Lecture 8 summary

2.2 Fokker – Planck equation

$$\frac{\partial}{\partial t} p(\vec{x},t) + \sum_i \frac{\partial}{\partial x_i} J_i(\vec{x},t) = 0 \quad \text{local balance equation}$$

with probability flow / flux / current $J_i(\vec{x},t)$:

$$J_i(\vec{x},t) = \overset{\text{drift}}{A_i(\vec{x},t)}\, p(\vec{x},t) - \frac{1}{2} \sum_j \frac{\partial}{\partial x_j} \left(B_{ij}(\vec{x},t)\, p(\vec{x},t) \right)$$

Boundary conditions

(a) reflecting $\quad \vec{n} \cdot \vec{J}(\vec{x},t) \Big|_{\vec{x} \in S} = 0$

(b) absorbing barrier $\quad p(\vec{x},t) \Big|_{\vec{x} \in S} = 0$

(c) discontinuity

$$\hat{n} \cdot \vec{J} \Big|_{S_+} = \hat{n} \cdot \vec{J} \Big|_{S_-}$$

$$p \Big|_{S_+} = p \Big|_{S_-}$$

(d) periodic

$$p(a,t) = p(b,t)$$
$$J(a,t) = J(b,t)$$

(e) natural

$A(a,t) = 0$ (velocity is zero; the boundary can never be reached)

Stationary solutions for hom. Markov processes:

$$J(x) = \text{const} = J(b) = J(a)$$

(i) reflecting boundary conditions $\quad J(a) = 0$

potential solution

$$p^*(x) = \frac{\mathcal{N}}{B(x)} \exp\left[2 \int_a^x dx' \, \frac{A(x')}{B(x')} \right]$$

(ii) periodic boundary conditions

here we have nonzero current J:

$$A(x)\, p^*(x) - \frac{1}{2} \frac{d}{dx} \left[B(x)\, p^*(x) \right] = J \qquad ☺☺$$

However, J is not arbitrary, but is determined by normalization and the periodic boundary conditions.

$$p^*(a) = p^*(b)$$
$$J(a) = J(b)$$

For convenience, define

$$\Psi(x) = \exp\left[2 \int_a^x dx' \, \frac{A(x')}{B(x')} \right]$$

Then we can easily integrate ☺☺ to get

$$p^*(x)\, B(x) / \Psi(x) = p^*(a)\, B(a) / \Psi(a) - 2J \int_a^x dx' / \Psi(x')$$

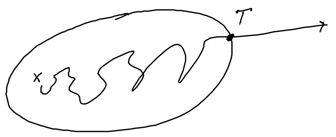
By imposing b.c. $p^*(a) = p^*(b)$ we find that

$$J = \left[\frac{B(b)}{\Psi(b)} - \frac{B(a)}{\Psi(a)} \right] \Big/ \left[\int_a^b dx' / \Psi(x') \right]$$

so that

$$p^*(x) = p^*(a) \left[\frac{\int_a^x \frac{dx'}{\psi(x')} \frac{B(b)}{\psi(b)} + \int_x^b \frac{dx'}{\psi(x')} \frac{B(a)}{\psi(a)}}{\frac{B(x)}{\psi(x)} \int_a^b \frac{dx'}{\psi(x')}} \right]$$

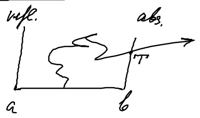
First passage times for homogen. processes



Q: How long will the particle remain in a certain region?

Particle between absorbing and reflecting barrier

Let the particle be initially at x at time $t=0$.



Q: How long will it remain in the interval (a, b)?

Goal: escape time T

The probability that the particle at time t is still in (a, b)

$$G(x,t) = \int_a^b dx'\, p(x',t/x,0)$$

Let the time that the particle leaves (a,b) be T.

Then $$\text{Prob.}(T \geq t) = \int_a^b dx'\, p(x',t/x,0)$$

Since the process is homog., we can write

$$p(x',t/x,0) = p(x',0/x,-t)$$ and

the backward FPE can be written (backward evolution for $t' < t$ from (x,t)):

$$\frac{\partial p(x,t/y,t')}{\partial t'} = -A(y,t') \frac{\partial p(x,t/y,t')}{\partial y} - \frac{1}{2} B(y,t') \frac{\partial^2 p(x,t/y,t')}{\partial y^2}$$

homogen. process $\Rightarrow$ A and B do not depend on time

$$\Rightarrow \frac{\partial}{\partial t} G(x,t) = -\frac{\partial}{\partial t'} \int_a^b dx'\, p(x',0/x,\underset{-t}{\underset{\parallel}{t'}})$$

$$\Rightarrow \frac{\partial}{\partial t} G(x,t) = A(x) \frac{\partial}{\partial x} G(x,t) + \frac{1}{2} B(x) \frac{\partial^2}{\partial x^2} G(x,t)$$

The boundary conditions

$$p(x',0|x,0) = \delta(x'-x) \Rightarrow$$

$$\Rightarrow G(x,0) = \begin{cases} 1, & a \le x \le b \\ 0, & \text{elsewhere} \end{cases}$$

If $x=b$, the particle is absorbed immediately, so $G(b,t)=0$

For $x=a$: $\partial_x G(a,t) = 0$

$\overset{\shortparallel}{\text{Prob.}}(T \geq t) = 0$ if $x=b$

Since $G(x,t)$ is the probability that $T \geq t$,

the mean of any function of T is

$$\langle f(T) \rangle = -\int_0^\infty f(t)\, dG(x,t)$$

Thus, the mean first passage time

$T(x) = \langle T \rangle$ is given by

$$T(x) = -\int_0^\infty t\, dG = -\int_0^\infty t \frac{\partial G(x,t)}{\partial t} dt \xlongequal[\text{by parts}]{\text{integrate}}$$

$$= \int_0^\infty G(x,t)\, dt$$

We can derive a simple ODE for $T(x)$ from backward FPE

We note $\displaystyle\int_0^\infty \frac{\partial}{\partial t} G(x,t)\, dt = \underbrace{G(x,\infty)}_{0} - \underbrace{G(x,0)}_{1} = -1$

and derive

$$A(x) \frac{\partial}{\partial x} T(x) + \frac{1}{2} B(x) \frac{\partial^2 T(x)}{\partial x^2} = -1 \quad (*)$$

Boundary conditions $T'(a) = 0$ (refl.), $T(b) = 0$ (abs.)

Equation $(*)$ can be solved by integration

The solution after some manipulation can be written

$$\psi(x) = \exp\left[2 \int_a^x dx' \frac{A(x')}{B(x')} \right]$$

One can find $\displaystyle T(x) = 2 \int_x^b \frac{dy}{\psi(y)} \int_a^y dz \frac{\psi(z)}{B(z)}$

<u>Proof</u>

$$T' = -\frac{2}{\psi(x)} \int_a^x dz \frac{\psi(z)}{B(z)}$$

$$T'' = -\frac{2}{\psi(x)^2} \Big[\frac{\psi(x)^2}{B(x)} - \psi'(x) \int_a^x dz \frac{\psi(z)}{B(z)} \Big]_{\frac{2A}{\psi}}$$

$$\overset{(*)}{\Longrightarrow} A T' + \frac{1}{2} B T'' = \cancel{-\frac{2A}{\psi} \int_a^x dz \frac{\psi}{B}} - \Big[1 - \cancel{\frac{B}{\psi^2} \psi' \int_a^x dz \frac{\psi}{B}} \Big] = \underline{-1}$$

$$\psi' = \frac{2A}{B} \psi \Rightarrow \frac{B \psi'}{\psi^2} = \frac{2A}{\psi}$$

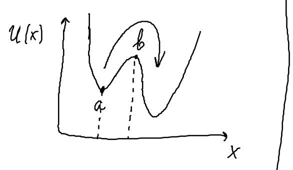
$$B.C.: \ T'(a) = \int_0^\infty dt \frac{\partial}{\partial x} G(x,t) \Big|_{x=a} = 0 \quad \checkmark$$

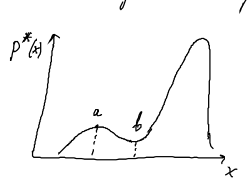
$$T(b) = 0 \quad \checkmark$$

$\square$

Application – escape over a potential barrier

Double well potential $U(x)$ | Stationary solution $p^*(x)$





We suppose that a point moves according FPE

$$\partial_t p(x,t) = \partial_x [U'(x) p(x,t)] + D \partial_x^2 p(x,t)$$

We suppose that motion is on an infinite range, which means the stationary solution

$$p^*(x) = \mathcal{N} \exp\left[\frac{-U(x)}{D}\right]$$

which is bimodal, so that there is a relatively high probability of being on the left or the right of b, but not near b.

Q: What is the mean escape time from the left hand well?

By this we mean, what is the mean first passage time from a to x, where x is the vicinity of b?

<u>substitutions</u>

$b \to x_0$

$a \to -\infty$

$x \to a$

$$T(a \to x_0) = \frac{1}{D} \int_a^{x_0} dy \exp\left[\frac{U(y)}{D}\right] \int_{-\infty}^{y} \exp\left[-\frac{U(z)}{D}\right] dz$$

If the central maximum of $U(x)$ is large and D is small then $\exp\left[\frac{U(y)}{D}\right]$ is sharply peaked at $x = b$, while $\exp\left[-\frac{U(z)}{D}\right]$ is very small near $z = b$. $\Rightarrow$

$\Rightarrow \int_{-\infty}^{y} \exp\left[-\frac{U(z)}{D}\right] dz$ is a very slowly varying function of y near $y = b$. This means that the value of the integral $\int_{-\infty}^{y} \exp\left[-\frac{U(z)}{D}\right] dz$ will be approximatly constant for those values of y which yield a value of $\exp\left[\frac{U(y)}{D}\right]$ which is significantly different from zero. $\Rightarrow$

$\Rightarrow$ in the inner integral, we can set $y = b$ and remove the resulting constant factor from inside the integral with respect to y $\Rightarrow$

$$\Rightarrow \quad T(a \to x_0) \simeq \left\{ \frac{1}{D} \int_{-\infty}^{b} dy \exp\left[-\frac{U(z)}{D} \right] \right\} \int_{a}^{x_0} dy \left[\frac{U(y)}{D} \right]$$

Definition of $p^*(x)$ $\Rightarrow$

$$\Rightarrow \quad \int_{-\infty}^{b} dy \exp\left[-\frac{U(z)}{D} \right] = \frac{n_a}{N}$$

which means that n_a is the probability that the particle is to the left of b when the system is stationary.