

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 $J_i(\vec{x}, t)$:

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

Boundary conditions

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

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

(c) discontinuity

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

(d) periodic

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

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

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

(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 $J(a) = 0$

potential solution

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

(ii) periodic boundary conditions

here we have nonzero current J :

$$A(x) p^*(x) - \frac{1}{2} \frac{d}{dx} [B(x) p^*(x)] = J \quad \text{☺ ☹}$$

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

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

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

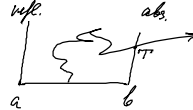


Q: How long will the particle remain in a certain region?

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 homogen., we can write

$$p(x, t/x, 0) = p(x', 0/x, -t) \text{ and}$$

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

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

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

The boundary conditions

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

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

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

For $x = a$: $\partial_x G(a, t) = 0$ \Downarrow
 $\text{Prob.}(T \geq t) = 0 \text{ if } x = b$

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

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

$$T(x) = - \int_0^{\infty} t dG = - \int_0^{\infty} t \frac{\partial G(x, t)}{\partial t} dt \quad \begin{array}{l} \text{integrate} \\ \text{by parts} \end{array}$$

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

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

We note $\int_0^{\infty} \frac{\partial}{\partial t} G(x, t) dt = \underbrace{G(x, \infty)}_0 - \underbrace{G(x, 0)}_1 = -1$

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

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

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

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

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

$$\Rightarrow (*) \quad A T' + \frac{1}{2} B T'' = - \frac{2A}{\psi} \int_a^x \frac{\psi}{B} - \left[1 - \frac{B \psi'}{\psi^2} \int_a^x \frac{\psi}{B} \right] = -1$$

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

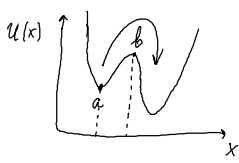
B.C.: $T'(a) = \int_0^{\infty} dt \frac{\partial}{\partial x} G(x, t) \Big|_{x=a} = 0 \quad \checkmark$

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

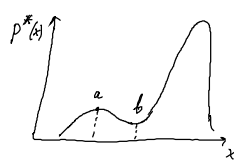
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Application - escape over a potential barrier

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

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

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 ?

Substitutions

$$b \rightarrow x_0$$

$$a \rightarrow -\infty$$

$$x \rightarrow a$$

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

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 approximately 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

$$\Rightarrow T(a \rightarrow x_0) \approx \left\{ \frac{1}{\mathcal{D}} \int_{-\infty}^b dy \exp \left[-\frac{u(z)}{\mathcal{D}} \right] \right\} \int_a^{x_0} dy \left[\frac{u'(z)}{\mathcal{D}} \right]$$

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

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

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