TD 12: First-Passage Problems - Solutions

Baptiste Coquinot & Antonio Costa

9 décembre 2021

An important quantity when studying stochastic processes, is to know the amount of time it takes before our fluctuating variables reaches a certain threshold. This is one of the simplest observations we can make from an experimental point of view, yet it captures some of properties of the underlying dynamics. The quantity of interest is the *first-passage time*, which is the average time to escape from an interval. It is in itself a stochastic variable with an associated probability distribution. As we will see, finding an expression for the full first-passage time distribution is very challenging except for a few simple systems. However, we can leverage the nature of the Fokker-Planck equation to compute moments of this distribution.

How can we obtain the mean first passage time $\overline{\tau}$?

1. Consider a point-like random walker starting at an initial condition $x \in [0, b]$ at time $t = 0$, jumping $\delta \ll 1$ to the right/left with equal probability after every time step $\Delta t \ll 1$. Show that the mean first-passage time $\overline{\tau}$ satisfies
$$\frac{d^2}{dx^2}\overline{\tau}(x) + \frac{1}{D} = 0,$$
where the diffusion constant $D = \frac{\delta^2}{2\Delta t}$.

2. Assume that the boundaries of the interval are absorbing. What does this imply for the boundary conditions of $\overline{\tau(x)}$ at $x = 0$ and $x = b$? Solve for $\overline{\tau}(x)$ with absorbing boundaries.

3. What is the average of $\overline{\tau}(x)$ if x is chosen uniformly at random in $[0, b]$?

Forward and backward Fokker-Planck equations and the mean-first passage time. Here, we derive the general expression of the mean-first passage time for a one-dimensional stochastic process driven by thermal noise

4. The propagator of the density dynamics of a system driven by thermal noise obeys the Fokker-Planck equation,
$$\partial_t p(x,t|x',t') = [-\partial_x D_1(x,t) + \partial_x^2 D_2(x,t)]p(x,t|x',t') \equiv \mathcal{L}p(x,t|x',t').$$
Multiply by $p(x',t'|x,t)$ and integrate by parts (assuming that probability vanishes sufficiently fast at $\pm\infty$) to derive the *adjoint* (also known as *backward*) Fokker-Planck equation,
$$-\partial_{t'} p(x,t|x',t') = [D_1(x',t')\partial_{x'} + D_2(x',t')\partial_{x'}^2]p(x,t|x',t') \equiv \mathcal{L}^+ p(x,t|x',t').$$

5. Consider the same situation as before but for general 1D Fokker-Planck dynamics with arbitrary drift and diffusion. We define the *survival probability* as the probability that the particle is still in the interval $[a, b]$ after a time t as
$$S(t|x) \equiv \int_a^b p(x',t|x,0)\mathrm{d}x'.$$
With absorbing boundaries $S(t|x)$ decreases in time such that $S(t|x) \overset{t\to\infty}{\to} 0$. The rate at which the probability decreases, i.e. the rate at which the particles in our ensemble reach the absorbing boundary, is given
$$f(t|x) = -\partial_t S(t|x).$$
Express the mean first-passage time $\overline{\tau}(x)$ using f and, assuming $tS(t|x) \overset{t\to\infty}{\to} 0$, simplify to show that
$$\overline{\tau}(x) = \int_0^\infty S(t|x)\mathrm{d}t.$$

6. The function $S(t|x)$ satisfies the initial condition $S(0|x) = 1 \forall x \in (a, b)$. Assume a stationary random process (D_1, D_2 do not depend on time), such that $p(x',t|x,t_0) = p(x',t-t_0|x,0)$. Apply $\mathcal{L}^+$ to $\overline{\tau}$ and show that
$$\mathcal{L}^+\overline{\tau}(x') = -1 \tag{1}$$
Check that that 1 agrees with problem 1. for $D_1 = 0, D_2 = D = const.$[1]

[1] One can derive an equation analogous to (1) for all higher moments of the first passage time distribution. In the simple case of $D_1 = 0$, $D_2 = D = cst$, one may even compute f exactly. It turns out to be a fairly wide distribution with a standard deviation comparable to the mean. This illustrates that the *mean* first passage time alone does not contain all information, but it is often the only thing one may hope to obtain analytically.

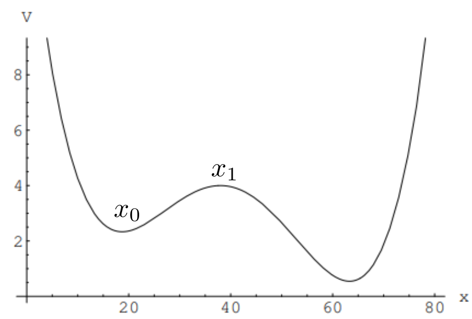

Figure 1: Sketch of the double-well potential $V(x)$ considered here.

7. *(Bonus)* Assume a to be reflecting, i.e. $\partial_x S(t|x)|_{x=a} = 0$, while b is absorbing. Show that the general solution to eq.(1) is

$$\overline{\tau}(x) = \int_x^b \mathrm{d}z \frac{1}{\phi(z)} \int_a^z \frac{\phi(y)}{D_2(y)} dy,$$

where

$$\phi(y) \equiv \exp\left(\int^y \mathrm{d}x \frac{D_1(x)}{D_2(x)}\right).$$

Example applications. We will compute the mean first passage times for some example dynamics.

8. Consider the case of $D_1(x) = -\lambda x$, $\lambda > 0$, $D_2(x) = D = const.$. It describes the dynamics of an overdamped particle in a quadratic potential subject to a space-independent random force, and is known as the *Ornstein Uhlenbeck-Process*. Let $a = 0$. Use the asymptotics $\int_0^x e^{t^2} dt \sim \frac{e^{x^2}}{2x}$ $(x \to \infty)$ to show that at leading order in $\eta = \lambda b^2/(2D) \gg 1$ (what does this limit mean physically?)

$$\overline{\tau}(x = 0) \sim \frac{\sqrt{\pi}}{2\lambda} \frac{e^{\eta^2}}{\eta}$$

Interpret this result.

9. Consider a double-well potential $V(x)$ as depicted in figure 1, with $D_1(x) = -\frac{dV}{dx}$. Let the starting point be x_0 at $t = 0$. We want know the mean first passage time for the escape, due to additive noise, over the potential barrier into the right potential well. Let the maximum be located at x_1. We choose $a = -\infty$ reflective and b lying somewhat to the right of x_1, absorbing. Consider appropriately small noise $D_2 = D$ and use the "saddle point" approximation, for a function $f(x)$ whose local maximum is at $x = x_*$, and a large parameter $\Lambda \to \infty$,

$$\int e^{\Lambda f(x)} dx \sim \sqrt{\frac{2\pi}{\Lambda |f''(x_*)|}} e^{\Lambda f(x_*)}, \tag{2}$$

to show that at leading order

$$\overline{\tau}(x_0) \approx \frac{2\pi}{\sqrt{V''(x_0)|V''(x_1)|}} e^{(V(x_1) - V(x_0))/D}.$$

Correction

1. After one time step, we recover the same problem but with the random walker at either $x + \delta$ or $x - \delta$ with equal probability, thus,

$$\overline{\tau}(x) = \Delta t + \frac{\overline{\tau}(x+\delta) + \overline{\tau}(x-\delta)}{2}.$$

Expanding for small δ gives,

$$\overline{\tau}(x) = \Delta t + \frac{\overline{\tau}(x) + \delta \partial_x \overline{\tau} + \frac{\delta^2}{2} \partial_x^2 \overline{\tau} + \overline{\tau}(x) - \delta \partial_x \overline{\tau} + \delta^2 \partial_x^2 \overline{\tau} + \mathcal{O}(\delta^2)}{2} \tag{3}$$

$$\partial_x^2 \overline{\tau} + \frac{2\Delta t}{\delta^2} = 0 \tag{4}$$

$$\partial_x^2 \overline{\tau} + \frac{1}{D} = 0, \tag{5}$$

where $D = \frac{\delta^2}{2\Delta t}$.

2. The fact that the boundaries are absorbing means that $\overline{\tau}(x^*) = 0$, meaning that the mean amount of time it takes from escape the region at $x^* = 0$ or $x^* = b$ is 0. The solution for $\overline{\tau}(x)$ can be obtained by integrating the previous equation twice,

$$\frac{d^2}{dx^2}\overline{\tau}(x) = -\frac{1}{D} \quad (6)$$

$$\frac{d}{dx}\overline{\tau}(x) = = -\frac{x}{D} + C_1 \quad (7)$$

$$\overline{\tau}(x) = = -\frac{x^2}{2D} + C_1 x + C_2. \quad (8)$$

Leveraging the boundary conditions we find $C_2 = 0$, $C_1 = \frac{b}{2D}$ and thus,

$$\overline{\tau}(x) = \frac{1}{2D} x(b-x).$$

3. The average of the mean first passage time is given by,

$$\langle \overline{\tau}(x) \rangle = \int_0^b \pi(x)\overline{\tau}(x) dx \quad (9)$$

Choosing x uniformly in the interval $[0, b]$ means that $\pi(x) = 1/b$ in this interval, as such,

$$\begin{aligned} \langle \overline{\tau}(x) \rangle &= \frac{1}{b}\int_0^b \overline{\tau}(x) dx \\ &= \frac{1}{b}\int_0^b \frac{1}{2D} x(b-x) dx \\ &= \frac{1}{b}\frac{1}{2D}\left(\frac{bx^2}{2} - \frac{x^3}{3}\right)\Big|_0^b dx \\ \langle \overline{\tau}(x) \rangle &= \frac{b^2}{12D} \end{aligned}$$

4. Multiplying by $p(x', t'|x, t)$ and integrating by parts the l.h.s. in t we get

$$\begin{aligned} \int dxdt p(x',t'|x,t)\partial_t p(x,t|x',t') &= \partial_t p(x',t'|x,t) p(x,t|x',t')\big|_{-\infty}^{\infty} \\ &\quad - \int dxdt \partial_t p(x',t'|x,t) p(x,t|x',t') \\ &= \int dxdt \left(-\partial_t p(x',t'|x,t)\right) p(x,t|x',t') \end{aligned}$$

Where we assume $p(x, t|x', t') = 0$ when $t = \pm\infty$. For the r.h.s we integrate by parts twice in x to get,

$$\begin{aligned} \int dxdt p(x',t'|x,t)\left[-\partial_x D_1(x,t) + \partial_x^2 D_2(x,t)\right] p(x,t|x',t') &= D_1(x,t)p(x,t|x',t')p(x',t'|x,t)\big|_{-\infty}^{\infty} \\ &\quad + \partial_x\left[D_2(x,t)p(x,t|x',t')\right] p(x',t'|x,t)\big|_{-\infty}^{\infty} \\ &\quad - \int dxdt D_1(x,t)\partial_x p(x',t'|x,t)p(x,t|x',t') \\ &\quad - \int dxdt \partial_x\left[D_2(x,t)p(x,t|x',t')\right]\partial_x p(x',t'|x,t) \\ &= - \int dxdt D_1(x,t)\partial_x p(x',t'|x,t)p(x,t|x',t') \\ &\quad - D_2(x,t)p(x,t|x',t')\partial_x p(x',t'|x,t)\big|_{-\infty}^{\infty} \\ &\quad + \int dxdt D_2(x,t)p(x,t|x',t')\partial_x^2 p(x',t'|x,t) \\ &= - \int dxdt D_1(x,t)\partial_x p(x',t'|x,t)p(x,t|x',t') \\ &\quad + \int dxdt D_2(x,t)\partial_x^2 p(x',t'|x,t)p(x,t|x',t') \\ &= \int dxdt \mathcal{L}^+ p(x',t'|x,t)p(x,t|x',t'). \end{aligned}$$

From this we find that,

$$\int dxdt \left(-\partial_t p(x',t'|x,t)\right) p(x,t|x',t') = \int dxdt \mathcal{L}^+ p(x',t'|x,t)p(x,t|x',t'),$$

and thus,

$$-\partial_t p(x',t'|x,t) = \mathcal{L}^+ p(x',t'|x,t),$$

where $\mathcal{L}^+ = D_1(x,t)\partial_x + D_2(x,t)\partial_x^2$. Changing $x \leftrightarrow x'$ and $t \leftrightarrow t'$ we get the required solution.

5. The mean first passage time is the average time weighted by the first passage time distribution, thus,

$$\overline{\tau}(x) = \int_0^\infty f(t|x)t dt,$$

which can be integrated by parts to give

$$\overline{\tau}(x) = -S(t|x)t|_0^\infty - \int_0^\infty -S(t|x)dt = \int_0^\infty S(t|x)dt$$

6. Since $\overline{\tau}(x') = \int_0^\infty \int_a^b p(x,t|x',0)dx$, we have

$$\begin{aligned}
\mathcal{L}^+\overline{\tau}(x') &= \int_0^\infty \int_a^b \mathcal{L}^+ p(x,t|x',0)dxdt \\
&= \int_0^\infty \int_a^b \mathcal{L}^+ p(x,0|x',-t)dxdt \\
&= \int_0^\infty \int_a^b -\frac{\partial}{\partial(-t)} p(x,0|x',-t)dxdt \\
&= \int_0^\infty \int_a^b \partial_t p(x,t|x',0)dxdt \\
&= \int_0^\infty \partial_t S(t|x)dt = \\
&= S(\infty|x) - S(0|x) = \\
\mathcal{L}^+\overline{\tau}(x') &= -1,
\end{aligned}$$

since $S(\infty|x) = 0$ and $S(0|x) = 1$. For brownian motion, $D1 = 0$ and $D2 = D$ we have,

$$\begin{aligned}
D\partial_x^2\overline{\tau}(x) &= -1 \\
\partial_x^2\overline{\tau}(x) + \frac{1}{D} &= 0,
\end{aligned}$$

and we recover the results of problem 1.

7. Let $u = \partial_x\overline{\tau}(x)$, then

$$\frac{D_1}{D_2}u + \partial_x u = -\frac{1}{D_2},$$

which admits the integrating factor $\phi(x) = \exp\left(\int^x \frac{D_1(y)}{D_2(y)}dy\right)$, such that

$$\partial_x(\phi(x)u(x)) = -\frac{\phi(x)}{D_2(x)}. \tag{10}$$

Integrating once, solving for $u(x) = \partial_x\overline{\tau}(x)$ and integrating again to get $\overline{\tau}(x)$, one finds

$$\overline{\tau}(x) = \int_x^{C_1} dz \frac{1}{\phi(z)} \int_{C_2}^z dy \frac{\phi(y)}{D_2(y)}. \tag{11}$$

with arbitrary constants of integration C_1, C_2. By the boundary conditions, one obtains $C_1 = b$ and $C_2 = a$, which is required for $\overline{\tau}(b) = 0$ and $\partial_x\overline{\tau}(a) = 0$.

8. For $D_1(x) = -\lambda x$, $\lambda > 0$, $D_2(x) = D = const.$, we find $\phi(x) = e^{-\frac{\lambda x^2}{2D}}$, and thus

$$\overline{\tau}(x=0) = \frac{1}{D}\int_0^b e^{\frac{\lambda z^2}{2D}} dz \int_0^z e^{-\frac{\lambda y^2}{2D}} dy.$$

Make the changes of variable $u^2 = \frac{\lambda y^2}{2D}$ and $v^2 = \frac{\lambda z^2}{2D}$. This leads to

$$\frac{2}{\lambda}\int_0^\eta e^{v^2} dv \int_0^v e^{-u^2} du, \tag{12}$$

where $\eta^2 = \frac{\lambda b^2}{2D}$. For large η, integral over v is dominated by contributions from $v \approx \eta$, since other contributions are exponentially small compared to e^{η^2}. Hence, it is reasonable to approximate $\int_0^v e^{-u^2} du \approx \int_0^\eta e^{-u^2} du \overset{\eta\to\infty}{\longrightarrow} \frac{\sqrt{\pi}}{2}$ and thus

$$\overline{\tau}(x) \sim \frac{\sqrt{\pi}}{\lambda} \underbrace{\int_0^\eta e^{v^2} dv}_{\sim \frac{e^{\eta^2}}{2\eta}} \sim \frac{\sqrt{\pi}}{2\lambda}\frac{e^{\eta^2}}{\eta}, \tag{13}$$

where we used the given leading-order asymptotic expansion for the integral. To derive the asymptotic behaviour, one may split the integral into a part from 0 to an intermediate value, e.g. 1, and from 1 to η. Then integrate by parts in latter integral, using that $e^{v^2} = \frac{1}{2v}\frac{d(\exp(v^2))}{dv}$. One thus finds that

$$\int_0^\eta e^{v^2} dv = \int_0^1 e^{v^2} dv - e/2 + \frac{e^{\eta^2}}{2\eta} + \underbrace{\int_1^\eta \frac{e^{v^2}}{2v^2} dv}_{=R(\eta)} \tag{14}$$

It is not hard to show using l'Hopital's rule that $R(\eta) \ll e^{\eta^2}/(2\eta)$ for $\eta \to \infty$, i.e that $\lim_{\eta\to\infty} R(\eta)/(e^{\eta^2}/(2\eta)) = 0$. This proves the given asymptotic expansion of the integral. Physically, the limit $\eta^2 = \lambda b^2/(2D) = (b^2/(2D))/(\lambda^{-1}) \gg 1$ means that the time scale associated with stochastic diffusion is much greater than the time scale associated with deterministic drift. In terms of dimensional analysis, this means that we expect the time $\overline{\tau}$ to scale as λ for a fixed value of the dimensionless parameter η. However, the solution still depends on the D through η and increases rapidly as b is increased for given λ, D or as D is decreased for given λ, b.

9. For a given double-well potential $V(x)$ as described in the problem statement, with $D_1 = -\frac{dV}{dx}$, and $D_2 = D = const.$ as depicted in figure 1,

$$\phi(x) = e^{-V(x)/D}.$$

Hence,

$$\overline{\tau}(x) = \frac{1}{D}\int_{x_0}^{b} dz e^{V(z)/D} \int_{-\infty}^{z} dy e^{-V(y)/D}.$$

Again, the integrals are dominated by contributions close to the maximum of the integrand. Hence,

$$\overline{\tau}(x) \approx \frac{1}{D}\left(\int_{x_0}^{b} dz e^{V(z)/D}\right)\left(\int_{-\infty}^{x_1} dy e^{-V(y)/D}\right).$$

Since $V(z)$ is maximum at x_1 in the given integration interval and $-V(y)$ is maximum at x_0 in the given integration interval, the saddle point approximation can be used for $V(x_*)/D \ll 1$ ("potential barrier high compared to noise amplitude"), where x_* is the location of the maximum, identifying $f = V/V(x_*)$, which gives

$$\overline{\tau}(x) \approx \frac{1}{D}\sqrt{\frac{2\pi D}{|V''(x_1)|}} e^{V(x_1)/D} \sqrt{\frac{2\pi D}{|V''(x_0)|}} e^{-V(x_0)/D} = \frac{2\pi}{\sqrt{V''(x_0)|V''(x_1)|}} e^{\Delta V/D}. \tag{15}$$

Note that D is related to temperature by the fluctuation-dissipation theorem. Hence, the escape time of an overdamped particle (think: a particle immersed in honey) from a potential well depends exponentially on the height of the potential barrier to be crossed, divided by the temperature of the honey! This is the Arrhenius law!