Minicourse

Exit time problems for swimming microorganisms

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28 May – 13 June, 2018

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Lecture 1

Drift and diffusion

1.1 Walls and exits

A particle starts at $(\boldsymbol{x}_0, t_0)$ inside a bounded, connected domain Ω. The particle is subject to a drift $\boldsymbol{u}(\boldsymbol{x}, t)$, which may include both a background fluid motion and a swimming velocity. The particle also undergoes diffusion with diffusivity D.

The domain boundary $\partial\Omega$ is divided into two types of regions: walls ($\partial\Omega_\mathrm{w}$) and exit regions ($\partial\Omega_\mathrm{e}$). The walls are impermeable to particles, though the drift might have a component through the wall. For the flow part of the drift, we can interpret this as walls having gratings that prevent particles from escaping the domain Ω. For the swimmer velocity part, this allows a swimmer to butt its head up against a rigid wall, without exiting.

We would like to understand what happens as we release particles at different initial locations in the domain. This is best expressed in terms of the transition probability density $p(\boldsymbol{x}, t \,|\, \boldsymbol{x}_0, t_0)$, which gives the probability density function (pdf) of finding a stochastic particle at $(\boldsymbol{x}, t)$ if it was initially at $(\boldsymbol{x}_0, t_0)$. That is

$$p(\boldsymbol{x}, t \,|\, \boldsymbol{x}_0, t_0)\,\mathrm{d}\boldsymbol{x} = \mathbb{P}(\boldsymbol{X}_t \in [\boldsymbol{x}, \boldsymbol{x} + \mathrm{d}\boldsymbol{x}) \,|\, \boldsymbol{X}_{t_0} = \boldsymbol{x}_0). \tag{1.1}$$

This probability density satisfies the Fokker–Planck equation (also called the Kolmogorov forward equation)

$$\partial_t p + \mathcal{L}p = 0, \quad t > t_0, \tag{1.2a}$$

with boundary conditions

$$\hat{\boldsymbol{n}} \cdot (\boldsymbol{u}p - D\nabla p)|_{\partial\Omega_\mathrm{w}} = 0, \tag{1.2b}$$

$$p|_{\partial\Omega_\mathrm{e}} = 0, \tag{1.2c}$$

and initial condition

$$p(\boldsymbol{x}, t_0 \,|\, \boldsymbol{x}_0, t_0) = \delta(\boldsymbol{x} - \boldsymbol{x}_0). \tag{1.2d}$$

Here the vector $\hat{\boldsymbol{n}}(\boldsymbol{x})$ is the outward unit normal at the surface, and the differential operator $\mathcal{L}$ is defined by[1]

$$\mathcal{L}g \coloneqq \nabla \cdot (\boldsymbol{u}g - D\nabla g) \tag{1.3}$$

for any differentiable function g. The wall boundary condition (1.2b) says the the *normal flux* of particles is zero at the walls. The exit boundary condition (1.2c) says that if a particle touches an exit, then its probability of being in the domain is immediately set to zero. The initial condition (2.12d) says that at $t = t_0$ the probability of finding the particle at $\boldsymbol{x}_0$ is one.

In this entire derivation, the diffusivity D could in principle be a function of $\boldsymbol{x}$ and t, though in practice we will never do this, and in some cases it does present some nontrivial challenges of interpretation [14]. More importantly, D could be a symmetric *tensor*, whose principal axes reflect different strengths of diffusivity according to direction. In this case we simply replace expressions such as $D\nabla p$ by $\mathbb{D} \cdot \nabla p$.

We will be presenting many examples througout. Most of the time, these examples will assume a constant scalar diffusivity D, and an initial time $t_0 = 0$, unless otherwise noted.

Example 1.1 (interval with diffusion only)**.** Set $\boldsymbol{u} = 0$ and take $\Omega = [0, 1]$, with $\partial\Omega_{\mathrm{w}} = \{0\}$ and $\partial\Omega_{\mathrm{e}} = \{1\}$. The Fokker–Planck equation (1.2) is then

$$\partial_t p = D\,\partial_x^2 p, \qquad \partial_x p|_{x=0} = p|_{x=1} = 0 \tag{1.4}$$

with $p(x, 0 \,|\, x_0, 0) = \delta(x - x_0)$. This is the standard heat equation in an interval, with solution [4]

$$p(x, t \,|\, x_0, 0) = 2 \sum_{n \text{ odd}} \cos(n\pi x/2) \cos(n\pi x_0/2)\, \mathrm{e}^{-(n\pi/2)^2 Dt}. \tag{1.5}$$

Figure 1.1 shows a plot of this pdf at different times. Ultimately the solution has the profile $\cos(\pi x/2)$, corresponding to the slowest-decaying eigenfunction.

Example 1.2 (interval with drift only)**.** Use the same setting as in Example (1.1), but with $\boldsymbol{u} = u\,\hat{\boldsymbol{x}}$ and $D = 0$. The Fokker–Planck equation (1.2) is then

$$\partial_t p = -u\,\partial_x p, \qquad p|_{x=0} = p|_{x=1} = 0 \tag{1.6}$$

[1] In stochastic calculus $\mathcal{L}$ is (minus) the adjoint of the *generator* for the process.

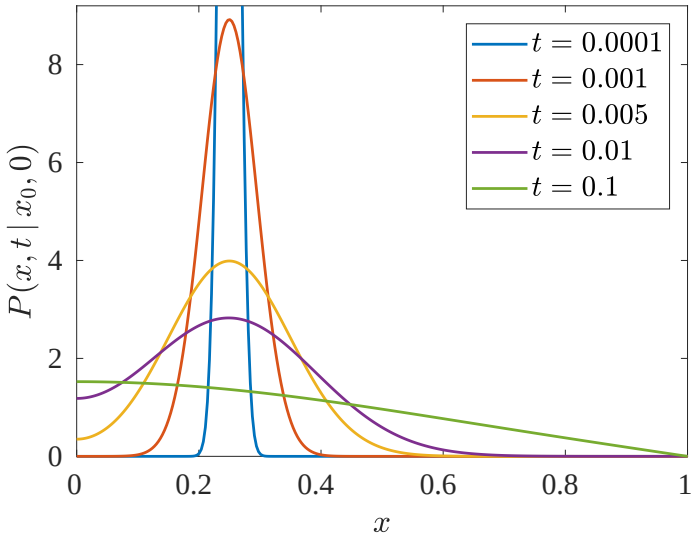


Figure 1.1: The pdf (1.5) for $D = 1$ and $x_0 = 0.25$, plotted at different times.

with $p(x, 0 \mid x_0, 0) = \delta(x - x_0)$. The solution to this is $\delta(x - x_0 - ut)$, which happens to satisfy the boundary conditions in (1.6), at least for a while, but we cannot possibly apply both conditions to this first-order equation. Intuitively, in this simple case the particles exits at $t = (1 - x_0)/u$ for $u > 0$. For $u < 0$ the particle reaches the left side in time $x_0/|u|$, and then just sits there. In general, in the absence of diffusion we only get to apply boundary conditions at the outflow regions, and for $u < 0$ it is pretty clear that (1.6) is not the appropriate limit as $D \to 0$.

Example 1.3 (interval with drift and diffusion)**.** Again, use the same setting as in Example (1.1), but with $\boldsymbol{u} = u\,\hat{\boldsymbol{x}}$ and $D = 1$. The Fokker–Planck equation (1.2) is then

$$\partial_t p = -u\,\partial_x p + \partial_x^2 p, \qquad u\,p - \partial_x p|_{x=0} = p|_{x=1} = 0 \tag{1.7}$$

with $p(x, 0 \mid x_0, 0) = \delta(x - x_0)$. The solution to this is significantly more involved than for Example 1.1, so we devote the next section to it (Section 1.2. The final result is

$$\begin{aligned} p(x, t \mid x_0, 0) = {} & 2\mathrm{e}^{u\,(x-x_0)/2}\,\frac{2\nu_0 \cosh \nu_0 x_< + u \sinh \nu_0 x_<}{(2+u)\cosh \nu_0 + 2\nu_0 \sinh \nu_0}\,\sinh \nu_0 (1 - x_>)\,\mathrm{e}^{-(u^2/4 - \nu_0^2)\,t} \\ & - 2\sum_{n=1}^{\infty} \mathrm{e}^{u\,(x-x_0)/2}\,\frac{2\omega_n \cos \omega_n x_< + u \sin \omega_n x_<}{(2+u)\cos \omega_n - 2\omega_n \sin \omega_n}\,\sin \omega_n (1 - x_>)\,\mathrm{e}^{-(\omega_n^2 + u^2/4)\,t}. \end{aligned} \tag{1.8}$$

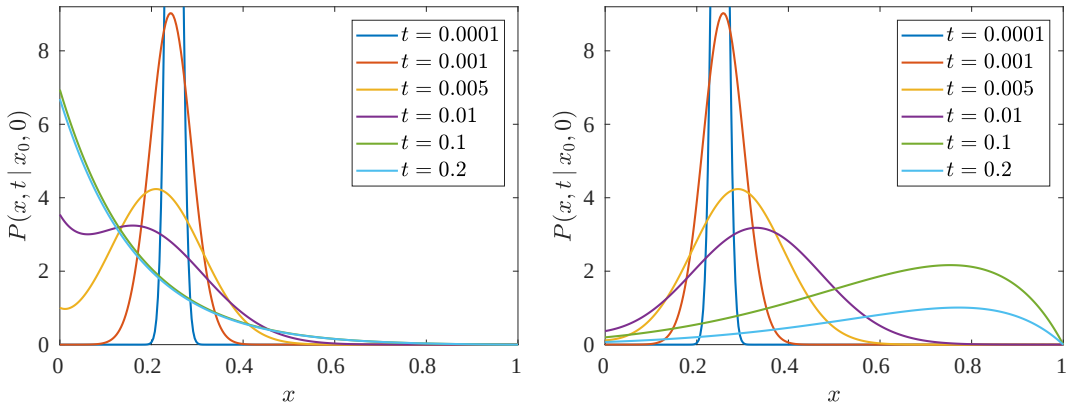


Figure 1.2: The pdf (1.8) with $x_0 = 0.25$, plotted at different times for (a) $u = -4$; (b) $u = 4$.

where $x_< = \min(x, x_0)$ and $x_> = \max(x, x_0)$. The eigenvalue ν_0 is the single real positive to

$$\tanh \nu_0 = (-2/u)\, \nu_0, \qquad u < -2, \tag{1.9}$$

which only exists for $u < -2$, and the ω_n are the the real positive solutions to

$$\tan \omega_n = (-2/u)\, \omega_n, \qquad n = 1, 2, 3, \ldots. \tag{1.10}$$

The exponentials in (1.8) are all decaying. For $u > 0$, the slowest-decaying eigenfunction can develop a 'bump' (Fig. 1.2(a) and (1.3)). For $u < 0$ the particles get pushed along the left wall, but diffusion always allows them to slowsly leak away (Fig. 1.2(b)). As $u \to -\infty$ we can predict this slow leakage rate by expanding the tanh for large argument in (1.9) to obtain

$$\nu_0 = -\tfrac{1}{2}u + u\, \mathrm{e}^{u} + \ldots \qquad u \to -\infty \tag{1.11}$$

which translates to an exponentially-small decay rate in the first term of (1.8) equal to

$$\mathrm{e}^{-(u^2/4 - \nu_0^2)\, t} = \mathrm{e}^{-u^2 \mathrm{e}^u t} + \mathrm{O}(\mathrm{e}^{-u^2 \mathrm{e}^{2u} t}), \qquad u \to -\infty. \tag{1.12}$$

Thus, diffusion allows the particles to leak very slowly against the prevailing leftward drift.

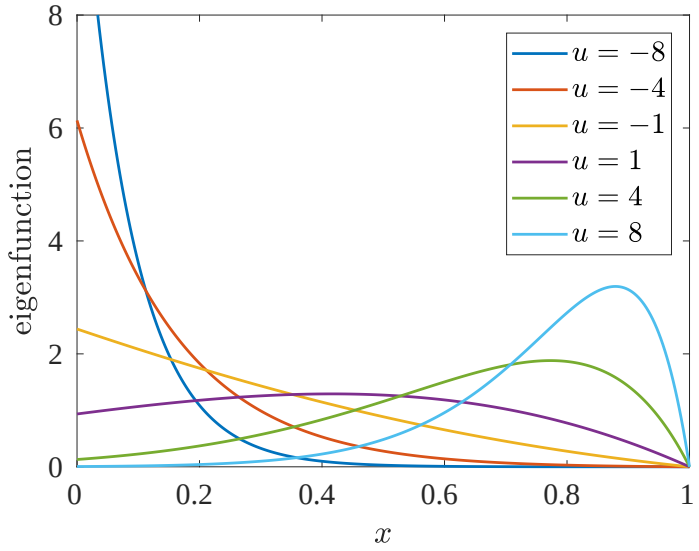


Figure 1.3: The normalized slowest-decaying eigenfunction for (1.8) with $x_0 = 0.25$ and different values of u.

1.2 Solving the advection–diffusion equation with Laplace transforms

To solve (1.7), start by taking its Laplace transform:

$$-\partial_x^2 \widetilde{p} + u\,\partial_x \widetilde{p} + s\widetilde{p} = \delta(x - x_0), \tag{1.13}$$

where $\widetilde{p}(x, s \,|\, x_0, 0)$ is

$$\widetilde{p}(x, s \,|\, x_0, 0) = \int_0^\infty p(x, t \,|\, x_0, 0)\, \mathrm{e}^{-st}\, \mathrm{d}t. \tag{1.14}$$

To the left and right of x_0 the solution to (1.13) is a linear combination of $\mathrm{e}^{\alpha_\pm x}$ with

$$\alpha_\pm = \tfrac{1}{2}u \pm \nu(s), \qquad \nu(s) \coloneqq \sqrt{s + \tfrac{1}{4}u^2}. \tag{1.15}$$

We create a composite solution that satisfies the boundary conditions in (1.7):

$$\widetilde{p}(x, s \,|\, x_0, 0) = \begin{cases} A_< \,\mathrm{e}^{ux/2}\left(u \sinh \nu x + 2\nu \cosh \nu x\right), & x < x_0; \\ A_> \,\mathrm{e}^{ux/2} \sinh(\nu(1 - x)), & x > x_0. \end{cases} \tag{1.16}$$

To determine $A_>$ and $A_<$ we impose continuity of $\widetilde{p}$ at $x = x_0$, and specify a jump in its derivative according to (1.13):

$$[\partial_x \widetilde{p}]_{x_0^-}^{x_0^+} = -1\,. \tag{1.17}$$

We find

$$\widetilde{p}(x, s \,|\, x_0, 0) = \mathrm{e}^{u\,(x-x_0)/2}\,\frac{2\nu\cosh\nu x_< + u\sinh\nu x_<}{\nu(2\nu\cosh\nu + u\sinh\nu)}\,\sinh\nu(1-x_>) \tag{1.18}$$

where $x_< = \min(x, x_0)$ and $x_> = \max(x, x_0)$.

We now recover the solution by taking the inverse Laplace transform of (1.18):

$$p(x, t \,|\, x_0, 0) = \frac{1}{2\pi\mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \widetilde{p}(x, s \,|\, x_0, 0)\,\mathrm{e}^{st}\,\mathrm{d}s \tag{1.19}$$

where c is a real constant that puts the contour to the right of all poles. The relevant features of (1.18) are the singularities in the complex plane where $2\nu\cosh\nu + u\sinh\nu = 0$, and the branch cut in $\nu(s)$ at $s = -u^2/4$. (The apparent singularity at $\nu = 0$ is removable.)

Along the branch cut, take $s_\pm = \frac{1}{4}u^2\left(-1 + \xi\,\mathrm{e}^{\pm\mathrm{i}\pi}\right)$, with $\xi \geq 0$ real and $\nu(s_\pm) = \frac{1}{2}u\sqrt{\xi\,\mathrm{e}^{\pm\mathrm{i}\pi}} = \frac{1}{2}u\sqrt{\xi}\,\mathrm{e}^{\pm\mathrm{i}\pi/2} = \pm\frac{1}{2}\mathrm{i}u\sqrt{\xi}$. The two sides of the branch cut will thus cancel, since $\widetilde{p}$ is an even function of ν. We conclude that the branch cut makes no contribution to the inverse Laplace transform.

Let ν_n, $n = 0, 1, 2, 3, \ldots$, correspond to the poles of (1.18) in the complex plane; then the inverse transform (1.19) can be evaluated as a sum over residues

$$p(x, t \,|\, x_0, 0) = 2\sum_{n=0}^{\infty} \mathrm{e}^{u\,(x-x_0)/2}\,\frac{2\nu_n\cosh\nu_n x_< + u\sinh\nu_n x_<}{(2+u)\cosh\nu_n + 2\nu_n\sinh\nu_n}\,\sinh\nu_n(1-x_>)\,\mathrm{e}^{(\nu_n^2 - u^2/4)\,t}. \tag{1.20}$$

Here we sum over just one member of each pair of singularities at $\pm\nu_n$, since these correspond to a single pole for $s = \nu^2 - \frac{1}{3}u^2$. We also took care to divide by $\nu'(s) = 1/2\nu$ since the integration variable is s, not ν.

The poles are located at

$$\tanh\nu = -\frac{2}{u}\,\nu. \tag{1.21}$$

There is one positive real solutions ν_0 only if $0 < -2/u < 1$, or $u < -2$. This corresponds to a strong flow to the *left*, away from the exit. From (1.15), the rate constant of that solution is recovered from

$$s_0 = \nu_0^2 - \tfrac{1}{4}u^2 = \tfrac{1}{4}u^2(\tanh^2\nu_0 - 1) < 0 \tag{1.22}$$

which means that $s_0 < 0$ for $u < -2$, indicating decay as required.

Now let $\nu = \mathrm{i}\omega$ in (1.21):

$$\tan\omega = -\frac{2}{u}\,\omega\,. \tag{1.23}$$

This clearly has an infinite number of positive real solutions ω_n, $n = 1, 2, 3, \ldots$. These give exponential time dependence $\mathrm{e}^{s_n t}$ with

$$s_n = -\omega_n^2 - \tfrac{1}{4}u^2 < 0 \tag{1.24}$$

again corresponding to decaying solutions. Note that for $u < -2$ the real solution to (1.21) is always the slowest-decaying eigenmode, and its decay rate approaches zero as $u \to -\infty$. We will discuss this further below.

Splitting the sum in (1.20) between real ν_0 and imaginary $\nu_n = \mathrm{i}\omega_n$ for $n \geq 1$, we can write the full solution as

$$\begin{aligned} p(x,t\,|\,x_0,0) = {} & 2\mathrm{e}^{u\,(x-x_0)/2}\,\frac{2\nu_0\cosh\nu_0 x_< + u\sinh\nu_0 x_<}{(2+u)\cosh\nu_0 + 2\nu_0\sinh\nu_0}\,\sinh\nu_0(1-x_>)\,\mathrm{e}^{-(u^2/4-\nu_0^2)\,t} \\ & - 2\sum_{n=1}^{\infty}\mathrm{e}^{u\,(x-x_0)/2}\,\frac{2\omega_n\cos\omega_n x_< + u\sin\omega_n x_<}{(2+u)\cos\omega_n - 2\omega_n\sin\omega_n}\,\sin\omega_n(1-x_>)\,\mathrm{e}^{-(\omega_n^2+u^2/4)\,t}, \end{aligned} \tag{1.25}$$

which is (1.8). For $u \geq -2$ we set $\nu_0 = 0$ and the first term simply drops out.

For $u \to 0$, we have $\omega_n = (n - \frac{1}{2})\pi$ and $\cos\omega_n = 0$:

$$\begin{aligned} p(x,t\,|\,x_0,0) &= -2\sum_{n=1}^{\infty}\frac{\cos\omega_n x_<}{-\sin\omega_n}\,\sin\omega_n(1-x_>)\,\mathrm{e}^{-\omega_n^2 t} \\ &= 2\sum_{n=1}^{\infty}\cos\omega_n x_<\,\cos\omega_n x_>\,\mathrm{e}^{-\omega_n^2 t} \\ &= 2\sum_{n=1}^{\infty}\cos\omega_n x\,\cos\omega_n x_0\,\mathrm{e}^{-\omega_n^2 t} \end{aligned} \tag{1.26}$$

which is the same as (1.5), as required.

Lecture 2

The mean exit time equation

2.1 The adjoint operator

A crucial operator will be the *adjoint* of $\mathcal{L}$ with respect to the inner product

$$\langle F, G\rangle = \int_\Omega F(\boldsymbol{x})\, G(\boldsymbol{x})\,\mathrm{d}V. \tag{2.1}$$

The adjoint of $\mathcal{L}$ is computed via integration by parts, which gives rise to boundary terms:

$$\begin{aligned}\langle f, \mathcal{L}g\rangle &= \int_\Omega f\,\nabla\cdot(\boldsymbol{u}g - D\nabla g)\,\mathrm{d}V \\ &= \int_{\partial\Omega} f\,(\boldsymbol{u}g - D\nabla g)\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S + \int_{\partial\Omega} g\,D\nabla f\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S + \int_\Omega g\,\mathcal{L}^* f\,\mathrm{d}V,\end{aligned} \tag{2.2}$$

where the adjoint operator is defined

$$\mathcal{L}^* f \coloneqq -\boldsymbol{u}\cdot\nabla f - \nabla\cdot(D\nabla f)\,. \tag{2.3}$$

The function g satisfies the same boundary conditions as p in (1.2); the first boundary term in (2.2) thus vanishes on $\partial\Omega_\mathrm{w}$. Hence,

$$\langle f, \mathcal{L}g\rangle = \int_{\partial\Omega_\mathrm{e}} f\,(\boldsymbol{u}g - D\nabla g)\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S + \int_{\partial\Omega_\mathrm{w}} g\,D\nabla f\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S + \langle\mathcal{L}^* f, g\rangle. \tag{2.4}$$

We still haven't imposed any boundary conditions on f. We use this freedom to get rid of the remaining boundary terms in (2.4), which we can do by requiring

$$\hat{\boldsymbol{n}}\cdot D\nabla f|_{\partial\Omega_\mathrm{w}} = 0, \tag{2.5a}$$

$$f|_{\partial\Omega_\mathrm{e}} = 0. \tag{2.5b}$$

We refer to (2.5) as the *adjoint boundary conditions*. We thus obtain the usual adjoint relation

$$\langle f, \mathcal{L}g \rangle = \langle \mathcal{L}^* f, g \rangle \tag{2.6}$$

for all functions g obeying (1.2b)–(1.2c) and functions f obeying (2.5). Note that we left the diffusivity D in (2.5a) instead of dividing through by D, to emphasize that (2.5a) becomes vacuous when $D = 0$, and so that (2.5a) is still valid for tensorial D.

2.2 Derivation of the exit time equation

The *survival probability* of finding the particle anywhere in Ω at time t is

$$S(t \,|\, \boldsymbol{x}_0, t_0) = \int_\Omega p(\boldsymbol{x}, t \,|\, \boldsymbol{x}_0, t_0) \, \mathrm{d}V. \tag{2.7}$$

We can also interpret $S(t \,|\, \boldsymbol{x}_0, t_0)$ as the fraction of particles remaining in the domain at time t. We can find its time evolution by integrating (1.2a):

$$\partial_t S(t \,|\, \boldsymbol{x}_0, t_0) = -\int_\Omega \nabla \cdot (\boldsymbol{u}p - D\nabla p) \, \mathrm{d}V = -\int_{\partial\Omega} (\boldsymbol{u}p - D\nabla p) \cdot \hat{\boldsymbol{n}} \, \mathrm{d}S. \tag{2.8}$$

By (1.2b), the surface integral vanishes on $\partial\Omega_\mathrm{w}$, and by (1.2c) p vanishes on $\partial\Omega_\mathrm{e}$. We are left with

$$\partial_t S(t \,|\, \boldsymbol{x}_0, t_0) = \int_{\partial\Omega_\mathrm{e}} D\nabla p \cdot \hat{\boldsymbol{n}} \, \mathrm{d}S \leq 0. \tag{2.9}$$

We can see that $\partial_t S$ is nonpositive as follows. Since $p \geq 0$ inside Ω and $p = 0$ on $\partial\Omega_\mathrm{e}$, $\nabla p|_{\partial\Omega_\mathrm{e}}$ points toward the interior, and so $\nabla p \cdot \hat{\boldsymbol{n}} \leq 0$. We conclude that $\partial_t S \leq 0$, and hence the only way to lose particles is at the exit boundaries $\partial\Omega_\mathrm{e}$.

From $S(t \,|\, \boldsymbol{x}_0, t_0)$ we find the *first passage time density* $f(t \,|\, \boldsymbol{x}_0, t_0)$, which is the probability density for a particle to have first reached the boundary at time t:

$$f(t \,|\, \boldsymbol{x}_0, t_0) = -\frac{\partial S}{\partial t} \geq 0. \tag{2.10}$$

The *expected exit time* or *mean exit time* $\tau(\boldsymbol{x}_0, t_0)$ (measured from t_0) is then

$$\begin{aligned}\tau(\boldsymbol{x}_0, t_0) &= \int_{t_0}^{\infty} (t - t_0) f(t \,|\, \boldsymbol{x}_0, t_0)\, \mathrm{d}t \\ &= -\int_{t_0}^{\infty} (t - t_0)\, \frac{\partial S}{\partial t}\, \mathrm{d}t \\ &= -[(t - t_0)S]_{t_0}^{\infty} + \int_{t_0}^{\infty} S(t \,|\, \boldsymbol{x}_0, t_0)\, \mathrm{d}t \\ &= \int_{t_0}^{\infty} S(t \,|\, \boldsymbol{x}_0, t_0)\, \mathrm{d}t. \end{aligned} \tag{2.11}$$

Note that this assumes that $S(t)$ decays faster than t^{-1} as $t \to \infty$. This is fine, as p should be asymptotically equal to the slowest-decaying eigenfunction of the operator $\mathcal{L}$, and so should decay exponentially.

Our ultimate goal is to derive a PDE for $\tau(\boldsymbol{x}_0, t_0)$. But first, an aside: in Appendix 2.A, we show that $p(\boldsymbol{x}, t \,|\, \boldsymbol{x}_0, t_0)$ satisfies the Kolmogorov backward equation with respect to $(\boldsymbol{x}_0, t_0)$:

$$-\partial_{t_0} p + \mathcal{L}^*_{\boldsymbol{x}_0, t_0} p = 0, \quad t_0 < t, \tag{2.12a}$$

with the adjoint boundary conditions (2.5)

$$\hat{\boldsymbol{n}} \cdot D \nabla_{\boldsymbol{x}_0} p|_{\partial\Omega_\mathrm{w}} = 0, \tag{2.12b}$$

$$p|_{\partial\Omega_\mathrm{e}} = 0, \tag{2.12c}$$

and terminal condition

$$p(\boldsymbol{x}, t \,|\, \boldsymbol{x}_0, t) = \delta(\boldsymbol{x} - \boldsymbol{x}_0). \tag{2.12d}$$

The subscripts on $\mathcal{L}^*_{\boldsymbol{x}_0, t_0}$ and $\nabla_{\boldsymbol{x}_0}$ remind us that the derivatives are with respect to $\boldsymbol{x}_0$, and the velocity field in the operator is evaluated at $\boldsymbol{x}_0$ and t_0. The system (2.12) is ill-posed forward in time, so it must be solved *backward* in time.

Given that $p(\boldsymbol{x}, t \,|\, \boldsymbol{x}_0, t_0)$ satisfies (2.12), we act on τ with $\mathcal{L}^*_{\boldsymbol{x}_0, t_0}$:

$$\begin{aligned}\mathcal{L}^*_{\boldsymbol{x}_0, t_0} \tau(\boldsymbol{x}_0, t_0) &= \int_{t_0}^{\infty} \mathcal{L}^*_{\boldsymbol{x}_0, t_0} S(t \,|\, \boldsymbol{x}_0, t_0)\, \mathrm{d}t \\ &= \int_{t_0}^{\infty} \int_{\Omega} \mathcal{L}^*_{\boldsymbol{x}_0, t_0} p(\boldsymbol{x}, t \,|\, \boldsymbol{x}_0, t_0)\, \mathrm{d}V\, \mathrm{d}t \\ &= \int_{\Omega} \int_{t_0}^{\infty} \partial_{t_0} p\, \mathrm{d}t\, \mathrm{d}V = \int_{t_0}^{\infty} \partial_{t_0} S\, \mathrm{d}t. \end{aligned}$$

For the last term, we use

$$\partial_{t_0}\tau = \partial_{t_0}\int_{t_0}^{\infty} S(t\,|\,\boldsymbol{x}_0,t_0)\,\mathrm{d}t = -S(t_0\,|\,\boldsymbol{x}_0,t_0) + \int_{t_0}^{\infty}\partial_{t_0}S\,\mathrm{d}t \tag{2.13}$$

with $S(t_0\,|\,\boldsymbol{x}_0,t_0)=1$. We thus obtain

$$-\partial_{t_0}\tau + \mathcal{L}^*_{\boldsymbol{x}_0,t_0}\tau = 1, \quad t_0<t, \tag{2.14a}$$

$$\hat{\boldsymbol{n}}\cdot D\nabla_{\boldsymbol{x}_0}\tau|_{\partial\Omega_\mathrm{w}} = 0, \tag{2.14b}$$

$$\tau|_{\partial\Omega_\mathrm{e}} = 0, \tag{2.14c}$$

where the boundary conditions on τ are inherited from those on p in Eq. (2.12). The exit time $\tau(\boldsymbol{x}_0,t_0)$ is measured from t_0, so if the velocity field is time-independent then τ does not depend on t_0 (autonomous drift), and we can drop the $-\partial_{t_0}\tau$ term in (2.14):

$$\mathcal{L}^*_{\boldsymbol{x}_0}\tau = 1, \quad \hat{\boldsymbol{n}}\cdot D\nabla_{\boldsymbol{x}_0}\tau|_{\partial\Omega_\mathrm{w}} = 0, \quad \tau|_{\partial\Omega_\mathrm{e}} = 0. \tag{2.15}$$

Note that when dealing only with τ and not with p it is customary to drop the zero subscripts, with the understanding that $\boldsymbol{x}$ now refers to an initial position.

Appendix 2.A The backward Kolmogorov equation

The probability density must satisfy a consistency property in the form of the Chapman–Kolmogorov equation:

$$\int_\Omega p(\boldsymbol{x},t\,|\,\boldsymbol{y},s)\,p(\boldsymbol{y},s\,|\,\boldsymbol{x}_0,t_0)\,\mathrm{d}V_{\boldsymbol{y}} = p(\boldsymbol{x},t\,|\,\boldsymbol{x}_0,t_0), \qquad t_0\le s\le t. \tag{2.16}$$

This says that if we integrate over all locations at some intermediate time, we must obtain the same result, independent of the choice of intermediate time s. Take a derivative with respect to s of (2.16), then set $s=t_0$:

$$\int_\Omega \left(\partial_{t_0}p(\boldsymbol{x},t\,|\,\boldsymbol{y},t_0)\,p(\boldsymbol{y},t_0\,|\,\boldsymbol{x}_0,t_0) + p(\boldsymbol{x},t\,|\,\boldsymbol{y},t_0)\,\partial_t p(\boldsymbol{y},t_0\,|\,\boldsymbol{x}_0,t_0)\right)\,\mathrm{d}V_{\boldsymbol{y}} = 0. \tag{2.17}$$

We use the forward equation (1.2a) to replace $\partial_t p$ by $-\mathcal{L}p$, as well as $p(\boldsymbol{y},t_0\,|\,\boldsymbol{x}_0,t_0) = \delta(\boldsymbol{y}-\boldsymbol{x}_0)$:

$$\int_\Omega \left(\partial_{t_0}p(\boldsymbol{x},t\,|\,\boldsymbol{y},t_0)\,\delta(\boldsymbol{y}-\boldsymbol{x}_0) - p(\boldsymbol{x},t\,|\,\boldsymbol{y},t_0)\,\mathcal{L}_{\boldsymbol{y},t_0}p(\boldsymbol{y},t_0\,|\,\boldsymbol{x}_0,t_0)\right)\,\mathrm{d}V_{\boldsymbol{y}} = 0. \tag{2.18}$$

We then integrate the delta function and use the adjoint property (2.6):

$$\partial_{t_0} p(\boldsymbol{x}, t \,|\, \boldsymbol{x}_0, t_0) - \int_\Omega \mathcal{L}^*_{\boldsymbol{y},t_0} p(\boldsymbol{x}, t \,|\, \boldsymbol{y}, t_0)\, p(\boldsymbol{y}, t_0 \,|\, \boldsymbol{x}_0, t_0)\, \mathrm{d}V_{\boldsymbol{y}} = 0. \tag{2.19}$$

The use of the adjoint requires that $p(\boldsymbol{x}, t \,|\, \boldsymbol{x}_0, t_0)$ satisfy the adjoint boundary conditions (2.12b)–(2.12c). Finally, we again use $p(\boldsymbol{y}, t_0 \,|\, \boldsymbol{x}_0, t_0) = \delta(\boldsymbol{y} - \boldsymbol{x}_0)$ and integrate to find

$$\partial_{t_0} p(\boldsymbol{x}, t \,|\, \boldsymbol{x}_0, t_0) - \mathcal{L}^*_{\boldsymbol{x}_0,t_0} p(\boldsymbol{x}, t \,|\, \boldsymbol{x}_0, t_0) = 0, \tag{2.20}$$

which is Eq. (2.12a).

Lecture 3

Examples of exit time calculations

In this lecture we explore several examples of solutions of the mean exit time equation (2.15) for an autonomous flow:

$$\mathcal{L}^*_{\boldsymbol{x}}\tau = 1, \quad \hat{\boldsymbol{n}} \cdot D\nabla_{\boldsymbol{x}}\tau\big|_{\partial\Omega_{\rm w}} = 0, \quad \tau\big|_{\partial\Omega_{\rm e}} = 0 \tag{3.1}$$

where $\mathcal{L}^*$ was defined in (2.3)

$$\mathcal{L}^* f \coloneqq -\boldsymbol{u} \cdot \nabla f - \nabla \cdot (D\nabla f)\,. \tag{3.2}$$

and we dropped the 0 subscript on initial quantities.

3.1 Exit from a one-dimensional interval

Example 3.1 (interval with diffusion only)**.** Set $\boldsymbol{u} = 0$ and take $\Omega = [0, 1]$, with $\partial\Omega_{\rm w} = \{0\}$ and $\partial\Omega_{\rm e} = \{1\}$. The exit time equation (2.15) for $\tau(x)$ is then

$$-D\tau'' = 1, \qquad \tau'(0) = 0, \quad \tau(1) = 0. \tag{3.3}$$

This has the simple solution

$$\tau(x) = \frac{1}{2D}(1 - x^2). \tag{3.4}$$

As a check, recall that in Lecture 1 we derived the pdf (1.26):

$$p(x, t \,|\, x_0, 0) = 2\sum_{n=1}^{\infty} \cos\omega_n x \, \cos\omega_n x_0 \, \mathrm{e}^{-\omega_n^2 Dt}, \qquad \omega_n = (n - \tfrac{1}{2})\pi. \tag{3.5}$$

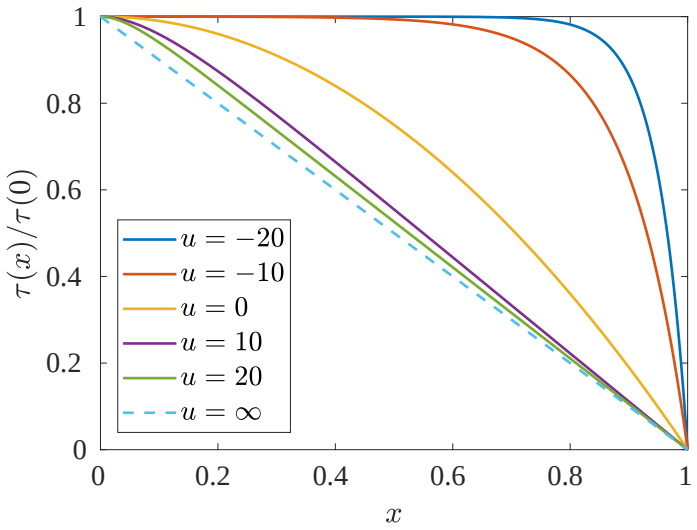


Figure 3.1: Mean exit time (3.10) for a particle, as a function of its initial position in the interval. We set $D = 1$ and the exit time is normalized by $\tau(0)$. The dashed line is the ballistic limit.

From this we can directly compute the survival probability (2.7):

$$S(t \,|\, x_0, 0) = \int_0^1 p(x, t \,|\, x_0, 0)\, \mathrm{d}x \tag{3.6}$$

$$= \frac{2}{D} \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{\omega_n} \cos \omega_n x_0 \, \mathrm{e}^{-\omega_n^2 t}, \tag{3.7}$$

and then the mean exit time (2.11):

$$\tau(x_0) = \int_0^\infty S(t \,|\, x_0, 0)\, \mathrm{d}t = \frac{2}{D} \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{\omega_n^3} \cos \omega_n x_0. \tag{3.8}$$

This is the generalized Fourier series expansion of (3.4) (with $x \to x_0$) in terms of the orthogonal functions $\cos \omega_n x_0$.

Example 3.2 (interval with drift and diffusion)**.** With the same setting as Example 3.1, we now allow for nonzero drift $\boldsymbol{u} = u\hat{\boldsymbol{x}}$; the exit time equation (2.15) is

$$-D\tau'' - u\tau' = 1, \qquad \tau'(0) = 0, \quad \tau(1) = 0 \tag{3.9}$$

with solution

$$\tau(x) = \frac{1-x}{u} + \frac{D}{u^2}\left(\mathrm{e}^{-u/D} - \mathrm{e}^{-ux/D}\right). \tag{3.10}$$

This solution is plotted in Fig. 3.1 for different values of u.

For large positive u the mean exit time is

$$\tau(x) = \frac{1-x}{u} + \mathrm{O}(\mathrm{e}^{-ux/D}), \qquad u \to \infty. \tag{3.11}$$

The quantity $(1-x)/u$ is the 'ballistic' exit time (i.e., nondiffusive), but there is a boundary layer in τ' at $x = 0$ of width D/u to ensure the wall condition $\tau'(0) = 0$.

For $u < 0$, write (3.10) as

$$\tau(x) = -\frac{1-x}{|u|} + \frac{D}{u^2}\left(\mathrm{e}^{|u|/D} - \mathrm{e}^{|u|x/D}\right), \qquad u < 0. \tag{3.12}$$

The largest term as $u \to -\infty$ is $\mathrm{e}^{|u|/D}$, independent of x. There is however a boundary layer on the right, of width $D/|u|$, to ensure the exit boundary condition $\tau(1) = 0$. This situation — an exit time independent of initial position, except in a boundary layer — will recur when we encounter the "Narrow Escape Problem." (See Example 3.4 and references such as [3, 8].) If a particle starts near the exit, inside the boundary layer, there's a good chance it will escape immediately. However, if it starts outside the boundary layer, the particle is likely to explore the interval many times over because it happens to enter the boundary layer. This wipes out any memory of the initial position of the particle, leading to a flat exit time.

3.2 Exit from a disk or sphere

Example 3.3 (disk or sphere with diffusion only)**.** Set $\boldsymbol{u} = 0$, in a disk or sphere of unit radius, and take $\partial\Omega_{\mathrm{w}} = \emptyset$ and $\partial\Omega_{\mathrm{e}} = \partial\Omega$. The mean exit time will depend only on r, so we write $\tau(r)$. Then (3.1) reads

$$-D\,\frac{1}{r^{d-1}}\left(r^{d-1}\,\tau'\right)' = 1, \qquad \tau'(0) = 0, \qquad \tau(1) = 0, \tag{3.13}$$

where $d = 2$ or 3, with solution

$$\tau(r) = \frac{1}{2Dd}\left(1 - r^2\right). \tag{3.14}$$

As intuition suggests, the mean exit time is maximized at the center of the disk or sphere.

Example 3.4 (disk or sphere with small exit, diffusion only)**.** Take a disk or sphere with a small exit at its center:

$$\Omega = \{\varepsilon < r < 1\}, \qquad \partial\Omega_{\rm e} = \{r = \varepsilon\}, \qquad \partial\Omega_{\rm w} = \{r = 1\}. \tag{3.15}$$

The outer boundary is a reflecting wall, and the exit is a disk or sphere centered on the origin. The exit time equation (3.1) with $D = 1$ is

$$-\frac{1}{r^{d-1}}\left(r^{d-1}\,\tau'\right)' = 1, \qquad \tau(\varepsilon) = 0, \qquad \tau'(1) = 0. \tag{3.16}$$

For a disk ($d = 2$), the solution is

$$\tau(r) = \tfrac{1}{4}\left(\varepsilon^2 - r^2 + 2\log(r/\varepsilon)\right). \tag{3.17}$$

As $\varepsilon \to 0$,

$$\tau(r) = \tfrac{1}{2}\log\varepsilon^{-1} + {\rm O}(\varepsilon^0), \qquad r \gtrsim \varepsilon, \tag{3.18}$$

that is, the exit time is roughly constant except in a boundary layer near the central exit. The mean exit time blows up logarithmically as $\varepsilon \to 0$.

For a sphere ($d = 3$), the solution is

$$\tau(r) = \tfrac{1}{3}(\varepsilon^{-1} - r^{-1}) + \tfrac{1}{6}(\varepsilon^2 - r^2) = \frac{1}{3\varepsilon} + {\rm O}(\varepsilon^0). \tag{3.19}$$

Again, the exit time is roughly constant except in a boundary layer of width ε near the central exit. However, here the exit time blows up as ε^{-1} with $\varepsilon \to 0$ rather than logarithmically. This reflects the fact that it is much harder in three dimensions for the particle to wander into the exit.

Example 3.5 (disk or sphere with small exit, with drift and diffusion)**.** For the same setup as in Example 3.4, the exit time equation with $D = 1$ and a symmetric flow $\boldsymbol{u}(r) = u(r)\,\hat{\boldsymbol{r}} + \ldots$ is

$$-\frac{1}{r^{d-1}}\left(r^{d-1}\,\tau'\right)' - u(r)\,\tau' = 1, \qquad \tau(\varepsilon) = 0, \qquad \tau'(1) = 0. \tag{3.20}$$

The components of $\boldsymbol{u}$ in directions perpendicular to $\hat{\boldsymbol{r}}$ do not contribute to $\boldsymbol{u}\cdot\nabla\tau$, since by symmetry the solution $\tau(r)$ depends on r only. We let $y(r) = r^{d-1}\,\tau'(r)$, so that (3.20) becomes

$$y' + u(r)\,y = -r^{d-1}, \qquad y(1) = 0. \tag{3.21}$$

Take

$$F(r) = \int u(r)\,{\rm d}r \tag{3.22}$$

to be any antiderivative of $u(r)$. Then $\mathrm{e}^{F(r)}$ is an integrating factor for (3.21):

$$\left(\mathrm{e}^{F(r)}\, y\right)' = -r^{d-1}\, \mathrm{e}^{F(r)} \tag{3.23}$$

which can then be integrated to give

$$y(r) = r^{d-1}\, \tau' = \mathrm{e}^{-F(r)} \int_r^1 t^{d-1}\, \mathrm{e}^{F(t)}\, \mathrm{d}t. \tag{3.24}$$

We divide by r^{d-1} and integrate this again from ε to r to find $\tau(r)$ with $\tau(\varepsilon) = 0$. We thus obtain the solution to (3.20) in the integral form

$$\tau(r) = \int_\varepsilon^r s^{-(d-1)}\, \mathrm{e}^{-F(s)} \int_s^1 t^{d-1}\, \mathrm{e}^{F(t)}\, \mathrm{d}t\, \mathrm{d}s\,. \tag{3.25}$$

Rewrite this as

$$\tau(r) = \int_\varepsilon^r s^{-(d-1)}\, \mathcal{G}(s)\, \mathrm{d}s, \qquad \mathcal{G}(s) := \mathrm{e}^{-F(s)} \int_s^1 t^{d-1}\, \mathrm{e}^{F(t)}\, \mathrm{d}t\,. \tag{3.26}$$

Unless $u(r)$ is singular at the origin, $\mathcal{G}(s)$ will have a Taylor series expansion at $s = 0$:

$$\mathcal{G}(s) = \mathcal{G}(0)\,(1 - u(0)s) + \mathrm{O}(s^2). \tag{3.27}$$

The integral for $\tau(r)$ in (3.26) will then be dominated by the singularity $s^{-(d-1)}$ as $\varepsilon \to 0$:

$$\tau(r) = \mathcal{G}(0) \left(\int_\varepsilon^r s^{-(d-1)}\, \mathrm{d}s - u(0) \int_\varepsilon^r s^{-d+2}\, \mathrm{d}s \right) + \dots \tag{3.28}$$

In particular, for $d = 2$ or 3:

$$\tau(r) = \mathcal{G}(0) \times \begin{cases} \log(r/\varepsilon) - u(0)\,(r - \varepsilon) + \mathrm{O}(\varepsilon^2, r^2), & d = 2; \\ \varepsilon^{-1} - r^{-1} - u(0) \log(r/\varepsilon) + \mathrm{O}(\varepsilon, r), & d = 3. \end{cases} \tag{3.29}$$

As $\varepsilon \to 0$, $\tau(r)$ becomes independent of r except in a small boundary layer of thickness ε near the exit, in a manner very similar to Example 3.4. The coefficient can be regarded as a kind of 'effective diffusivity'

$$D_{\text{eff}} = D/\mathcal{G}(0)d \tag{3.30}$$

which measures the enhancement or suppression of the exit time by the flow. Note that $\mathcal{G}(0) = 1/d$ for $u \equiv 0$, so (3.30) reduces to D in the absence of flow.

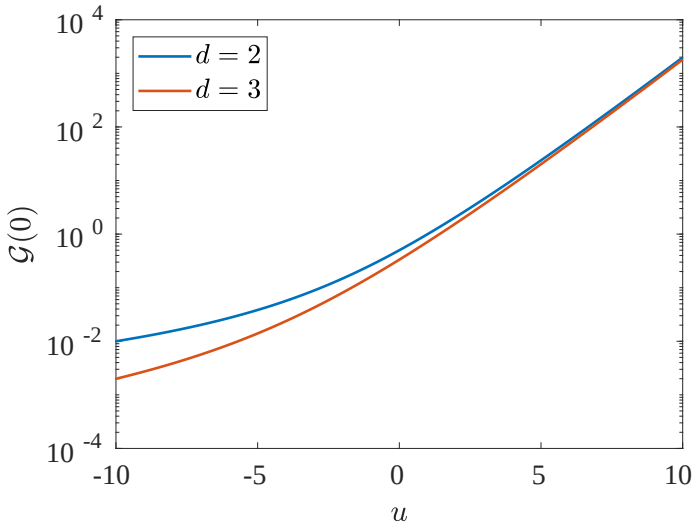


Figure 3.2: The function $\mathcal{G}(0)$ for the case $u = \text{const.}$, as given by Eq. (3.31).

For the case $u = \text{const.}$, we have

$$\mathcal{G}(0) = (-u)^{-d}\left\{\Gamma(d) - \Gamma(d,-u)\right\} = \begin{cases} \left((u-1)\,\mathrm{e}^u + 1\right)/u^2, & d = 2; \\ \left((u^2-2u+2)\,\mathrm{e}^u - 2\right)/u^3, & d = 3. \end{cases} \tag{3.31}$$

These are plotted in Fig. 3.2. For positive u there is an exponential suppression of the exit time, $\mathcal{G}(0) \sim \mathrm{e}^u/u$ independent of d, consistent with the flow pushing particles away from the exit. For negative u there is an enhancement. We get the asymptotic result

$$\mathcal{G}(0) \sim \frac{(d-1)!}{|u|^d}, \qquad u \to -\infty, \tag{3.32}$$

or from (3.30)

$$D_{\text{eff}} \sim D\,|u|^d/d!\,, \qquad u \to -\infty. \tag{3.33}$$

This suggests an enhancement that can become arbitrarily large, but this is a figment of taking small ε first.

Lecture 4

The swimming Brownian needle

4.1 Basic equation

We call a needle an infinitely thin segment of length ℓ. We will confine ourselves to two dimensions. We define a coordinate X to be along the length of the needle, with positive X corresponding to the 'head,' and Y the perpendicular direction to X. These are relative coordinates defined in the frame of the needle, or 'body frame.' The coordinates x and y are the absolute 'lab frame' coordinates.

The needle moves due to diffusion of its center of mass, and its angle θ with respect to the absolute horizontal also undergoes diffusion. The needle is propelled at some speed U along its long direction, in the positive X direction.

The basic stochastic differential equation (SDE) for the swimming Brownian needle are inspired by [8, p. 235]. We add to their formulation a drift term in the X direction in the needle frame:

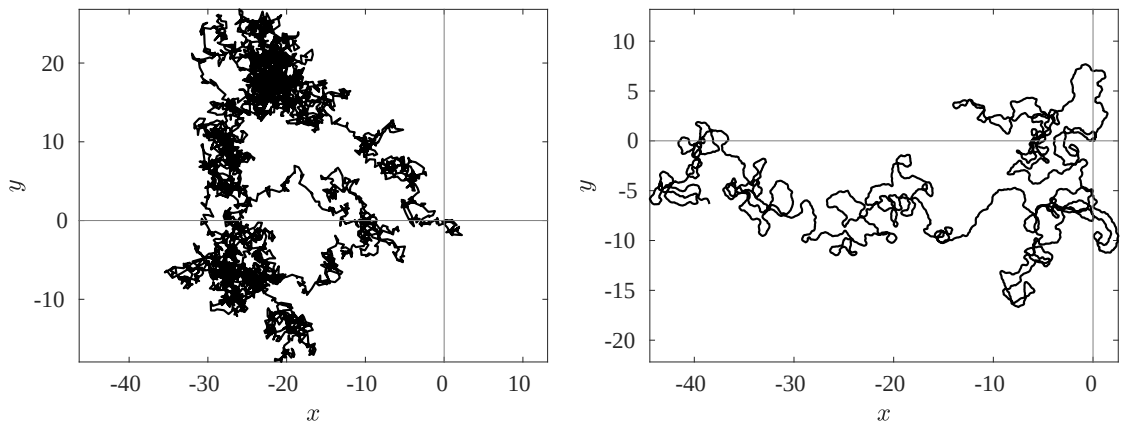
$$\mathrm{d}X = U\,\mathrm{d}t + \sqrt{2D_X}\,\mathrm{d}W_1\,; \tag{4.1a}$$

$$\mathrm{d}Y = \sqrt{2D_Y}\,\mathrm{d}W_2\,; \tag{4.1b}$$

$$\mathrm{d}\theta = \sqrt{2D_\theta}\,\mathrm{d}W_3\,. \tag{4.1c}$$

Here $\mathrm{d}X$ is the change in the needle's position in its long direction, $\mathrm{d}Y$ in the perpendicular direction, and $\mathrm{d}\theta$ the change to its angle. The increments $(\mathrm{d}X, \mathrm{d}Y)$ in body frame coordinates are related to those in lab frame coordinates $(\mathrm{d}x, \mathrm{d}y)$ by a rotation:

$$\begin{pmatrix} \mathrm{d}X \\ \mathrm{d}Y \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \mathrm{d}x \\ \mathrm{d}y \end{pmatrix}. \tag{4.2}$$



(a) (b)

Figure 4.1: (a) Sample path for a purely Brownian needle ($D_X = D_Y = 1, U = D_\theta = 0$) starting from the origin, and (b) for a swimming Brownian needle ($D_X = D_Y = 0$, $U = D_\theta = 1$). The swimming case is much smoother-looking.

We apply the rotation (4.2) to the SDEs (4.1) to obtain the Itô stochastic equations[1]

$$\mathrm{d}x = \Big(U(x,y,t)\,\mathrm{d}t + \sqrt{2D_X}\,\mathrm{d}W_1\Big)\cos\theta - \sin\theta\,\sqrt{2D_Y}\,\mathrm{d}W_2\,; \tag{4.3a}$$

$$\mathrm{d}y = \Big(U(x,y,t)\,\mathrm{d}t + \sqrt{2D_X}\,\mathrm{d}W_1\Big)\sin\theta + \cos\theta\,\sqrt{2D_Y}\,\mathrm{d}W_2\,; \tag{4.3b}$$

$$\mathrm{d}\theta = \sqrt{2D_\theta}\,\mathrm{d}W_3\,. \tag{4.3c}$$

These can be rewritten in matrix form as

$$\begin{pmatrix}\mathrm{d}x\\ \mathrm{d}y\\ \mathrm{d}\theta\end{pmatrix} = \boldsymbol{\mu}\,\mathrm{d}t + \upsigma\cdot\begin{pmatrix}\mathrm{d}W_1\\ dW_2\\ dW_3\end{pmatrix}, \tag{4.4}$$

with

$$\boldsymbol{\mu} = \begin{pmatrix}U\cos\theta\\ U\sin\theta\\ 0\end{pmatrix}, \qquad \upsigma = \begin{pmatrix}\sqrt{2D_X}\,\cos\theta & -\sqrt{2D_Y}\,\sin\theta & 0\\ \sqrt{2D_X}\,\sin\theta & \sqrt{2D_Y}\,\cos\theta & 0\\ 0 & 0 & \sqrt{2D_\theta}\end{pmatrix}. \tag{4.5}$$

[1]Here we are avoiding the thorny modeling issue of interpretation of the SDE as Itô, Stratonovich, or something else. This issue goes away in our simplified equation (4.8), which has constant diffusivity. See [13, 14] for a lot more on this subtle point.

The Fokker–Planck equation for the probability density $p(x, y, \theta, t)$ is then

$$\partial_t p = -\partial_{x_i} \left(\mu_i(x, y, \theta, t)\, p\right) + \partial^2_{x_i x_j} \left(D_{ij}(x, y, \theta)\, p\right) \tag{4.6}$$

with

$$[D_{ij}] = \mathbb{D} = \tfrac{1}{2}\sigma\sigma^T = \begin{pmatrix} D_X \cos^2\theta + D_Y \sin^2\theta & \frac{1}{2}(D_X - D_Y)\sin 2\theta & 0 \\ \frac{1}{2}(D_X - D_Y)\sin 2\theta & D_X \sin^2\theta + D_Y \cos^2\theta & 0 \\ 0 & 0 & D_\theta \end{pmatrix}. \tag{4.7}$$

We thus have an example of a system in which the diffusivity is both a tensor and depends on one of the coordinates, here θ, though this dependence goes away when $D_X = D_Y$. However, we can effect a tremendous simplification: the problem is still interesting even if we set $D_X = D_Y = 0$, since the needle will still swim throughout the entire domain by varying its direction. (See Fig. 4.1 for typical paths in the diffusive and swimming case.) The Fokker–Planck equatoin (4.6) then simplifies to

$$\partial_t p = -\partial_x(U\cos\theta\, p) - \partial_y(U\sin\theta\, p) + D_\theta\, \partial^2_{\theta\theta}\, p\,. \tag{4.8}$$

For any volume Ω we have

$$\begin{aligned} \partial_t \int_\Omega p \, \mathrm{d}V &= -\int_\Omega \left\{\partial_x(U\cos\theta\, p) + \partial_y(U\sin\theta\, p) + D_\theta\, \partial^2_{\theta\theta}\, p\right\} \mathrm{d}V \\ &= -\int_\Omega \nabla_{x,y,\theta} \cdot (U\cos\theta\, p\,,\, U\sin\theta\, p\,,\, D_\theta\, \partial_\theta p)\, \mathrm{d}V \\ &= -\int_{\partial\Omega} (U\cos\theta\, p\,,\, U\sin\theta\, p\,,\, D_\theta\, \partial_\theta p) \cdot \hat{\boldsymbol{n}}\, \mathrm{d}S. \end{aligned}$$

Thus, on the reflecting (wall) parts of the boundary we require

$$(U\cos\theta\, p\,,\, U\sin\theta\, p\,,\, D_\theta\, \partial_\theta p) \cdot \hat{\boldsymbol{n}} = 0, \quad \text{on} \quad \partial\Omega_{\mathrm{w}} \tag{4.9}$$

where $\hat{\boldsymbol{n}}$ is the outer unit normal to the boundary.

The mean exit time equation corresponding to (4.8) is

$$U\cos\theta\, \partial_x\tau + U\sin\theta\, \partial_y\tau + D_\theta\, \partial^2_{\theta\theta}\, \tau = -1\,. \tag{4.10}$$

We will return later to this equation. For now, in the next Section, we'd like to attack the SDE directly in the case where there are no boundaries.

4.2 Solving the SDE in an infinite domain

Let's solve (4.3) with $D_X = D_Y = 0$ and U constant, for the case where there are no exits or walls and $\Omega = \mathbb{R}^2 \times [-\pi, \pi]$:

$$\mathrm{d}x = U\cos\theta(t)\,\mathrm{d}t\,; \tag{4.11a}$$

$$\mathrm{d}y = U\sin\theta(t)\,\mathrm{d}t\,; \tag{4.11b}$$

$$\mathrm{d}\theta = \sqrt{2D_\theta}\,\mathrm{d}W_t\,. \tag{4.11c}$$

(We have altered the notation a bit: the time-dependence is indicated by a subscript on $\mathrm{d}W_t$, since there is now only one Brownian motion.) Change this to the dimensionless variables $t' = 2D_\theta t$ and $\boldsymbol{x}' = (2D_\theta/U)\boldsymbol{x}$:

$$\mathrm{d}x' = \cos\theta(t')\,\mathrm{d}t'\,; \tag{4.12a}$$

$$\mathrm{d}y' = \sin\theta(t')\,\mathrm{d}t'\,; \tag{4.12b}$$

$$\mathrm{d}\theta = \mathrm{d}W_{t'}\,, \tag{4.12c}$$

so that now W_t is standard Brownian motion. We drop the primes in (4.12). We can immediately solve for $\theta(t) = \theta_0 + W_t$ and then find an integral form for $\boldsymbol{x}(t)$:

$$\boldsymbol{x}(t) = \boldsymbol{x}_0 + \int_0^t \hat{\boldsymbol{r}}(\theta_0 + W_s)\,\mathrm{d}s, \qquad \hat{\boldsymbol{r}}(\theta) = \begin{pmatrix}\cos\theta\\ \sin\theta\end{pmatrix}. \tag{4.13}$$

The solution (4.13) is exact, but is not yet very useful. One thing we can do is use it to compute expectations of $\boldsymbol{x}(t)$ and its moments. To simplify the calculation from here, let's set $\boldsymbol{x}_0 = \theta_0 = 0$ and rotate the answer at the end.

Expectations of functions of W_t are computed using the Gaussian heat kernel,

$$\mathbb{E}f(W_t) = \int_{-\infty}^{\infty} f(w)\,\frac{\mathrm{e}^{-w^2/2t}}{\sqrt{2\pi t}}\,\mathrm{d}w. \tag{4.14}$$

Using this in (4.13) with $\theta_0 = 0$, we have

$$\mathbb{E}\boldsymbol{x}(t) = \mathbb{E}\int_0^t \begin{pmatrix}\cos W_s\\ \sin W_s\end{pmatrix}\mathrm{d}s = 2(1-\mathrm{e}^{-t/2})\begin{pmatrix}1\\0\end{pmatrix}. \tag{4.15}$$

Here, using Fubini's theorem, we brought the expectation inside the integral. Perhaps surprisingly, the expectation (4.15) does not go to $\boldsymbol{x}_0 = 0$ as $t \to \infty$, because there is a bias determined by the initial motion in the $\hat{\boldsymbol{x}}$ direction. Of course, averaging over the initial angle would eliminate the bias. For small time, (4.15) gives

$$\mathbb{E}x(t) = t + \mathrm{O}(t^2), \qquad t \to 0, \tag{4.16}$$

exhibiting the initial ballistic motion of the needle. Equation (4.15) is compared to numerical simulations in Fig. 4.2(a).

Now for the mean-squared displacement. We have the quadratic expectation

$$\begin{aligned}\mathbb{E}(\boldsymbol{x}(t)\otimes\boldsymbol{x}(t)) &= \mathbb{E}\left\{\int_0^t \hat{\boldsymbol{r}}(W_s)\,\mathrm{d}s \otimes \int_0^t \hat{\boldsymbol{r}}(W_s)\,\mathrm{d}s\right\}\\ &= \mathbb{E}\int_0^t\int_0^t \hat{\boldsymbol{r}}(W_s)\otimes\hat{\boldsymbol{r}}(W_{s'})\;\mathrm{d}s\,\mathrm{d}s'.\end{aligned}$$

The covariance of a vector $\boldsymbol{x}(t)$ is[2]

$$\mathrm{Cov}\{\boldsymbol{x}(t),\boldsymbol{x}(t)\} = \mathbb{E}\{\boldsymbol{x}(t)\otimes\boldsymbol{x}(t)\} - \mathbb{E}\boldsymbol{x}(t)\otimes\mathbb{E}\boldsymbol{x}(t) \tag{4.17}$$

so that

$$\mathrm{Cov}\{\boldsymbol{x}(t),\boldsymbol{x}(t)\} = \int_0^t\int_0^t \mathrm{Cov}\{\hat{\boldsymbol{r}}(W_s),\hat{\boldsymbol{r}}(W_{s'})\}\,\mathrm{d}s\,\mathrm{d}s'. \tag{4.18}$$

We thus need to compute the expectation $\mathbb{E}\{\hat{\boldsymbol{r}}(W_s),\hat{\boldsymbol{r}}(W_{s'})\}$ at different times s and s'. For $t>s$, we use the independence of $W_t - W_s$ and W_s:

$$\begin{aligned}\mathbb{E}\{\cos W_t\cos W_s\} &= \mathbb{E}\{\cos(W_t - W_s + W_s)\cos W_s\}\\ &= \mathbb{E}\{(\cos(W_t-W_s)\cos W_s - \sin(W_t-W_s)\sin W_s)\cos W_s\}\\ &= \mathbb{E}\cos W_{t-s}\,\mathbb{E}\cos^2 W_s - \mathbb{E}\sin W_{t-s}\,\mathbb{E}\{\sin W_s\cos W_s\}\\ &= (\mathrm{e}^{-(t-s)/2})(\mathrm{e}^{-s}\cosh s) - 0\\ &= \mathrm{e}^{-(t+s)/2}\,\cosh s,\end{aligned}$$

and similarly for the other entries, to obtain

$$\mathbb{E}\{\hat{\boldsymbol{r}}(W_t)\otimes\hat{\boldsymbol{r}}(W_s)\} = \mathrm{e}^{-(t+s)/2}\begin{pmatrix}\cosh s & 0\\ 0 & \sinh s\end{pmatrix}, \qquad t>s. \tag{4.19}$$

We also have

$$\mathbb{E}\hat{\boldsymbol{r}}(W_t)\otimes\mathbb{E}\hat{\boldsymbol{r}}(W_s) = \mathrm{e}^{-(t+s)/2}\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}, \tag{4.20}$$

so that

$$\mathrm{Cov}\{\hat{\boldsymbol{r}}(W_t),\hat{\boldsymbol{r}}(W_s)\} = \mathrm{e}^{-(t+s)/2}\begin{pmatrix}\cosh s - 1 & 0\\ 0 & \sinh s\end{pmatrix}, \qquad t>s. \tag{4.21}$$

[2]Feller [5, p. 82] defines this as the variance of a vector. It seems more natural call this a covariance and reserve variance for $\mathrm{Var}\{\boldsymbol{x}(t)\} = \mathrm{Tr}\,\mathrm{Cov}\{\boldsymbol{x}(t),\boldsymbol{x}(t)\}$.

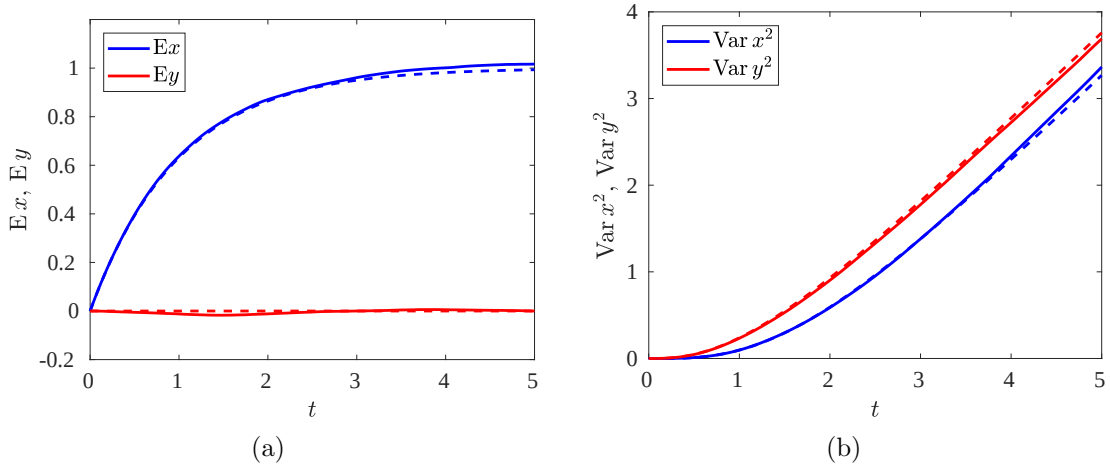


Figure 4.2: (a) Components of expected displacement $\mathbb{E}\boldsymbol{x}(t)$ for a swimming needle with $D_X = D_Y = 0$, $U = D_\theta = 1$, and $\boldsymbol{x}_0 = \theta_0 = 0$, averaged over 3000 paths. The dashed lines are the components of (4.15). (b) Variance of x and y for the same parameters, compared to the diagonal elements of (4.22).

Inserting this into (4.18) we find

$$\begin{aligned}\mathrm{Cov}\{\boldsymbol{x}(t),\boldsymbol{x}(t)\} &= 2\int_0^t \mathrm{d}s \int_0^s \mathrm{d}s'\ \mathrm{Cov}\{\hat{\boldsymbol{r}}(s),\hat{\boldsymbol{r}}(s')\} \\ &= 2\int_0^t \mathrm{d}s \int_0^s \mathrm{d}s'\ \mathrm{e}^{-(s+s')/2}\begin{pmatrix}\cosh s'-1 & 0\\ 0 & \sinh s'\end{pmatrix} \\ &= 2(t-3+4\mathrm{e}^{-t/2}-\mathrm{e}^{-t})\,\mathbb{I} \\ &\quad -\left(1-\tfrac{1}{3}\mathrm{e}^{-2t}\left(1-6\mathrm{e}^{t}+8\mathrm{e}^{3t/2}\right)\right)\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \end{aligned} \tag{4.22}$$

This expression is compared to numerical simulations in Fig. 4.2(b).

The variance of $\boldsymbol{x}(t)$ is then

$$\mathrm{Var}\{\boldsymbol{x}(t)\} = \mathbb{E}\|\boldsymbol{x}(t)-\mathbb{E}\boldsymbol{x}(t)\|^2 = \mathrm{Tr}\,\mathrm{Cov}\{\boldsymbol{x}(t),\boldsymbol{x}(t)\} = 4(t-3+4\mathrm{e}^{-t/2}-\mathrm{e}^{-t}). \tag{4.23}$$

This is diffusive (linear in t) for large t. The long-time effective diffusivity is read off from

$$\mathrm{Var}\{\boldsymbol{x}(t)\} \sim 4D_{\mathrm{eff}}\,t, \qquad t\longrightarrow\infty, \tag{4.24}$$

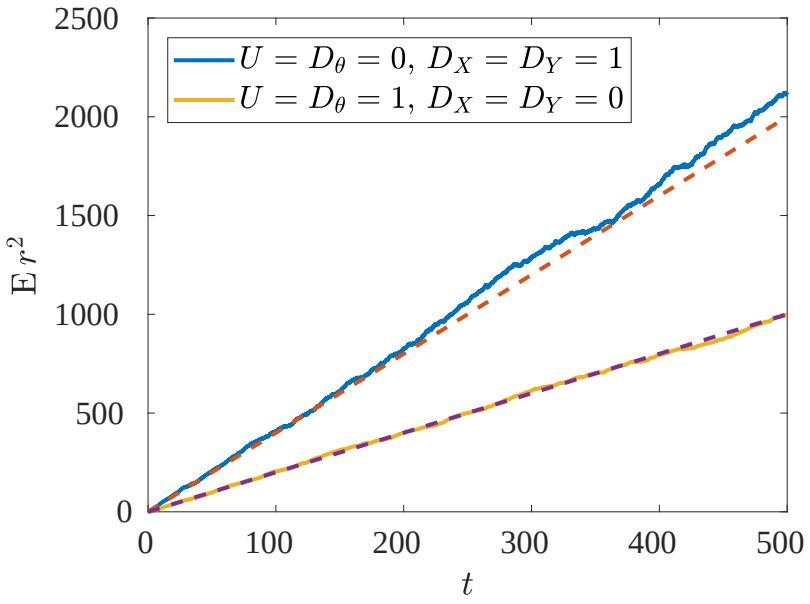


Figure 4.3: The mean-squared displacement for a purely Brownian needle, and a swimming needle. The dashed lines are the predicted effective diffusivities: $D_X + D_Y$ for the first case, $D_{\text{eff}} = U^2/2D_\theta$ for the second.

which gives $D_{\text{eff}} = 1$. In terms of the original units, this is

$$D_{\text{eff}} = U^2/2D_\theta. \tag{4.25}$$

For small t (4.22) can be expanded as

$$\mathrm{Cov}\{\boldsymbol{x}(t), \boldsymbol{x}(t)\} = \begin{pmatrix} \frac{1}{12}t^4 & 0 \\ 0 & \frac{1}{3}t^3 - \frac{5}{24}t^4 \end{pmatrix} + \mathrm{O}(t^5). \tag{4.26}$$

For a general initial angle θ_0, we can transform (4.22) with the rotation (4.2):

$$\begin{pmatrix} \cos\theta_0 & -\sin\theta_0 \\ \sin\theta_0 & \cos\theta_0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \cos\theta_0 & -\sin\theta_0 \\ \sin\theta_0 & \cos\theta_0 \end{pmatrix}^T = \begin{pmatrix} \cos 2\theta_0 & \sin 2\theta_0 \\ \sin 2\theta_0 & -\cos 2\theta_0 \end{pmatrix}. \tag{4.27}$$

Lecture 5

Introduction to stochastic calculus

This lecture is a bit out of order since we solved an SDE in the previous lecture, but people expressed interest in learning more, so here we go. This short introduction will be far from rigorous; rather we will focus on intuition and on practical calculations. A good non-rigorous reference is the book by Gardiner [6]; a standard rigorous reference is Øksendal [10].

5.1 Brownian motion

The basic building block in SDEs is Brownian motion, which a time-dependent stochastic process W_t. As mentioned in Lecture 4, $W_t \sim N(0,t)$, i.e., it is normally-distributed (Gaussian) with mean zero and variance t. Expected values of functions of Brownian motion are computed according to

$$\mathbb{E}f(W_t) = \int_{-\infty}^{\infty} f(w)\,\frac{\mathrm{e}^{-w^2/2t}}{\sqrt{2\pi t}}\,\mathrm{d}w. \tag{5.1}$$

This the Gaussian probability density corresponding to a heat kernel with mean zero and variance t:

$$\mathbb{E}W_t = 0; \qquad \mathbb{E}W_t^2 = t. \tag{5.2}$$

The *increments* of the Brownian process are of the form

$$W_t - W_s, \qquad t > s\,, \tag{5.3}$$

and $W_t - W_s$ is independent of W_s if $t > s$. For $t > s$, we have the correlation

$$\begin{aligned}\mathbb{E}\{W_t W_s\} &= \mathbb{E}\{(W_t - W_s + W_s)W_s\} \\ &= \mathbb{E}\{(W_t - W_s)\,W_s\} + \mathbb{E}\{W_s^2\} \\ &= 0 + s, \qquad t > s. \end{aligned} \tag{5.4}$$

We rewrite this as

$$\mathbb{E}\{W_t W_s\} = \min\{t, s\}. \tag{5.5}$$

5.2 The stochastic integral

A *stochastic differential equation* is an equation of the form

$$\mathrm{d}X_t = \mu(X_t, t)\,\mathrm{d}t + \sigma(X_t, t)\,\mathrm{d}W_t \tag{5.6}$$

for some sufficiently smooth functions f and σ. The infinitesimal increment $\mathrm{d}W_t$ is the limit $W_{t+\Delta s} - W_t$ as $\Delta s \to 0$. Integrate (5.6) to give

$$X_t = X_0 + \int_0^t \mu(X_s, s)\,\mathrm{d}s + \int_0^t \sigma(X_s, s)\,\mathrm{d}W_s. \tag{5.7}$$

The first integral does not cause any problems: we just integrate with rest to s as we would normally. The second is more problematic: $\mathrm{d}W_s$ is an increment of Brownian motion. To interpret the integral, we divide up the interval as we normally would for a Riemann integral:

$$s_n = n\Delta s, \qquad n = 0, \ldots N, \qquad \Delta s = t/N. \tag{5.8}$$

The last integral in (5.7) then becomes

$$\int_0^t \sigma(X_s, s)\,\mathrm{d}W_s = \lim_{N\to\infty} \sum_{n=0}^{N-1} \sigma(X_{s_n}, s_n)\,\Delta W_{s_n}. \tag{5.9}$$

where

$$\Delta W_{s_n} \coloneqq W_{s_n+\Delta s} - W_{s_n}. \tag{5.10}$$

Example 5.1 (Integral of Brownian motion)**.** As an example, let's integrate Brownian motion itself:

$$\begin{aligned}\int_0^t W_s \,\mathrm{d}W_s &= \lim_{N\to\infty} \sum_{n=0}^{N-1} W_{s_n}\,\Delta W_{s_n} \\ &= \lim_{N\to\infty} \sum_{n=0}^{N-1} (W_{s_n}\,W_{s_n+\Delta s} - W_{s_n}^2) \\ &= \lim_{N\to\infty} \sum_{n=0}^{N-1} \tfrac{1}{2}\left(W_{s_n+\Delta s}^2 - W_{s_n}^2\right) - \tfrac{1}{2}(W_{s_n+\Delta s} - W_{s_n})^2.\end{aligned} \tag{5.11}$$

The first term is a telescoping sum with value $\frac{1}{2}\,(W_t^2 - W_0^2)$ with $W_0 = 0$. The second is a sum over $(\Delta W_{s_n})^2$, and these converge in the mean-squared sense to Δs (see p. 30); hence,

$$\int_0^t W_s \,\mathrm{d}W_s = \tfrac{1}{2}W_t^2 - \tfrac{1}{2}t. \tag{5.12}$$

The integral is different than we might expect from the normal chain rule, which would imply $W_s \mathrm{d}W_s = \mathrm{d}(\frac{1}{2}W_t^2)$. The expected value of the integral vanishes:

$$\mathbb{E}\int_0^t W_s \,\mathrm{d}W_s = \tfrac{1}{2}(\mathbb{E}W_t^2 - t) = 0. \tag{5.13}$$

For the stochastic integral of a general differentiable function $f(W_s)$, we write

$$\int_0^t f(W_s)\,\mathrm{d}W_s = \lim_{N\to\infty} \sum_{n=0}^{N-1} f(W_{s_n})\,\Delta W_{s_n}. \tag{5.14}$$

The expectation again vanishes:

$$\mathbb{E}\int_0^t f(W_s)\,\mathrm{d}W_s = \lim_{N\to\infty} \sum_{n=0}^{N-1} \mathbb{E}\{f(W_{s_n})\Delta W_{s_n}\} = 0, \tag{5.15}$$

since W_{s_n} is independent of ΔW_{s_n} and $\mathbb{E}\Delta W_{s_n} = 0$. In fact, we can write something resembling the fundamental theorem of calculus:

$$\int_{t_0}^t f(W_s)\,\mathrm{d}W_s = F(W_t) - F(W_{t_0}) - \tfrac{1}{2}\int_{t_0}^t f'(W_s)\,\mathrm{d}s, \tag{5.16}$$

where $F(w)$ is and antiderivative of $f(w)$, which will follow from Itô formula (Eq. (6.2)).

What about a differentiable function of the stochastic process $f(X_t)$? We define the integral in the same way:

$$\int_0^t f(X_s)\,\mathrm{d}W_s = \lim_{N\to\infty} \sum_{n=0}^{N-1} f(X_{s_n})\,\Delta W_{s_n}. \tag{5.17}$$

This is the *Itô integral*, with expected value zero since X_{s_n} is independent of ΔW_{s_n}.

An integral in $(\mathrm{d}W_s)^2$ is equal to one in $\mathrm{d}s$ in expectation:

$$\mathbb{E}\left\{\int_0^t f(X_s)(\mathrm{d}W_s)^2 - \int_0^t f(X_s)\,\mathrm{d}s\right\} = \lim_{N\to\infty}\sum_{n=0}^{N-1}\mathbb{E}\left\{f(X_{s_n})\left((\Delta W_{s_n})^2 - \Delta s\right)\right\} = 0.$$

Moreover, the Riemann sums defining these integrals converge to each other in the mean-squared sense, as can be see by first writing

$$\mathbb{E}\left\{\left(\int_0^t f(X_s)(\mathrm{d}W_s)^2 - \int_0^t f(X_s)\,\mathrm{d}s\right)^2\right\} =$$

$$\lim_{N,N'\to\infty}\sum_{n=0}^{N-1}\sum_{n'=0}^{N'-1}\mathbb{E}\left\{f(X_{s_n})f(X_{s_{n'}})\left((\Delta W_{s_n})^2 - \Delta s\right)\left((\Delta W_{s_{n'}})^2 - \Delta s'\right)\right\}.$$

For $n < n'$ we have $f(X_{s_n})f(X_{s_{n'}})\left((\Delta W_{s_n})^2 - \Delta s\right)$ independent of $\left((\Delta W_{s_{n'}})^2 - \Delta s'\right)$, so the expectation vanishes, and similarly for $n > n'$. Hence,

$$\mathbb{E}\left\{\left(\int_0^t f(X_s)(\mathrm{d}W_s)^2 - \int_0^t f(X_s)\,\mathrm{d}s\right)^2\right\} =$$

$$\lim_{N\to\infty}\sum_{n=0}^{N-1}\mathbb{E}\{f^2(X_{s_n})\}\,\mathbb{E}\left\{(\Delta W_{s_n})^4 - 2(\Delta W_{s_n})^2\Delta s + (\Delta s)^2\right\}.$$

On the right-hand side we use $\mathbb{E}(\Delta W_{s_n})^2 = \Delta s$ and $\mathbb{E}(\Delta W_{s_n})^4 = 3\mathbb{E}(\Delta W_{s_n})^2 = 3(\Delta s)^2$, which follows from ΔW_{s_n} being Gaussian. We thus have

$$\mathbb{E}\left\{\left(\int_0^t f(X_s)(\mathrm{d}W_s)^2 - \int_0^t f(X_s)\,\mathrm{d}s\right)^2\right\} = \lim_{N\to\infty}\sum_{n=0}^{N-1}\mathbb{E}\{f^2(X_{s_n})\}\,2(\Delta s)^2 = 0$$

which vanishes because $(\Delta s)^2 \sim 1/N^2$ and there are only N terms in the series (f is bounded since it is continuous on a closed interval). We conclude that the two integrals converge to each other in the mean-squared sense for any function $f(x)$, and thus it makes sense to write [10, p. 44, Theorem 4.1.2]

$$(\mathrm{d}W_s)^2 = \mathrm{d}s, \qquad (\Delta W_{s_n})^2 = \Delta s \tag{5.18}$$

even without expectation.

5.3 Other definitions of the stochastic integral

But wait! We made a big assumption in writing down (5.11): when we evaluated W_s in an interval inside the sum, we chose to evaluate it at the *start* of the interval. We could have equally well have evaluated it at the end of the interval:

$$\int_0^t W_s \, \mathrm{d}W_s = \lim_{N\to\infty} \sum_{n=0}^{N-1} W_{s+\Delta s} \, \Delta W_{s_n}. \tag{5.19}$$

The expected value is then

$$\begin{aligned} \mathbb{E} \int_0^t W_s \, \mathrm{d}W_s &= \lim_{N\to\infty} \sum_{n=0}^{N-1} (\mathbb{E} W_{s_n+\Delta s}^2 - \mathbb{E}\{W_{s_n+\Delta s} W_{s_n}\}) \\ &= \lim_{N\to\infty} \sum_{n=0}^{N-1} (s_n + \Delta s - s_n) = t. \end{aligned} \tag{5.20}$$

Oops... we get a different answer. What about if we use a trapezoidal rule to approximate the integral, by averaging the values at the start and end of the interval? This leads to

$$\int_0^t W_s \, \mathrm{d}W_s = \lim_{N\to\infty} \sum_{n=0}^{N-1} \tfrac{1}{2} \left(W_{s_n} + W_{s_n+\Delta s}\right) \Delta W_{s_n}. \tag{5.21}$$

By linearity, the expected value is the average of (5.13) and (5.20):

$$\mathbb{E} \int_0^t W_s \, \mathrm{d}W_s = \tfrac{1}{2} t \tag{5.22}$$

which is different yet again. We can combine all these cases by using an arbitrary weight $0 \le \beta \le 1$:

$$\int_0^t W_s \, \mathrm{d}W_s = \lim_{N\to\infty} \sum_{n=0}^{N-1} \left((1-\beta) W_{s_n} + \beta W_{s_n+\Delta s}\right) \Delta W_{s_n} \tag{5.23}$$

so the expectation is

$$\mathbb{E} \int_0^t W_s \, \mathrm{d}W_s = \beta t. \tag{5.24}$$

The cases we looked at before correspond to $\beta = 0$ (start of interval), $\beta = \frac{1}{2}$ (average of start and end), and $\beta = 1$ (end of interval).

Note that instead of averaging the two endpoint values we can also decide to evaluate the Brownian motion at an intermediate point inside the interval:

$$\int_0^t W_s \,\mathrm{d}W_s = \lim_{N\to\infty} \sum_{n=0}^{N-1} W_{s_n+\beta\Delta s}\, \Delta W_{s_n} \tag{5.25}$$

which gives the expectation

$$\begin{aligned}\mathbb{E}\int_0^t W_s \,\mathrm{d}W_s &= \lim_{N\to\infty} \sum_{n=0}^{N-1} \left(\mathbb{E}\{W_{s_n+\beta\Delta s} W_{s_n+\Delta s}\} - \mathbb{E}\{W_{s_n+\beta\Delta s} W_{s_n}\}\right) \\ &= \lim_{N\to\infty} \sum_{n=0}^{N-1} \left((s_n+\beta\Delta s) - s_n\right) = \beta t, \end{aligned} \tag{5.26}$$

i.e., the same as (5.24). So it makes no difference whether we interpret the stochastic integral as (5.23) or (5.25).

Because the choice of β affects the value of the stochastic integral, we introduce the somewhat kludgy notation

$$\int_0^t f \circ_\beta \,\mathrm{d}W_s \tag{5.27}$$

to indicate the choice of β in interpreting the stochastic integral. However, the absence of $\circ_\beta$ indicates the Itô convention $\beta = 0$, which is the default in most stochastic calculus texts. Another common convention is the *Stratonovich integral*, $\beta = \frac{1}{2}$, which is usually denoted by a plain circle $\circ$.

For the integral of functions of the stochastic process $f(X_t)$, the integral using weighted endpoints is

$$\begin{aligned}\int_0^t f(X_s) \circ_\beta \mathrm{d}W_s &= \lim_{N\to\infty} \sum_{n=0}^{N-1} f((1-\beta)\, X_{s_n} + \beta\, X_{s_n+\Delta s}))\, \Delta W_{s_n} \\ &= \lim_{N\to\infty} \sum_{n=0}^{N-1} f(X_{s_n} + \beta\,(X_{s_n+\Delta s} - X_{s_n}))\, \Delta W_{s_n} \\ &= \lim_{N\to\infty} \sum_{n=0}^{N-1} (f(X_{s_n}) + \beta\, f'(X_{s_n})\, \Delta X_{s_n} + \cdots)\, \Delta W_{s_n} \end{aligned}$$

where higher-order terms can be neglected in the limit. As $\Delta s \to 0$ the increment ΔX_{s_n} tends to $\mathrm{d}X_{s_n}$, so we can use (5.6):

$$\int_0^t f(X_s) \circ_\beta \mathrm{d}W_s = \lim_{N\to\infty} \sum_{n=0}^{N-1} (f(X_{s_n}) + \beta\, f'(X_{s_n})\, \sigma(X_{s_n}, s_n)\, \Delta W_{s_n})\, \Delta W_{s_n}.$$

Substituting $(\Delta W_{s_n})^2 = \Delta s$, we obtain

$$\int_0^t f(X_s) \circ_\beta \mathrm{d}W_s = \int_0^t f(X_s)\,\mathrm{d}W_s + \beta \int_0^t f'(X_s)\,\sigma(X_s, s)\,\mathrm{d}s \tag{5.28}$$

where the first term on the right is an Itô integral (5.17). Equation (5.28) is a conversion formula between the Itô integral and any other convention. Thus, there is no real loss in generality in using Itô calculus, as long as we remember to do the conversion. Indeed, supposed we are faced with a general SDE of the form

$$\mathrm{d}X_t = \mu(X_s, s)\,\mathrm{d}s + \sigma(X_s, s) \circ_\beta \mathrm{d}W_s. \tag{5.29}$$

Then we apply (the time-derivative of) (5.28) and obtain the Itô equation

$$\mathrm{d}X_t = (\mu(X_s, s) + \beta\,\sigma(X_s, s)\,\partial_x\sigma(X_s, s))\,\mathrm{d}s + \sigma(X_s, s)\,\mathrm{d}W_s. \tag{5.30}$$

Hence, an SDE (5.29) with an arbitrary value of β is an Itô SDE (5.6) with the substitution

$$\mu(x,t) \;\longrightarrow\; \mu(x,t) + \beta\,\sigma(x,t)\,\partial_x\sigma(x,t). \tag{5.31}$$

Note that in the case where $\partial_x\sigma = 0$ there is no difference between the different conventions. The case with $\partial_x\sigma \neq 0$ is referred to as *multiplicative noise*.

If we take $X_s = W_s$ so that $\sigma \equiv 1$, the relationship (5.28) can be used with the 'Itô fundamental theorem' (5.16) to get a fundamental theorem for general choice of β:

$$\int_{t_0}^t f(W_s) \circ_\beta \mathrm{d}W_s = F(W_t) - F(W_{t_0}) + (\beta - \tfrac{1}{2}) \int_{t_0}^t f'(W_s)\,\mathrm{d}s. \tag{5.32}$$

In the Stratonovich case ($\beta = \frac{1}{2}$), we have the elegant result

$$\int_{t_0}^t f(W_s) \circ \mathrm{d}W_s = F(W_t) - F(W_{t_0}), \tag{5.33}$$

that is, the chain rule $\mathrm{d}f(W_s) = f'(W_s) \circ \mathrm{d}W_s$ is satisfied just as in ordinary calculus. This is why it is sometimes preferred, but bear in mind that then the expectation of stochastic integrals does not vanish.

Lecture 6

The Fokker–Planck equation

In this lecture we'll (hopefully) complete our basic introduction to stochastic calculus. In addition, we'll devote some time to the so-called 'Itô vs Stratonovich dilemma,' a modeling issue that is not often addressed in mathematical SDE courses, but is relevant in physics and applied math.

6.1 Itô's formula

Let $f(x,t)$ be a differentiable function. We wish to find the stochastic calculus version of the chain rule. We have by Taylor expansion

$$\mathrm{d}f(X_t,t) = \partial_t f(X_t,t)\,\mathrm{d}t + \mathrm{d}_x f(X_t,t)\,\mathrm{d}X_t + \tfrac{1}{2}\partial_x^2 f(X_t,t)\,(\mathrm{d}X_t)^2 + \mathrm{O}(\mathrm{d}X_t^3). \quad (6.1)$$

Here $\mathrm{d}X_t$ satisfies the Itô SDE (5.6), so to leading order $(\mathrm{d}X_t)^2 = \sigma^2\,(\mathrm{d}W_t)^2 = \sigma^2\mathrm{d}t$, after using (5.18). We thus obtain *Itô's formula*

$$\mathrm{d}f(X_t,t) = \big(\partial_t f(X_t,t) + \mu(X_t,t)\,\partial_x f(X_t,t) + \tfrac{1}{2}\sigma^2(X_t,t)\,\partial_x^2 f(X_t,t)\big)\,\mathrm{d}t \\ + \partial_x f(X_t,t)\,\sigma(X_t,t)\,\mathrm{d}W_t. \quad (6.2)$$

Itô's formula can be regarded as a transformation rule for changing variables in (5.6).

Define the *generator* of the stochastic process as the differential operator

$$\mathcal{A}_{x,t} f(x) := \mu(x,t)\,f'(x) + \tfrac{1}{2}\sigma^2(x,t) f''(x). \quad (6.3)$$

Then Itô's formula can be recast as

$$\mathrm{d}f(X_t,t) = (\partial_t f(X_t,t) + \mathcal{A}_{X_t,t} f(X_t,t))\,\mathrm{d}t + \partial_x f(X_t,t)\,\sigma(X_t,t)\,\mathrm{d}W_t \quad (6.4)$$

or in integral form as

$$f(X_t,t) - f(X_0,t_0) = \int_{t_0}^{t} (\partial_s + \mathcal{A}_{X_s,s}) f(X_s,s)\,\mathrm{d}s + \int_{t_0}^{t} \partial_x f(X_s)\,\sigma(X_s,s)\,\mathrm{d}W_s. \quad (6.5)$$

6.2 The forward and backward Kolmogorov equations

For some differentiable function $g(x)$, define the quantity

$$u(t \,|\, x_0, t_0) \coloneqq \mathbb{E}^{x_0,t_0} g(X_t), \quad (6.6)$$

where we used the notation

$$\mathbb{E}^{x_0,t_0} g(X_t) \coloneqq \mathbb{E}\{g(X_t) \,|\, X_{t_0} = x_0\}. \quad (6.7)$$

We have

$$u(t \,|\, x_0, t) = g(x_0) \quad (6.8)$$

which we regard as a terminal value for $u(t \,|\, x_0, t_0)$, $t_0 \le t$. In fact another way to write $u(t \,|\, x_0, t_0)$ is in terms of the transition probability density function $p(\boldsymbol{x}, t \,|\, \boldsymbol{x}_0, t_0)$ introduced in Lecture 1:

$$u(t \,|\, x_0, t_0) = \int_\Omega g(x')\, p(x', t \,|\, x_0, t_0)\,\mathrm{d}V_x\,. \quad (6.9)$$

From the definition of p, we see that the indices x_0, t_0 on the right are exactly the statement that a stochastic particle started at that point, and the integral over x is the expectation (6.7). Putting $g(x') = \delta(x - x')$ gives $u(t \,|\, x_0, t_0) = p(x, t \,|\, x_0, t_0)$, so that p can be deduced from u.

To get a differential equation for u, consider the integral form (6.5) of Itô's formula applied to $f(x,t) = u(\tau \,|\, x, t)$:

$$u(\tau \,|\, X_t, t) - u(\tau \,|\, X_0, t_0) = \int_{t_0}^{t} (\partial_s + \mathcal{A}_{X_s,s})\, u(\tau \,|\, X_s, s)\,\mathrm{d}s + \int_{t_0}^{t} \partial_x u(\tau \,|\, X_s, s)\,\sigma(X_s,s)\,\mathrm{d}W_s. \quad (6.10)$$

Now take expectation $\mathbb{E}^{x_0,t_0}$ on both sides of (6.10). On the left we have

$$\begin{aligned} \mathbb{E}^{x_0,t_0}\{u(\tau \,|\, X_t, t) - u(\tau \,|\, X_0, t_0)\} &= E^{x_0,t_0}\mathbb{E}^{x_0,t_0} g(X_\tau) - u(\tau \,|\, x_0, t_0) \\ &= \mathbb{E}^{x_0,t_0} g(X_\tau) - u(\tau \,|\, x_0, t_0) \\ &= 0. \end{aligned}$$

On the right of (6.10), after taking expectation $\mathbb{E}^{x_0,t_0}$, divide by $t - t_0$, and take the limit $t \to t_0$:

$$\begin{aligned} 0 &= \mathbb{E}^{x_0,t_0} \lim_{t\to t_0} \frac{1}{t-t_0} \int_{t_0}^{t} (\partial_s + \mathcal{A}_{X_s,s})\, u(\tau \,|\, X_s, s)\, \mathrm{d}s \\ &= \mathbb{E}^{x_0,t_0} \left(\partial_{t_0} + \mathcal{A}_{X_0,t_0}\right) u(\tau \,|\, X_0, t_0) \\ &= \left(\partial_{t_0} + \mathcal{A}_{x_0,t_0}\right) u(\tau \,|\, x_0, t_0). \end{aligned} \tag{6.11}$$

After setting $\tau = t$, we thus obtain the *Kolmogorov backward equation*

$$\partial_{t_0} u(t \,|\, x_0, t_0) + \mathcal{A}_{x_0,t_0} u(t \,|\, x_0, t_0) = 0, \qquad t_0 < t, \qquad u(t \,|\, x_0, t) = g(x_0). \tag{6.12}$$

The PDE (6.12) can easily be transformed to a PDE for $p(x, t \,|\, x_0, t_0)$ using (6.9) with $g(x') = \delta(x - x')$. Comparing this to (2.12) from Lecture 2: we can see that the generator $\mathcal{A}$ is related to $\mathcal{L}^*$ by

$$\mathcal{A}_{x_0,t_0} = -\mathcal{L}^*_{x_0,t_0}. \tag{6.13}$$

Now we proceed as in Lecture 2 when we found the adjoint $\mathcal{L}^*$, but going the other way. We obtain the *Kolmogorov forward* or *Fokker–Planck* equation:

$$\partial_{t_0} v(x, t \,|\, t_0) = \mathcal{A}^*_{x,t} v(x, t \,|\, t_0), \qquad t < t_0, \qquad v(x, t_0 \,|\, t_0) = f(x), \tag{6.14}$$

where the adjoint to the generator is

$$\mathcal{A}^*_{x,t} f(x) \coloneqq -(\mu(x,t) f(x))' + \tfrac{1}{2}(\sigma^2(x,t) f(x))''. \tag{6.15}$$

Comparing to (1.3), we have

$$\mathcal{A}^*_{x,t} = -\mathcal{L}_{x,t}. \tag{6.16}$$

Notice that the forward equation requires more regularity the the backward one, since μ and σ appear inside derivatives.

6.3 Itô vs Stratonovich vs Hänggi

As we saw in the previous lecture, changing the convention for the stochastic integral is simply a matter of effecting the substitution (5.31), which modifies the drift μ in the generator (6.3) to give

$$\mathcal{A}_{x,t} f(x) = (\mu + \beta\, \sigma\, \partial_x \sigma)\, f'(x) + \tfrac{1}{2}\sigma^2 f''(x). \tag{6.17}$$

We can instead move the extra β term to the diffusion term:

$$\mathcal{A}_{x,t} f(x) = \mu\, \partial_x f + \tfrac{1}{2}\sigma^{2(1-\beta)}\, \partial_x \left(\sigma^{2\beta} \partial_x f\right). \tag{6.18}$$

The adjoint appearing in the forward equation is

$$\mathcal{A}^*_{x,t} f(x) = -\partial_x(\mu\, f) + \tfrac{1}{2}\partial_x \left(\sigma^{2\beta}\, \partial_x(\sigma^{2(1-\beta)} f)\right). \tag{6.19}$$

Thus, the different conventions for the stochastic integral can be interpreted as different models of diffusion.

For $\beta = 0$, the diffusion term is

$$\partial_x^2\, (D f)\,, \qquad D = \tfrac{1}{2}\sigma^2, \qquad (\beta = 0, \text{ Itô}), \tag{6.20}$$

whereas for $\beta = 1$ it is

$$\partial_x\, (D\, \partial_x f)\,, \qquad D = \tfrac{1}{2}\sigma^2, \qquad (\beta = 1, \text{ Hänggi}). \tag{6.21}$$

This last one resembles Fick's law of diffusion, which says that the flux is proportional to the gradient: $F = -D(x)\, \partial_x f$. Finally, the Stratonich choice splits the difference:

$$\partial_x\, (\sigma\, \partial_x(\sigma\, f))\,, \qquad (\beta = \tfrac{1}{2}, \text{ Stratonovich}). \tag{6.22}$$

Of course, when σ is constant these are all the same. The appropriate choice of β is a modeling issue.

- The Stratonovich integral is the limit of a non-white noise y^ε with short correlation time ε:
$$\frac{\mathrm{d}x^\varepsilon}{\mathrm{d}t} = h(x^\varepsilon) + \frac{1}{\varepsilon}\, f(x^\varepsilon)\, y^\varepsilon(t) \tag{6.23}$$
This limits to
$$\mathrm{d}X_t = h(X_t) + \sigma\, f(X_t) \cdot \mathrm{d}W_t. \tag{6.24}$$

- Stratonovich also makes sense when there is a differential constraint. For instance, to constrain Brownian motion to a sphere, a natural choice is the Itô process
$$\mathrm{d}\boldsymbol{X}_t = \mathbb{P}(\boldsymbol{X}_t) \cdot \mathrm{d}\boldsymbol{W}_t \tag{6.25}$$
where $\mathbb{P}$ is the orthogonal projection to the tangent space of the sphere's surface, and $\boldsymbol{W}_t \in \mathbb{R}^d$ is a d-dimensional Brownian motion. The projection operator can be taken to be
$$\mathbb{P}(\boldsymbol{x}) = \mathbb{I} - \frac{\boldsymbol{x} \otimes \boldsymbol{x}}{\|\boldsymbol{x}\|^2}\,. \tag{6.26}$$

The length of $\boldsymbol{X}_t$ appears to be preserved by the process, since $\boldsymbol{x} \cdot \mathbb{P}(\boldsymbol{x}) = 0$ and so $\boldsymbol{X}_t \cdot \mathrm{d}\boldsymbol{X}_t = 0$. However, all is not as well as it seems, which we can see by integrating the equation to find $\|\boldsymbol{X}_t\|^2$.

The multidimensional generalization of the Itô formula (6.2) for a function $f(\boldsymbol{x})$ is

$$\mathrm{d}f(\boldsymbol{X}_t) = \tfrac{1}{2}\boldsymbol{\sigma}\boldsymbol{\sigma}^T : \nabla\nabla f \,\mathrm{d}t + \nabla f \cdot \boldsymbol{\sigma} \cdot \mathrm{d}\boldsymbol{W}_t. \tag{6.27}$$

We set $\mu = 0$, $\boldsymbol{\sigma}(\boldsymbol{x}) = \mathbb{P}(\boldsymbol{x})$, $f(\boldsymbol{x}) = \frac{1}{2}\|\boldsymbol{x}\|^2$, $\nabla f = \boldsymbol{x}$, $\nabla\nabla f = \mathbb{I}$, to get

$$\mathrm{d}(\tfrac{1}{2}\|\boldsymbol{X}_t\|^2) = \tfrac{1}{2}\,\mathrm{Tr}\,\boldsymbol{\sigma}\boldsymbol{\sigma}^T \,\mathrm{d}t + \boldsymbol{X}_t \cdot \mathbb{P} \cdot \mathrm{d}\boldsymbol{W}_t. \tag{6.28}$$

The last term above vanishes, and $\boldsymbol{\sigma}\boldsymbol{\sigma}^T = \mathbb{P}\,\mathbb{P}^T = \mathbb{P}^2 = \mathbb{P}$, so that

$$\mathrm{Tr}\,\boldsymbol{\sigma}\boldsymbol{\sigma}^T = \mathrm{Tr}\,\mathbb{P} = d - 1, \tag{6.29}$$

where d is the dimension. Integrating (6.28) from 0 to t, we find

$$\|\boldsymbol{X}_t\|^2 = \|\boldsymbol{X}_0\|^2 + (d-1)\,t. \tag{6.30}$$

If the initial vector has unit length, $\|\boldsymbol{X}_0\|^2 = 1$, we see that the length drifts away from unity with time! We are using the wrong calculus, since for compatibility we need $\mathrm{d}(\frac{1}{2}\|\boldsymbol{X}_t\|^2) = \boldsymbol{X}_t \circ \mathrm{d}\boldsymbol{X}_t$ and we should really use the Stratonovich definition.

We modify Eq. (6.25) for the Stratonovich case by using [10, p. 83, Eq. (6.1.3)]

$$\mathrm{d}\boldsymbol{X}_t = \boldsymbol{\sigma} \circ \mathrm{d}\boldsymbol{W}_t = \tfrac{1}{2}\partial_{x_k}\sigma_{ij}\,\sigma_{kj}\,\hat{\boldsymbol{e}}_i \,\mathrm{d}t + \boldsymbol{\sigma} \cdot \mathrm{d}\boldsymbol{W}_t \tag{6.31}$$

with $\boldsymbol{\sigma} = \mathbb{P}$. After a bit of manipulation we find

$$\mathrm{d}\boldsymbol{X}_t = -\tfrac{1}{2}(d-1)\frac{\boldsymbol{X}_t}{\|\boldsymbol{X}_t\|^2}\,\mathrm{d}t + \mathbb{P}(\boldsymbol{X}_t) \cdot \mathrm{d}\boldsymbol{W}_t\,. \tag{6.32}$$

This is the correct Itô equation to solve in order to constraint $\boldsymbol{X}_t$ to the surface of a sphere. The generator is

$$\mathcal{A}_{\boldsymbol{x},t} f = -\tfrac{1}{2}(d-1)\frac{\boldsymbol{x}}{\|\boldsymbol{x}\|^2} \cdot \nabla f + \tfrac{1}{2}\mathbb{P}(\boldsymbol{x}) : \nabla\nabla f \tag{6.33}$$

with adjoint

$$\begin{aligned}
\mathcal{A}^*_{\boldsymbol{x},t} f &= \tfrac{1}{2}\nabla \cdot \left((d-1)\frac{\boldsymbol{x}}{\|\boldsymbol{x}\|^2}\, f + \nabla \cdot (\mathbb{P}(\boldsymbol{x}) f) \right) \\
&= \tfrac{1}{2}\nabla \cdot \left(-(\nabla \cdot \mathbb{P})\, f + \nabla \cdot (\mathbb{P}(\boldsymbol{x}) f) \right) \\
&= \tfrac{1}{2}\nabla \cdot (\mathbb{P}(\boldsymbol{x}) \cdot \nabla f)\,,
\end{aligned}$$

where we used $\nabla \cdot \mathbb{P} = -(d-1)\boldsymbol{x}/\|\boldsymbol{x}\|^2$. To make the role of the projection clearer, decompose the gradient into two parts:

$$\nabla = \mathbb{P}(\boldsymbol{x}) \cdot \nabla + \hat{\boldsymbol{x}}\,(\hat{\boldsymbol{x}} \cdot \nabla) = \nabla_\perp + \nabla_\parallel \tag{6.34}$$

with $\nabla_\parallel \mathbb{P}(\boldsymbol{x}) = 0$. Then

$$\begin{aligned}
\mathcal{A}^*_{\boldsymbol{x},t} f &= \tfrac{1}{2}(\nabla_\perp^2 f + \nabla_\parallel \cdot (\nabla_\perp f)) \\
&= \tfrac{1}{2}(\nabla_\perp^2 f + \nabla_\parallel \cdot (\mathbb{P} \cdot \nabla f)) \\
&= \tfrac{1}{2}(\nabla_\perp^2 f + \mathbb{P} \cdot \nabla_\parallel \cdot (\nabla f)) \\
&= \tfrac{1}{2}\nabla_\perp^2 f.
\end{aligned}$$

Challenge: characterize some interesting solution on the sphere. In 3D, relate to polar angles. Which is easier to solve?

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