

Lecture 8 ... still on O-U process

It is
hard to solve

$$\Delta X = -\theta x dt + \sigma dW$$

(or even comprehend) an SDE...

Instead, it would be better
if we had $P(x, t)$

then normal calculus rules

How to systematically derive $P(x, t)$
from the SDE.

Start with Evolution Eq.

$$P(x, t+dt) = \int G(x, t+dt | y, t) P(y, t) dy$$

Normally we
think of a propagator $G(x|y)$ with
fixed initial y , variable target x .

Here, the variable is y ...

To address this, take $\Delta x = x - y$,
 so $y = x - \Delta x$

$$P(x, t + \Delta t) = \int G(\overbrace{x - \Delta x + \Delta x}^x, t + \Delta t) P(\underbrace{x - \Delta x}_{\text{uniform shift}}, t) d(-\Delta x)$$

• G "steps" from $(x - \Delta x)$ into $(x - \Delta x) + \Delta x$:

• We have a uniform function of $(x - \Delta x)$

Taylor expand it:

$$P(x, t + \Delta t) = \int \sum_{n=0}^{\infty} \frac{(-\Delta x)^n}{n!} \frac{\partial^n}{\partial x^n} G(\overbrace{x + \Delta x}^{\text{step } \Delta x} | \underbrace{x}_{\text{whole range!}}) P(x) d(\Delta x)$$

Define moments:

$$\langle \Delta x^0 \rangle = 1 \quad : \quad G \text{ normalised for } 0 \rightarrow \infty$$

$$\langle \Delta x^1 \rangle = \int \Delta x G(x + \Delta x | x) d\Delta x \rightarrow -\partial_x \cdot \Delta t$$

$$\langle \Delta x^2 \rangle = \int \Delta x^2 G(x + \Delta x | x) d\Delta x \rightarrow \sigma^2 \Delta t$$

...

$$P(x, t + \Delta t) = P(x, t) - \frac{\partial}{\partial x} (\langle \Delta x \rangle P) + \frac{1}{2} \frac{\partial^2}{\partial x^2} (\langle \Delta x^2 \rangle P)$$

terms $\sim \Delta t$

+ ...
(no more)

Now substitute moments:

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x} (\theta x \cdot P(x,t)) + \frac{\sigma^2}{2} \frac{\partial^2}{\partial x^2} P(x,t)$$

for $O-U$ process. No more terms $\sim dt$ in r.h.s.

(limit $dt \rightarrow 0$)

external force

diffusion constant

$$D = \frac{1}{2} \sigma^2$$

This was an example of using "Kramers-Moyal expansion"



Evolution \rightarrow Expand kernel in powers of "step"

identify \leftarrow moments \rightarrow

form the PDE for $P(x,t)$

Kramers - Moyal Expansion (general)

Evolution

$$P(x, t+\Delta t) = \int G(x, t+\Delta t | y, t) P(y, t) dy$$

or it could be Kolmogorov - Chapman if we care about the initial condition:

$$P(x, t+\Delta t | x_0, t_0) = \int G(x, t+\Delta t | y, t) P(y, t | x_0, t_0) dy$$

Again: $\Delta x = x - y$, so $y = x - \Delta x$

$$P(x, t+\Delta t) = \int G(\underbrace{x - \Delta x + \Delta x}_{\text{shifted argument}} | \underbrace{x - \Delta x}_{\text{step}}) P(\underbrace{x - \Delta x}_{\text{shifted argument}}, t) d(-\Delta x)$$

shifted argument

Taylor expand (it)

$$= \int \sum_{n=0}^{\infty} \frac{(-\Delta x)^n}{n!} \frac{\partial^n}{\partial x^n} G(x + \Delta x | x) P(x, t) d(\Delta x)$$

Define "Kramers - Moyal coefficients"

$$D^{(n)}(x) = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int \frac{(\Delta x)^n}{n!} G(x + \Delta x | x) d\Delta x$$

Note that this is general (whatever G is), for any SDE. (For Wiener SDE, only two $D^{(1)}$ and $D^{(2)}$ are non-zero)

Then we have:

$$\frac{\partial P(x,t)}{\partial t} = \sum_{n=1}^{\infty} (-1)^n \frac{\partial^2}{\partial x^n} \left[D_{(x)}^{(n)} P(x,t) \right]$$

for \forall SDE, not necessarily Wiener, or

$$\frac{\partial P}{\partial t} = \hat{L}_{KM} P(x,t)$$

\hat{L}_{KM} operator

$D_{(x)}^{(n)}$ carry all information about the nature of stochastic proc.

(for Wiener process, there are only two non-zero K-M coeffs)

Practice:

①

$$\dot{v} = -\frac{\gamma}{m} v + \frac{\sqrt{2kT\gamma}}{m} \xi(t)$$

$$dv = -\frac{\gamma}{m} v dt + \frac{\sqrt{2kT\gamma}}{m} dw$$

standard O-U format

$$\langle dv \rangle = -\frac{\gamma}{m} v dt$$

$$\langle dv^2 \rangle = \frac{2kT\gamma}{m^2} \langle dw^2 \rangle \quad \leftarrow dt$$

then:

$$\frac{\partial P(v,t)}{\partial t} = \frac{\gamma}{m} \frac{\partial}{\partial v} (v \cdot P) + \frac{2kT\gamma}{2m^2} \frac{\partial^2 P}{\partial v^2}$$

This equation describes relaxation of $P(v,t)$ towards the equilibrium Maxwell distribution

test the steady state (eq.):

$$0 = \frac{\partial}{\partial v} \left[\frac{\gamma}{m} v \cdot P + \frac{kT\gamma}{m^2} \frac{\partial P}{\partial v} \right]$$

$$\frac{\partial P}{\partial v} = \frac{m^2}{kT\gamma} \left(-\frac{\gamma}{m} v \cdot P \right)$$

$$\int \frac{dP}{P} = - \int \frac{m}{kT} v dv$$

thermostat equilb. $P = \text{norm} e^{-\frac{mv^2}{2kT}}$

(2) Relaxation to a fixed equilibrium (in a harmonic potential $V(x)$)

overdamped limit

will test later

$$\gamma \dot{x} = -\theta(x - x_0) + \sqrt{2kT\gamma} \cdot \xi(t)$$

$$dx = -\frac{\theta}{\gamma}(x - x_0) + \sqrt{\frac{2kT}{\gamma}} dw$$

standard O-U format

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x} \left(\frac{\theta}{\gamma}(x - x_0) P \right) + \frac{kT}{2\gamma} \frac{\partial^2 P}{\partial x^2}$$

Smoluchowski equation:
(diffusion with external force)

Test: steady state: $\frac{dP}{dx} = -\frac{\theta}{kT}(x - x_0)P$: $P = P_0 e^{-\frac{\theta(x-x_0)^2}{2kT}}$

i.e. Boltzmann distr.

③ GBM $ds = \mu s dt + \sigma s dw$

$$\langle ds \rangle = \mu s dt$$

$$\langle ds^2 \rangle = \sigma^2 s^2 \langle dw^2 \rangle = dt$$

$$\frac{\partial P(s,t)}{\partial t} = -\frac{\partial}{\partial s} (\mu s P(s,t)) + \frac{\sigma^2}{2} \frac{\partial^2}{\partial s^2} (s^2 P)$$

④ Multi-variable process.
(see the last lecture for 'matrix notation')

Brownian motion with force

$$\begin{cases} m\dot{v} = -\gamma v - \theta(x-x_0) + \sqrt{2kT\gamma} \xi(t) \\ \dot{x} = v \end{cases}$$

Annotations: $v(t)$ and $x(t)$ are indicated by red arrows pointing to the variables in the equations. Red arrows also point to v and $x-x_0$ in the equations.

O-U process

linear drift terms.

Matrices:

$$\underline{\underline{\theta}} = \begin{pmatrix} \frac{\gamma}{m} & \frac{\theta}{m} \\ -1 & 0 \end{pmatrix}; \quad \underline{\underline{G}} = \begin{pmatrix} \frac{\sqrt{2kT\gamma}}{m} & 0 \\ 0 & 0 \end{pmatrix}$$

Let us work out the PDE
for $P(v, x, t) \dots$

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x_i} \left(\Theta_{ik} x_k \cdot P \right) + \frac{1}{2} (GG^T)_{ik} \frac{\partial^2 P}{\partial x_i \partial x_k}$$

$$= \frac{\partial}{\partial v} \left(\frac{\gamma}{m} v \cdot P \right) + \frac{\partial}{\partial v} \left(\frac{\partial}{m} (x - x_0) P \right)$$

$$- \frac{\partial}{\partial x} (v P) + \frac{2kT\gamma}{m^2} \frac{\partial^2 P}{\partial v^2}$$

$$\underbrace{\frac{\partial P(v, x, t)}{\partial t} + \frac{\partial}{\partial x} (v \cdot P)}_{\text{convective derivative}} = \frac{\partial}{\partial v} \left(\underbrace{\frac{\gamma v + \partial(x - x_0)}{m}}_{\text{full force}} \cdot P \right) + \frac{kT\gamma}{m^2} \frac{\partial^2 P}{\partial v^2}$$

General Fokker-Planck equation
for Brownian motion in $\uparrow V / \text{pot.}$