Chapter 2: Itō calculus

In the absence of external potential, the simplest dynamics of an overdamped colloid is given by

$$\dot{x}(t) = \sqrt{\sigma}\,\eta(t) \qquad (1)$$

where $\eta(t)$ is a Gaussian white noise satisfying $\langle \eta(t) \rangle = 0$
$\langle \eta(t)\eta(t') \rangle = \delta(t-t')$

Two problems

(I) $\dfrac{x(t+\tau)-x(t)}{\tau} \sim \sqrt{\dfrac{\sigma}{\tau}} \xrightarrow[\tau\to 0]{} \infty \Rightarrow x(t)$ not differentiable

(II) Chain rule + causality predicts $\langle x^2(t) \rangle = C^{st}$ which is wrong

Itō-calculus

$$\dot{x} = F(x) + \eta(t) \iff \underbrace{dx(t)}_{x(t+dt)-x(t)} = F(\overbrace{x(t)}^{x(t)\text{ for causality}})dt + d\eta$$

(I) $\dot{x}(t)$ is just a notation, only $\int^t ds\, \dot{x}(s)$ makes sense

(II) Save causality & modify the chain rule:

$$\boxed{\frac{d}{dt}\left[f(x(t))\right] = f'(x(t))\,\dot{x}(t) + \frac{\sigma}{2} f''(x(t))} \qquad (7)$$

Stratonovich: $\dot{x} = F(x) + \eta(t) \overset{\int_t^{t+dt}}{\iff} dx = F\left(x_t + \underbrace{\frac{dx}{2}}_{\frac{1}{2}[x(t+dt)+x(t)]}\right)dt + d\eta$ $\Rightarrow$ breaks causality

$$(7) \iff df(x(t)) = \underbrace{f'(x(t))\,dx}_{\text{not symmetrized} \Rightarrow \text{not a Stratonovich prescription}} + \frac{\sigma}{2} f''(x(t))\,dt$$

$$f'(x(t)) = f'\left(x(t)+\frac{dx}{2}-\frac{dx}{2}\right) = f'\Big(\underbrace{x(t)+\frac{dx}{2}}_{\text{symmetric}}\Big) - \frac{dx}{2} f''(x(t)) + O(dx^2)$$ (2)

$$f'(x(t))\,dx = f'\left(x(t)+\frac{dx}{2}\right)dx - \frac{1}{2} f''(x(t))\, dx^2$$

but to order dt, $dx^2 = d\eta^2 = \sigma dt$ $\Rightarrow$ exactly cancels $\frac{\sigma}{2} f''$ in (7)

$$\Rightarrow df(x(t)) = f'\left(x(t)+\frac{dx}{2}\right)dx \iff \frac{df}{dt} = f'(x)\,\dot{x} \quad \text{(Strato)}$$

$\Rightarrow$ simple formula but complicated symmetrization

2.2) Generalization to $f(x(t),t)$

The derivation above generalizes directly to

$$\boxed{\frac{d}{dt} f(x(t),t) = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\dot{x}(t) + \frac{\sigma}{2}\frac{\partial^2 f}{\partial x^2}}$$

2.3) N-dimensional Itō formula

$\dot{x}_i = F_i(x_1,\dots,x_N) + \eta_i$ where the $\{\eta_i\}$ are correlated GWN s.t.

$$\langle \eta_i(t)\rangle = 0 \quad \langle \eta_i(t)\eta_k(t')\rangle = \sigma_{ik}\,\delta(t-t')$$

Then $$\boxed{\frac{d}{dt} f(x_1(t),\dots,x_N(t)) = \sum_i \frac{\partial f}{\partial x_i}\dot{x}_i + \frac{1}{2}\sum_{i,k}\frac{\partial^2 f}{\partial x_i \partial x_k}\sigma_{ik}} \quad (8)$$

Comment: Very useful in the presence of deterministic & stochastic variable.

E.g. $\dot{x} = v$; $m\dot{v} = -\gamma v - V'(x) + \sqrt{2\gamma k T}\,\eta(t)$

$$\iff \dot{x} = v + \xi_x \; ; \; \dot{v} = -\frac{\gamma}{m}v - \frac{1}{m}V'(x) + \xi_y$$

where $\langle \xi_x(t) \rangle = 0$; $\langle \xi_x(t)\, \xi_x(t') \rangle = 0$

$$\langle \xi_y(t) \rangle = 0; \quad \langle \xi_y(t)\, \xi_y(t') \rangle = \frac{2\gamma k_B T}{m^2}\,\delta(t-t')$$

$$\langle \xi_x(t)\, \xi_y(t') \rangle = 0$$

$$\frac{d}{dt} f(x(t), v(t)) = \frac{\partial f}{\partial x}\dot{x} + \frac{\partial f}{\partial v}\dot{v} + \frac{\gamma k_B T}{m^2}\frac{\partial^2 f}{\partial v^2}$$

$\Rightarrow$ only the stochastic variable leads to a second order derivative.

2.4) Back to the paradox

$f(x(t)) = x^2(t)$ & $\dot{x}(t) = \sqrt{2D}\,\eta(t)$

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

$$\frac{d}{dt} f(x(t)) = \frac{\partial f}{\partial x}\cdot\dot{x} + \frac{1}{2}\cdot\frac{\partial^2 f}{\partial x^2}\cdot 2D = 2x\dot{x} + 2D = 2D + \sqrt{8D}\,x\,\eta(t)$$

$$x^2(t) = 2Dt + \sqrt{8D}\int_0^t ds\, \eta(s)$$

$\rightarrow$ ① we recover $\langle x^2(t) \rangle = 2Dt$

② we can characterize the fluctuations of $x^2(t)$ around its mean $2Dt$.

Also works for higher moments:

$$\frac{d}{dt}\langle x^4(t) \rangle = 4\langle x^3 \dot{x} \rangle + \frac{1}{2}\cdot 2D\cdot 12\langle x^2 \rangle$$

$$= 4\langle x^3 \rangle \underbrace{\langle \sqrt{2D}\,\eta(t) \rangle}_{=0} + 12D\underbrace{\langle x^2 \rangle}_{2Dt}$$

$\Rightarrow \langle x^4(t) \rangle = 12 D^2 t^2 = 3\times(2Dt)^2 = 3\langle x^2(t) \rangle^2$ as expected for a GRV.

3) Probability of noise realization

If we say that $\{\eta(t)\}$ forms a set of GRV, it would be nice to be able to write their probability weight $P[\{\eta(t)\}] = ?$

Start with N random variables η_j such that $\vec{\eta} = (\eta_1, \dots, \eta_N)$ 4

$$P(\vec{\eta}) = \frac{1}{Z} \exp\left[-\frac{1}{2}\vec{\eta}\cdot(\Gamma\ \vec{\eta})\right] \quad (9)$$

with Γ a matrix symmetric positive definite.

From the pset you know that $\langle \eta_i \eta_j \rangle = K_{ij}$, with $K = \Gamma^{-1}$.

From $\langle \eta_i \eta_j \rangle = K_{ij}$, we can build $\Gamma = K^{-1}$ & $P(\vec{\eta})$. Can we do the same from $\langle \eta(t)\eta(t')\rangle$?

Now let's call $t_i = i\,dt$ and $\eta_i = \eta(t_i)$ and take the limit $dt \to 0$ keeping $N dt = t$ fixed. We then rewrite

$$\vec{\eta}\cdot(\Gamma\vec{\eta}) = \sum_{i,j} \eta_i \Gamma_{ij} \eta_j = \sum_{i,j} dt^2\, \eta(t_i) \frac{\Gamma_{ij}}{dt^2} \eta(t_j)$$

$$\vec{\eta}\cdot(\Gamma\vec{\eta}) \sim \int dt\,dt'\, \eta(t)\eta(t')\Gamma_c(t,t') \quad \text{where } \boxed{\Gamma_c(t_i,t_j) = \frac{1}{dt^2}\Gamma_{ij}} \quad (10)$$

① Can we build $K_c(t_i,t_j)$?

$$K = \Gamma^{-1} \Rightarrow \sum_k K_{ik}\Gamma_{kj} = \delta_{i,j} \quad (11)$$

Take a function $f(t)$ & denote $f_i = f(t_i)$. Then (11) implies

$$\sum_{j,k} K_{ik}\Gamma_{kj} f_j = \sum_j \delta_{ij} f_j = f_i$$

$$\Leftrightarrow \sum_{j,k} dt^2\, K_{ik} \frac{\Gamma_{kj}}{dt^2} f_j = f_i$$

$$\Leftrightarrow \int dt'' dt'\, K_c(t,t')\Gamma_c(t',t'') f(t'') = f(t) \quad \text{with } \boxed{K_c(t_i,t_j) = K_{ij}}$$

$$\Leftrightarrow \int dt'' f(t'') \left[\int dt'\, K_c(t,t')\Gamma_c(t',t'')\right] = f(t)$$

Since this holds for any function f, one has that

$$\Rightarrow \boxed{\int dt'\, K_c(t,t')\, \Gamma_c(t',t'') = \delta(t-t'')}$$

This is the generalisation of $K \cdot \Gamma = Id$ for convolution kernel.

(ii) Going back to the GWN: $\langle \eta(t)\eta(t')\rangle = 2kT\,\delta(t-t') = K_c(t,t')$

$\Rightarrow$ What is Γ_c ?

$* \int dt\, f(t)\,\delta(t-t_j) \simeq f(t_j) = f_j = \sum_i f_i\,\delta_{ij} = \sum_i dt\, f_i\, \frac{\delta_{ij}}{dt} \Rightarrow \delta(t_i - t_j) \simeq \frac{\delta_{ij}}{dt}$

$* \langle \eta(t_i)\eta(t_j)\rangle = 2kT\,\frac{\delta_{ij}}{dt} \Rightarrow K_{ij} = 2kT\,\frac{\delta_{ij}}{dt}$.

Eq (11) thus leads to $\Gamma_{jk} = \frac{1}{2k_BT}\, dt\, \delta_{jk}$

Then, Eq (10) $\Rightarrow \Gamma_c(t_i,t_j) = \frac{1}{2k_BT}\,\frac{\delta_{jk}}{dt} \simeq \frac{\delta(t_i-t_j)}{2k_BT}$

Indeed, we check that

$$\int dt\, K(t,t')\,\Gamma(t',t'') = \frac{2k_BT}{2k_BT}\int dt'\,\delta(t-t')\,\delta(t'-t'') = \delta(t-t'')$$

From there, we can build the noise probability distribution:

$$\Rightarrow P[\{\eta(t)\}] = \frac{1}{Z}\exp\left[-\frac{1}{4kT}\int dt\,dt'\,\eta(t)\eta(t')\,\delta(t-t')\right]$$

$$\boxed{P[\{\eta(t)\}] = \frac{1}{Z}\exp\left[-\frac{1}{4kT}\int dt\,\eta(t)^2\right]}$$:-)

Colored noise: If $\langle \eta(t)\eta(t')\rangle = K(t-t')$

then $P[\{\eta(t)\}] = \frac{1}{Z}\exp\left[-\int dt\,dt'\,\eta(t)\,\Gamma(t-t')\,\eta(t')\right]$

when Γ is such that $\int dt'\, K(t-t')\,\Gamma(t'-t'') = \delta(t-t'')$

4) Probability of trajectories $\{x(t)\}$

If we know $P[\{\eta(t)\}]$ and we know $x(t,\{\eta(s)\})$, can we get $P[\{x(t)\}]$? Yes, but this is painful...

Changing variable N rdm variables $x_1,-,x_N$ & a new set of coordinates $y_i(x_1,-,x_N)$

Conservation of probability means that $P(x_1,-,x_N)\,dx_1-dx_N = P(y_1,-,y_N)\,dy_1-dy_N$

$$\Rightarrow P(y_1,-,y_N) = P(x_1,-,x_N)\cdot\underbrace{\left|\frac{dx_1-dx_N}{dy_1-dy_N}\right|}_{\text{Jacobian of the change of variable}}$$

Here $P[\{x(t)\}] = P[\{\eta(t)\}]\cdot\det J$, where J "=" $\left|\frac{\partial \eta(t)}{\partial x(t')}\right|$

Q: How do we give a meaning to J?

Let's time-discretize the Langevin equation $\dot{x} = f(x)+\eta(t)$

x_0 fixed, $x_i = x(t_i)$, $t_i = i\,dt$. $x_1,-,x_N$ are N RVs. Then, we define

$$\tilde{\eta}_i \equiv \int_{t_{i-1}}^{t_i}\eta(s)\,ds \quad \text{so that } \tilde{\eta}_i \text{ leads from } x_{i-1} \text{ to } x_i:$$

$$x_{i+1} = x_i + \int_{t_i}^{t_{i+1}} f(x(s))\,ds + \tilde{\eta}_{i+1} \Rightarrow \tilde{\eta}_1,\dots,\tilde{\eta}_N \text{ are } N \text{ GRVs.}$$

$$\Rightarrow \frac{\partial\tilde{\eta}_{i+1}}{\partial x_j} = \frac{\partial}{\partial x_j}\Big[\underbrace{x_{i+1}-x_i}_{\text{easy}} - \underbrace{\int_{t_i}^{t_{i+1}} f(x(s))\,ds}_{}\Big]$$

$$=?= f(x_i)\,dt\,?$$
$$= f(x_{i+1})\,dt\,?$$
$$= f(x_i^\alpha)\,dt \quad \text{with } x_i^\alpha = \alpha x_{i+1} + (1-\alpha)x_i \;?$$
$$= x_i + \alpha(x_{i+1}-x_i)$$

All appear equivalent to order dt... Let's keep α arbitrary for now.

$\Rightarrow$ the matrix $\frac{\partial\tilde{\eta}_{i+1}}{\partial x_j}$ is an upper triangular matrix

$$\Rightarrow \det = \prod_i \frac{\partial \tilde{x}_i}{\partial x_i} = \prod_i \left(1-\alpha\, dt\, f'(x_i^\alpha)\right) \underset{dt\to 0}{\simeq} \prod_i e^{-\alpha dt f'(x_i^\alpha)}$$ 7

$$\simeq e^{-\alpha \sum_i dt\, f'(x^\alpha_{i+1})} \simeq e^{-\alpha\int_0^t ds\, f'(x(s))}$$

$$P[\{x(t)\}] = \frac{1}{Z} e^{-\int dt\left[\frac{\eta^2(t)}{4uT} + \alpha f'(x(s))\right]}$$

But we know that $\dot{x} = f(x) + \eta(t) \Rightarrow \eta(t) = \dot{x} - f(x)$

$$\Rightarrow \boxed{P[\{x(t)\}] = \frac{1}{Z} e^{-\int dt \frac{(\dot{x}-f(x))^2}{4uT} + \alpha f'(x(s))}}$$

Comment: Causality makes us again choose $\alpha = 0$. Then

$$\boxed{P[\{x(t)\}] = \frac{1}{Z} e^{-\int dt \frac{(\dot{x}-f(x))^2}{4uT}}}$$

Then, we need to use Itō calculus to compute time-derivatives in the integral.

If we use $\alpha = \frac{1}{2}$, we use what is called Stratonovich time discretization. We can use standard calculus in the exponent, but the computation of averages is harder since η_{i+1} and x_{i+1} are now correlated $\Rightarrow \langle x(t)\eta(t)\rangle \neq 0$.

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