VII Functionals of stochastic processes: the Feynman-Kac correspondance

An important motivation for studying such questions comes from the field of stochastic thermodynamics, that emerged ca 1997 (Sekimoto). The idea is to assign a work performed by some operator, and the heat exchanged with some thermal bath, for a single trajectory of a stochastic process → they are functionals of the whole trajectories. What are their statistical properties?

1°) The Feynman-Kac correspondance

We consider the Langevin eq

$$\dot{x}(t) = \mu F(x) + \sqrt{2D}\,\xi(t) \quad ; \quad \langle \xi(t)\rangle = 0 \; ; \; \langle \xi(t)\xi(t')\rangle = \delta(t-t')$$

and we define an arbitrary functional Ω of the trajectory, as

$$\Omega = \int_0^t V[x(t')]\,dt'$$

V has nothing to do with the potential from which $F(x)$ derives (when it does) unless otherwise stated, and the analysis to follow also holds when $V[x(t'), t']$ has an explicit time dependence (useful for stochastic thermodynamics). The goal is to characterize exponential averages of the type $\langle e^{-p\Omega}\rangle$, where $\langle\ \rangle$ denote average over all possible trajectories (as before), with various constraints (such as fixing the final point $x(t)$, or averaging over it). If we can compute $\langle e^{p\Omega}\rangle$ for all p, then we have the Laplace transform of the pdf of Ω, $p(\Omega)$

$$\langle e^{-p\Omega}\rangle = \int_{-\infty}^{+\infty} e^{-p\Omega}\,p(\Omega)\,d\Omega$$

For the time being, redefining pV into V, we take $p=1$ without loss of generality.

We will consider two types of questions

$$Q_f(x,t) = \left\langle e^{-p\Omega(t)}\,\delta(x(t)-x)\right\rangle \qquad \text{for arbitrary initial conditions @ } t=0$$

$$Q_b(x_0,t) = \left\langle e^{-p\Omega(t)}\right\rangle_{x(0)=x_0 \text{ fixed}} \qquad \text{i.e. averaging ~~also~~ on final } x(t) \text{ for a fixed initial condition}$$

Q_f obeys a "forward"-type of equation, Q_b a "backwards" one, both of the "Schrödinger / Fokker-Planck" form. This connexion between stochastic processes and PDE was realized ~ 1947 by Feynman and Kac, both at Cornell who understood they were working on the same problem from different perspectives.

1) a) The forward formulation

The joint pdf $p(x, \Omega, t)$ of x and Ω is the key here. We are dealing with the process $(x(t), \Omega(t))$ with

$$\begin{cases} \dot{x} = \mu F(x(t)) + \sqrt{2D}\, \xi(t) \\ \dot{\Omega} = V[x(t)] \end{cases} \qquad \left(\text{and actually } \begin{Bmatrix} F(x,t) \\ V[x(t),t] \end{Bmatrix} \text{ is allowed}\right).$$

$\hookrightarrow$ useful for stochastic thermodynamics

for which the Fokker-Planck equation reads

$$\partial_t p(x, \Omega, t) = -V(x)\,\partial_\Omega p - \mu\,\partial_x[F(x)p] + D\,\partial_x^2 p \,;$$

note $\partial_\Omega[V(x)p(x,\Omega,t)] = V(x)\,\partial_\Omega p$. This gives the evolution eq for

$$\boxed{Q_f(x,t) \text{, from its very definition } = \int d\Omega\, e^{-\Omega} p(x, \Omega, t)}$$

$$\begin{aligned} \partial_t Q_f(x,t) &= \int d\Omega\, e^{-\Omega}\, \partial_t p(x,\Omega,t) \\ &= \int d\Omega\, e^{-\Omega}\left[-V(x)\,\partial_\Omega p - \mu\,\partial_x(Fp) + D\,\partial_x^2 p\right] \\ &= -V(x) \underbrace{\int d\Omega\, e^{-\Omega}\,\partial_\Omega p}_{\left[e^{-\Omega} p\right]_{-\infty}^{+\infty} + \int d\Omega\, e^{-\Omega} p \;\; Q_f} - \mu\,\partial_x(FQ_f) + D\,\partial_x^2 Q_f \end{aligned}$$

Assuming that the boundary term ↑ does vanish (how do we prove this?),

$$\boxed{\partial_t Q_f(x,t) = -V(x)\,Q_f - \mu\,\partial_x[F(x)\,Q_f] + D\,\partial_x^2 Q_f(x,t)}$$

The initial condition is arbitrary: at $t=0$, $\Omega(0)=0$, $Q_f(x,t=0) = p(x,t=0)$

also holds for $V(x,t)$ and $F(x,t)$ (exercise).

1) b) The backward formulation

Compared to Q_f, Q_b is obtained by averaging over $x(t)$, but at a fixed initial condition $x(0) = x_0$. To find its evolution equation, we introduce the propagator $p(x, \Omega, t \mid x_0, \Omega_0, t_0)$ and it is understood that $\Omega(t) = \Omega_0 + \int_{t_0}^{t} V(x(\tau))\,d\tau$

$$\begin{aligned} \partial_t p(x,\Omega,t \mid x_0,\Omega_0,t_0) &= -V(x)\,\partial_\Omega p - \mu\,\partial_x[F(x)p] + D\,\partial_x^2 p \\ &\equiv \mathcal{L}_{x,\Omega}\, p \end{aligned}$$

$$\begin{aligned} \Rightarrow \partial_{t_0} p(x,\Omega,t \mid x_0,\Omega_0,t_0) &= -\mathcal{L}^{+}_{x_0,\Omega_0}\, p \\ &= -V(x_0)\,\partial_{\Omega_0} p - \mu F(x_0)\,\partial_{x_0} p - D\,\partial_{x_0}^2 p \end{aligned}$$

and we are interested in

$$Q_f(x_0,t,t_0) = \left\langle e^{-[\Omega(t)-\Omega_0]} \right\rangle_{x(t_0)=x_0}$$

$$Q_f(x_0,t,t_0) = \int d\Omega\, dx\; e^{-(\Omega-\Omega_0)}\; p(x,\Omega,t|x_0,\Omega_0,t_0)$$

does not depend on Ω_0

$$\Rightarrow \partial_{t_0} Q_f(x_0,t,t_0) = \int d\Omega\, dx\; e^{-\Omega+\Omega_0}\; \partial_{t_0} p$$

$$= -\int d\Omega\, dx\; e^{\Omega_0-\Omega}\left[V(x_0)\partial_{\Omega_0} p + \mu F(x_0)\partial_{x_0} p + D\partial^2_{x_0} p\right]$$

$$= -V(x_0)e^{\Omega_0}\partial_{\Omega_0}\left\langle e^{-\Omega}\right\rangle_{x_0} - \mu F(x_0)\partial_{x_0} Q_f - D\partial^2_{x_0} Q_f$$

$$= \partial_{\Omega_0}\left(e^{-\Omega_0} Q_f\right) = -e^{-\Omega_0} Q_f \;;\; \partial_{\Omega_0} Q_f = 0$$

$$\Rightarrow \boxed{\partial_{t_0} Q_f(x_0,t,t_0) = V(x_0,t)\, Q_f - \mu\, F(x_0,t)\,\partial_{x_0} Q_f - D\,\partial^2_{x_0} Q_f}$$

we make explicit this t dependence

This relation is sometimes found in a $\neq t$ form, when there is no explicit time dependence in $V(x)$ and $F(x)$, and we thus have time translation invariance with dependence on $t-t_0$:

$$Q_f(x_0,t,t_0) = Q_f(x_0,t-t_0) \quad \therefore \quad \partial_t Q_f = -\partial_{t_0} Q_f, \text{ so that}$$

$$\partial_t Q_f(x_0,t-t_0) = -V(x_0)\,Q_f(x_0,t-t_0) + \mu F(x_0)\,\partial_{x_0} Q_f + D\,\partial^2_{x_0} Q_f$$

This result can be recovered from a more direct argument, still with $V(x,\cancel{t})$, $F(x,\cancel{t})$

$$Q_f(x_0,t) = \left\langle e^{-\int_0^t V(x(\tau))\,d\tau}\right\rangle_{x(0)=x_0}$$

$$= \left\langle \exp\left(-\int_0^{\Delta t} V(x(\tau))\,d\tau - \int_{\Delta t}^t V(x(\tau))\,d\tau\right)\right\rangle_{x(0)=x_0}$$

$$x(\Delta t) = \underbrace{x(0)}_{x_0} + \mu F(x_0)\Delta t + \sqrt{2D}\underbrace{\int_t^{t+\Delta t}\xi(t')\,dt'}_{B_{\Delta t}} \;;\; \langle B_{\Delta t}\rangle = 0,\; \langle B^2_{\Delta t}\rangle = \Delta t$$

$$Q_f(x_0,t) = e^{-V(x_0)\Delta t}\left\langle e^{-\int_{\Delta t}^t V(x(\tau))\,d\tau}\right\rangle_{x(0)=x_0}$$

↳ this average is performed in 2 steps. First at fixed $x(\Delta t)$ which yields $Q_f(x(\Delta t), t-\Delta t)$ and then averaging over $x(\Delta t)$, ie over $B_{\Delta t}$

$$Q_f(x_0,t) = e^{-V(x_0)\Delta t}\left\langle Q_f(x(\Delta t), t-\Delta t)\right\rangle$$

→ this bracket means average of $B_{\Delta t}$

$$\simeq (1-V(x_0)\Delta t)\left\langle Q_f\left(x_0 + F(x_0)\Delta t + \sqrt{2D}B_{\Delta t},\; t-\Delta t\right)\right\rangle$$

$$= (1-V(x_0)\Delta t)\left\langle Q_f(x_0,t) + \left(F(x_0)\Delta t + \sqrt{2D}B_{\Delta t}\right)\partial_{x_0} Q_f + \frac{1}{2}\left(F(x_0)\Delta t + \sqrt{2D}B_{\Delta t}\right)^2 \partial^2_{x_0} Q_f - \Delta t\,\partial_t Q_f\right\rangle$$

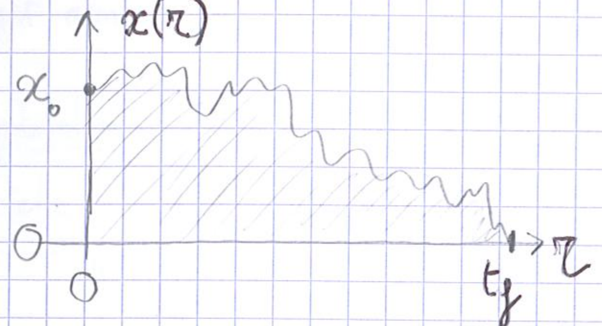
$$= (1-V(x_0)\Delta t)\left\{Q_f(x_0,t) + F(x_0)\Delta t\,\partial_{x_0} Q_f + D\,\partial^2_{x_0} Q_f\,\Delta t - \Delta t\,\partial_t Q_f\right\}$$

$$\cancel{Q_f(x_0,t)} = \cancel{Q_f(x_0,t)} + F(x_0)\,\partial_{x_0} Q_f\,\Delta t + \Delta t\, D\,\partial^2_{x_0} Q_f - \Delta t\,\partial_t Q_f - V(x_0)\Delta t\, Q_f$$

$$\Rightarrow \partial_t Q_f = -V(x_0)\,Q_f(x_0,t) + F(x_0)\,\partial_{x_0} Q_f + D\,\partial^2_{x_0} Q_f \qquad \square$$

2°) First-passage functionals

We have so far considered functionals like $Q = \left\langle e^{-\int_0^t V(x(\tau))\,d\tau} \right\rangle$ and we could also have worked out $\left\langle \varphi(x(t))\, e^{-\int_0^t V(x(\tau))\,d\tau} \right\rangle$. Yet, in some situations, the time t is itself stochastic. If it is exponentially distributed, averaging over t corresponds to taking the Laplace transform of Q. We will address a different family of problems, where the functional stops at the first passage time (at some point, that we take to be $x = 0$):



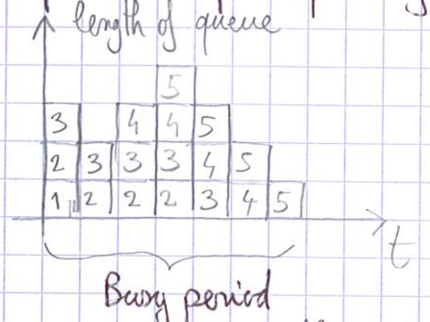
t_f is the first-passage time

$$\boxed{\Omega = \int_0^{t_f} V(x(\tau))\,d\tau}\,,\quad \text{what is } P(\Omega, x_0)?$$

If $V(x) = 1$, $\quad \Omega = t_f$ itself

$V(x) = x$, $\quad \Omega$ is the hatched area

An example comes from queuing theory



"Customer 1" is being served; then 2 becomes ahead; customer 4 arrives, then 5, before 2 is finally served; then 3, 4 and 5 are served without any new arrival

The total time spent by all of the customers during busy period = area under the curve.

A simple model for the evolution of the queue length at time n, ℓ_n, is

$$\ell_n = \ell_{n-1} + \xi_n \;; \quad \xi_n \longrightarrow 1 \text{ with proba } p \text{ (a new customer arrives)}$$

$$A = \sum_{n=1}^{t_f} \ell_n \qquad\qquad \longrightarrow -1 \;\;\text{"}\;\;\text{"}\;\; q \text{ (the first in line is served and leaves)}$$

What is $P(A, \ell_0)$?

As above, we define the average

$$Q_f(x_0) = \left\langle e^{-\Omega} \right\rangle_{x(0) = x_0 \text{ fixed}}$$

Quite remarkably, $Q_f(x)$ obeys an equation that is closely related to that for $Q_f(x_0, t)$

$$Q(x_0) = \left\langle e^{-\int_0^{\Delta t} \cdots - \int_{\Delta t}^{t_f} \cdots} \right\rangle$$

$$= e^{-\Delta t\, V(x_0)} \left\langle Q_f(x_0 + \Delta x) \right\rangle \quad \text{average over } \Delta x = x(\Delta t) - x_0 \text{ i.e. over } B_{\Delta t}$$

$$\Delta x = \mu F(x_0)\Delta t + \sqrt{2D}\, B_{\Delta t}$$

$$Q_f(x_0) \simeq (1 - V(x_0)\Delta t)\left\langle Q_f(x_0) + \Delta x\, \partial_{x_0} Q_f + \frac{(\Delta x)^2}{2} \partial^2_{x_0} Q_f \right\rangle$$ (8.9)

∂_{x_0} are $\frac{d}{dx_0}$

$$\simeq (1 - V(x_0)\Delta t)\left[Q_f(x_0) + \mu F(x_0)\partial_{x_0} Q_f \Delta t + D\, \partial^2_{x_0} Q_f \Delta t \right]$$

$$= Q_f(x_0) + \Delta t\left[\mu F(x_0)\partial_{x_0} Q_f + D\, \partial^2_{x_0} Q_f - V(x_0) Q_f \right]$$

$$\Rightarrow D \frac{d^2 Q_f}{dx_0^2} + F(x_0)\frac{dQ_f}{dx_0} - V(x_0) Q_f(x_0) = 0$$

with boundary conditions : $x_0 \to 0,\ t_f \to 0 \Rightarrow Q_f(0) = 1$

$x_0 \to \infty,\ t_f \to \infty \Rightarrow Q_f(\infty) = 0$

We get almost the equation for $Q_f(x_0, t)$, but without the time derivative

Application : statistics of the first-passage time for the Wiener process (no force, $F(x)=0$).

We take $V(x) = s$, independent from x, s arbitrary :

$$D \frac{d^2 Q_f}{dx_0^2} = s\, Q_f \quad \text{with} \quad Q_f(0) = 1,\ Q_f(\infty) = 0 \quad \Rightarrow Q_f(x_0) = e^{-\sqrt{s/D}\, x_0}$$

$$\Rightarrow \left\langle e^{-s t_f} \right\rangle_{x_0} = \exp\left(-x_0\sqrt{\frac{s}{D}}\right)$$, which is the Laplace transform of

$$= \int_0^\infty e^{-s t_f} p(t_f)\, dt_f$$ $p(t_f)$, the pdf of t_f

We have already met such a Laplace form, when studying Lévy-stable distribution : this is indeed the Fréchet distribution, of Pareto index $\mu = 1/2$ (hence a tail for large t_f in $t_f^{-3/2} = t_f^{-(1+\mu)}$. Remember indeed that Lévy stable laws are most conveniently expressed in Fourier space, and have form in $\langle e^{ikx}\rangle = e^{-\gamma |k|^\mu}$

Finally, we have here :

$$P(t_f) = \frac{|x_0|}{\sqrt{4\pi D}} \frac{1}{t_f^{3/2}} e^{-x_0^2/4Dt_f}$$

$\Rightarrow \langle t_f \rangle = +\infty$ as a result of large excursions with $x > 0$

We had already met a behaviour in $(t_f)^{-3/2}$ for the survival probability of a symmetric discrete random walk (starting from $x = 0$, proba $S(t)$ to remain on the positive sector, $x > 0$)

Motivation for studying first passage properties

First passage properties underlie a wide range of stochastic processes, from micro $\to$ macro

- diffusion-limited reactions : diffusing p have to meet before a reaction can happen
- neuron firing

- protein looking for target site on DNA
- ions searching for ion channels in cell membranes
- proteins that must exit from organelle where they were produced / synthetized, before accomplishing their biological function
- gambler's ruin ; different models where a critical threshold has to be reached
- triggering of stock options etc.