an officer. He also refused to be exempted from military service. As a convinced socialist (communist ??), he chose to be drafted as a simple soldier, and WWII started.

During the phoney war ("drôle de guerre"), he tried to maintain his mathematical research activity, which was extremely difficult. He used as notebooks what he could buy at the village shop nearby. He was working on stochastic processes, and the Chapman-Kolmogorov / Fokker Planck equations (that he called "the Kolmogorov equation"). During the winter 39-40, he sends some of his notes as a pli cacheté to the Académie des Sciences.

He is sent to the Ligne Maginot, and when he realizes that the Wehrmacht troops, he burns his latest mathematical works, ID papers, and chooses to die (1940)

He is buried as an unknown soldier in Housras (Vosges), and will only be identified in 1944, 4 years later.

The "pli cacheté" (sealed envelope) was only mentioned in a letter to Fréchet, that went unnoticed until the 1990s. It was opened in 2000, and was quite a shock to the probabilist's community. Among other results that were (independently of course) discovered in the 1940s to 1960s, it contains the key ideas behind Itô stochastic calculus... Itô was also born in 1915, never met Döblin, and obtained his first important result in 1942. We quite clearly have 2 rather isolated "geniuses", who never communicated, but had the same ideas almost at the same time → this illustrates the importance of the "community" as an "aligning field", a "thermal bath" that plays a key role in the progression of ideas: science is not this individualistic activity, sometimes put forward, where leaps of ideas are due to gifted individuals only.

Rather than Itô calculus, we will from now on use terminology Itô-Doblin calculus

5) Numerical integration

This is the domain of Brownian dynamics, a popular mesoscopic simulation technique. Because the underlying suspending fluid (or, more generally, the thermal bath at the origin of the Langevin force) is not taken into account explicitly, but implicitly, such an approach is much more efficient than Molecular Dynamics, that would integrate all equations of motion (fluid + Brownian object). It has of course limitations (like hydrodynamics interaction, not taken into account, and that influence the relative motion of interacting Brownian objects).

Back to the overdamped Langevin: $\dot{x} = \mu F(x,t) + \sqrt{2D}\,\eta(t)$

Discretize: $x(t+\Delta t) = x(t) + \mu F(x(t),t)\Delta t + \sqrt{2D}\underbrace{\int_t^{t+\Delta t}\eta(t')dt'}_{B_{\Delta t}}$; the B's at ≠t times are independent

$B_{\Delta t}$ is a $\mathcal{G}(0,\sqrt{\Delta t})$ random variable.

It can be generated by the Box-Muller technique:

Take y_1 and y_2 uniform in $[0;1]$ independent : $\left.\begin{array}{l}\sqrt{-2\ln y_1}\,\cos(2\pi y_2)\\ \sqrt{-2\ln y_1}\,\sin(2\pi y_2)\end{array}\right\}$ provide 2 independ. $\mathcal{G}(0,1)$ variables

A historic but approximate variant is to consider $\left(\sum_{i=1}^{12} y_i\right) - 6$ where the y_i are IID uniform on $[0,1]$ again. Why 12? Why does this $\simeq$ work?

$\longrightarrow$ from $x(t_0)$, we compute $x(t_0) + F\Delta t + B_{\Delta t} = x(t_0 + \Delta t)$.

we then draw at random another $B_{\Delta t} \rightarrow x(t_0 + 2\Delta t) \ldots$

Called the Euler - Maruyama method