Langevin to Fokker-Planck

We show a general recipe on a simple example:

Consider the active Ornstein-Uhlenbeck process on an infinite line.

Position: $\dot{x}_t = \frac{\gamma_a}{\gamma} v_t + \frac{1}{\gamma} F(x(t)) + \sqrt{\frac{2 k_0 T}{\gamma}}\, \xi_t$ $\quad \langle \xi_t \rangle = 0$, $\langle \xi_t \xi_{t'} \rangle = \delta(t-t')$

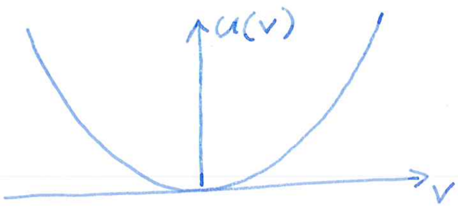
Velocity: $\dot{v}_t = -\frac{1}{\tau_a} v_t + \sqrt{2 D_a}\, \eta_t$ $\quad \langle \eta_t \rangle = 0$, $\langle \eta_t \eta_{t'} \rangle = \delta(t-t')$

We consider only the Langevin equation for the velocity. ~~The extension to the~~
Given the recipe, it is straightforward to get the Fokker-Planck eq. for $P_t(x,v)$.

1) We need the ~~Wiener process~~!

$$\dot{v}_t = -\frac{1}{\tau_a} v_t + \sqrt{2 D_a}\, \eta_t \quad (*)$$

describes the random walk of a particle in a harmonic potential



$$u(v) = \frac{1}{2\tau_a} v^2 \Rightarrow \underbrace{F}_{\text{force}} = -\frac{\partial}{\partial v} u(v) = \underbrace{-\frac{1}{\tau_a} v}_{\text{compare with } (*)}$$

Goal: discretise $(*)$ in time; let dt be our finite time step

$$(*) \Rightarrow \frac{v(t+dt) - v(t)}{dt} = -\frac{1}{\tau_a} v(t) + \sqrt{2 D_a}\, \eta(t)$$

$$\Leftrightarrow v(t+dt) = v(t) - \frac{1}{\tau_a} v(t)\, dt + \sqrt{2 D_a}\, \underbrace{\eta(t)\, dt}$$

what are the properties of this random number?

We define the Wiener dw(t) process and derive the properties:

$$\boxed{dw(t) := \eta(t)\, dt}$$

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What are the propedies of $\omega(t)$? ②

$$\langle \omega(s)\rangle = \int_0^s \underbrace{\langle \eta(t)\rangle}_{0} dt = 0$$

$$\langle \omega(s)\omega(s')\rangle = \int_0^s\int_0^{s'} \langle \eta(t)\eta(t')\rangle dt\,dt' = \underbrace{\int_0^s\int_0^{s'} \delta(t-t')\,dt\,dt' = \min(s,s')}$$

this means also

$$\langle \omega(s)^2\rangle = s$$

e.g. $\underline{s>s'}$ & discrete $\Rightarrow$

$$\sum_{t=0}^{s}\sum_{t'=0}^{s'} \delta(t-t') =$$

$$\sum_{t=0}^{s}\left[\delta(t-0)+\delta(t-1)+\dots+\delta(t-s')\right]$$

$$=\left[\delta(0-0)+\delta(0-1)+\dots+\delta(0-s')\right]+$$

$$\left[\delta(1-0)+\delta(1-1)+\dots+\delta(1-s')\right]+$$

$$\vdots$$

$$\left[\delta(s-0)+\delta(s-1)+\dots+\delta(s-s')\right]$$

$$= s'$$

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with this:

$$\langle \omega(t+dt)-\omega(t)\rangle \overset{=\langle d\omega(t)\rangle}{=} \underbrace{\langle\omega(t+dt)\rangle}_{0} - \underbrace{\langle\omega(t)\rangle}_{0} = 0$$

$$\langle d\omega(t)^2\rangle = \langle(\omega(t+dt)-\omega(t))^2\rangle$$

$$= \underbrace{\langle\omega(t+dt)^2\rangle}_{t+dt} + \underbrace{\langle\omega(t)^2\rangle}_{t} - 2\underbrace{\langle\omega(t+dt)\omega(t)\rangle}_{t} = t+dt+t-2t = \underline{\underline{dt}}$$

$\Rightarrow$ we know $d\omega(t)=\eta(t)dt$ is a random number of

mean $\underline{\langle d\omega(t)\rangle = 0}$ & variance $\langle(d\omega(t)-\overbrace{\langle d\omega(t)\rangle}^{0})^2\rangle$

$\boxed{\text{we will need this}}$ $\longrightarrow$ $= \underline{\langle d\omega(t)^2\rangle = dt}$

$\Rightarrow$ therefore we can generate the random number $d\omega(t)$ at everery time step with

$$\underline{d\omega = \sqrt{dt}\,\xi}\,,\quad \text{with } \langle\xi\rangle = 0\quad \langle\xi^2\rangle = 1$$

ξ can be generated from a gaussian distributed random number with mean 0 and variance 1

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2) Langevin to Fokker-Planck

Recipe

(A) discredizise your Langevin eq.

$$\dot{v}_t = -\frac{1}{\tau_a} v_t + \sqrt{2D_a}\,\eta_t \longrightarrow v(t+dt) = v(t) - \frac{1}{\tau_a} v(t)\,dt + \sqrt{2D_a}\, d\omega(t)$$

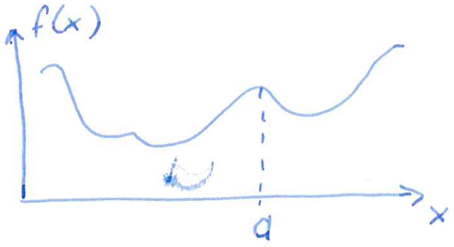
(B) define a test function $R(v_t)$ such that

$$\langle R(v_t)\rangle = \int_{-\infty}^{\infty} dv\, \underbrace{P_t(v)}_{\text{depends on } t}\, \underbrace{R(v)}_{\text{does not depend on } t}$$

(C) consider $\langle R(v_{\underline{t+dt}})\rangle = \int_{-\infty}^{\infty} dv\, P_{\underline{t+dt}}(v)\, R(v)$

(C.1) Taylor expend $R(v_{t+dt}) = R\big(\underbrace{v(t)}_{a} \underbrace{- \frac{1}{\tau_a} v(t)\,dt + \sqrt{2D_a}\, d\omega(t)}_{\varepsilon}\big)$

Reminder:



$$\underbrace{Tf(x;a)}_{\text{taylor exp. of } f(x) \text{ around } x=a} = T f_a(\underbrace{a+\varepsilon}_{x})$$

$$= f(a) + f'(a)\,\varepsilon + \frac{f''(a)}{2}\varepsilon^2 + \dots$$

$$= f(a) + f'(a)(x-a) + \frac{f''(a)}{2}(x-a)^2 + \dots$$

$$\Rightarrow R(v_{t+dt}) = \underbrace{R(v_t) - R'(v_t)\frac{1}{\tau_a} v_t\,dt + R'(v_t)\sqrt{2D_a}\,d\omega(t) + \frac{R''(v_t)}{2}\frac{1}{\tau_a^2} v_t^2\,dt^2 + \frac{R''(v_t)}{\cancel{2}}\cancel{2}D_a\,d\omega(t)^2 - \frac{R''(v_t)}{2}\frac{1}{\tau_a} v_t\,dt\sqrt{2D_a}\dots + \dots}_{\boxed{\text{Eq. C.1}}}$$

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C.2 split $\langle R(v_{t+dt})\rangle$ into average

a) over the possible histories just until time t

$$\langle f(v_t)\rangle_{H\to t} = \int_{-\infty}^{\infty} dv\, f(v) P_t(v)$$

b) & the noise at t (which is $d\omega_t$) that leads to the state at $t+dt$ $\langle d\omega_t\rangle_{d\omega}$

see page 2 for definition

with C.1

$$\Rightarrow \langle R(v_{t+dt})\rangle = \left\langle \left\langle Eq\ C.1 \right\rangle_{H\to t} \right\rangle_{d\omega}$$

$$= \langle R(v_t)\rangle_{H\to t} - \langle R'(v_t)\, v_t\rangle_{H\to t} \frac{1}{\tau_a} dt + \sqrt{2D_a}\, \langle R'(v_t)\rangle_{H\to t} \underbrace{\langle d\omega(t)\rangle_{d\omega}}_{0}$$

$$+ \frac{1}{2\tau_a^2} \underbrace{dt^2}_{0 \text{ for } dt\to 0} \langle R''(v_t)\, v_t^2\rangle_{H\to t} + D_a \langle R''(v_t)\rangle_{H\to t} \underbrace{\langle d\omega(t)^2\rangle_{d\omega}}_{dt}$$

$$- \frac{1}{2\tau_a} dt \sqrt{2D_a}\, \langle R''(v_t)\, v_t\rangle_{H\to t} \underbrace{\langle d\omega_t\rangle_{d\omega}}_{0}$$

$$= \langle R(v_t)\rangle_{H\to t} - \frac{1}{\tau_a} dt\, \langle R'(v_t)\, v_t\rangle_{H\to t} + D_a\, dt\, \langle R''(v_t)\rangle_{H\to t} \qquad \boxed{Eq.\ C.2}$$

C.3 we get rid of all the derivatives in R (eg. R' & R'') in the above expressions by integration by parts

$$\hookrightarrow \int_a^b u(x)\, v'(x)\, dx = \left[u(x)\, v(x)\right]_a^b - \int_a^b u'(x)\, v(x)\, dx$$

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$$\langle R'(v_t)\, v_t \rangle_{H \to t} = \int_{-\infty}^{\infty} dv \; R'(v)\, v\, P_t(v)$$

$$= \underbrace{\Big[R(v)\, v\, P_t(v) \Big]_{-\infty}^{\infty}}_{\substack{=0, \text{ as } P_t(\pm\infty) = 0 \\ [v \text{ is confined in } u(x)?]}} - \underline{\int_{-\infty}^{\infty} dv \; R(v) \frac{d}{dv}\Big[v\, P_t(v) \Big]} \qquad (\text{Eq C.3.1})$$

$$\langle R''(v_t) \rangle_{H \to t} = \int_{-\infty}^{\infty} dv \; R''(v)\, P_t(v)$$

$$= \underbrace{\Big[R'(v)\, P_t(v) \Big]_{v=-\infty}^{\infty}}_{=0, \text{ see above}} - \int_{-\infty}^{\infty} dv \; R'(v) \frac{d}{dv}\Big[P_t(v) \Big]$$

$$= - \underbrace{\Big[R(v) \frac{d}{dv}\big[P_t(v) \big] \Big]_{v=-\infty}^{\infty}}_{=0, \text{ similar argument as above}} + \underline{\int_{-\infty}^{\infty} dv \; R(v) \frac{d^2}{dv^2} P_t(v)} \qquad (\text{Eq. C.3.2})$$

C.4 put (Eq C.3.1) & (Eq C.3.2) in (Eq C.2) & exprm (Eq. C.2) only with integrals

$$\int_{-\infty}^{\infty} dv \; R(v)\, P_{\underline{t+dt}}(v) = \int_{-\infty}^{\infty} dv \; R(v) \Big[P_t(v) + \frac{1}{\tau_a} dt \frac{d}{dv}\big[v P_t(v) \big] + D_a\, dt \frac{d^2}{dv^2} P_t(v) \Big]$$

$$\Leftrightarrow \quad P_{t+dt}(v) = P_t(v) + \frac{1}{\tau_a} dt \frac{d}{dv}\big[v P_t(v) \big] + D_a\, dt \frac{d^2}{dv^2} P_t(v)$$

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$$\Longleftrightarrow \quad \boxed{\frac{P_{t+dt}(v) - P_t(v)}{dt} = \frac{1}{\tau_a}\frac{d}{dv}\left[v P_t(v)\right] + D_a \frac{d^2}{dv^2} P_t(v)}$$

$dt \to 0$

$$\boxed{\frac{dP_t(v)}{dt} = \frac{1}{\tau_a}\frac{d}{dv}\left(v P_t(v)\right) + D_a \frac{d^2}{dv^2} P_t(v)}$$

unconfined

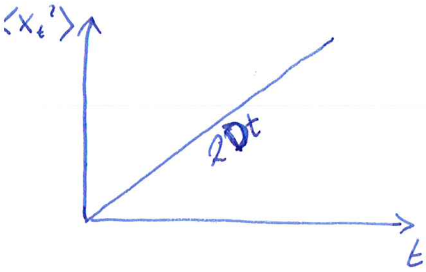
$$\Rightarrow \quad \frac{dP_t(v)}{dt} = D_a \frac{d^2}{dv^2} P_t(v)$$

$x = v$

$$P_t(x) = \frac{e^{-x^2/4Dt}}{\sqrt{4\pi D t}}$$

$$\langle x_t \rangle = \int_{-\infty}^{\infty} dx \, x \, P_t(x) = 0$$

$$\langle x_t^2 \rangle = \int_{-\infty}^{\infty} dx \, x^2 P_t(x) = 2 D_a t$$



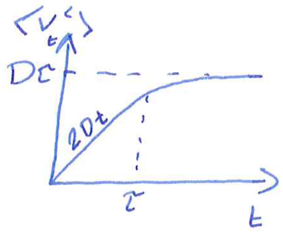
confined

$$\frac{dP_t(v)}{dt} = \frac{1}{\tau_a}\frac{d}{dv}\left(v P_t(v)\right) + D_a \frac{d^2}{dv^2} P_t$$

$$P_t(v) = \frac{e^{-\frac{v^2}{4A_t}}}{\sqrt{4\pi A_t}} \; ; \; A_t = \frac{D\tau}{2}\left(1 - e^{-\frac{2t}{\tau}}\right)$$

$$\langle v_t \rangle = 0$$

$$\langle v_t^2 \rangle = 2A_t = D\tau\left(1 - e^{-\frac{2t}{\tau}}\right) = \begin{cases} 2Dt & \text{for } t \ll \tau \\ D\tau & \text{for } t \gg \tau \end{cases}$$



Langevin eq. $\xrightarrow{\text{always}}$ Fokker-Planck $\xleftarrow{\text{condition: jumps in one time step are small; continuous time \& space}}$ Master eq.

Langevin eq. $\xleftarrow[\text{not always}]{}$ Fokker-Planck $\xrightarrow[\text{discretize space of configs.}]{}$ Master eq.

not always
e.g. if $\vec{F} \neq -\text{grad}\, U(\vec{x})$

discretize space of configs.
always

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