4 Worked examples: reaction, diffusion, and advection

We gather together a selection of worked examples demonstrating problems involving (stochastic) reaction-diffusion-advection models which can be solved with the techniques we have developed. Often there are gaps left in the working for you to fill.

We use standard notation throughout, i.e., $D > 0$ will represent a diffusion coefficient, W will represent Brownian motion, and so forth.

4.1 Brownian particle on a half-line with absorbing boundary

Consider Brownian particles diffusing according to

$$\mathrm{d}X = \sqrt{2D}\,\mathrm{d}W$$

on $[0, \infty)$ with an absorbing boundary at $x = 0$, and initial concentration $K > 0$ on $(0, \infty)$.

The evolving distribution. The corresponding F-P equation and BCs are

$$c_t = Dc_{xx}, \quad c(x, 0) = K, \quad c(0, t) = 0\,.$$

We first check that

$$c(x, t) = K\,\mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right),$$

solves this initial-boundary value problem. (Here, as usual, $\mathrm{erf}(z) := \frac{2}{\sqrt{\pi}}\int_0^z e^{-s^2}\,\mathrm{d}s$ is the error function.) We then show how to derive this solution.

Showing that given solution solves the problem. By the fundamental theorem of calculus and the chain rule we have

$$c_t = \frac{2K}{\sqrt{\pi}}e^{-x^2/4Dt}\left(\frac{-x}{4t\sqrt{Dt}}\right), \quad c_x = \frac{2K}{\sqrt{\pi}}e^{-x^2/4Dt}\left(\frac{1}{2\sqrt{Dt}}\right), \quad c_{xx} = \frac{2K}{\sqrt{\pi}}e^{-x^2/4Dt}\left(\frac{-x}{4Dt\sqrt{Dt}}\right),$$

confirming that the PDE is satisfied. It is clear that $c(0, t) = 0$ for all $t > 0$. We define $c(x, 0) = \lim_{t\to 0+} c(x, t)$ from which $c(x, 0) = 1$ follows from the fact that $\lim_{z\to\infty} \mathrm{erf}\, z = 1$.

Deriving the given solution. We first extend the initial condition antisymmetrically to the whole line, i.e., define the initial value of c to be

$$c(x, 0) = \begin{cases} -K & (x < 0)\,, \\ 0 & (x = 0)\,, \\ K & (x > 0)\,. \end{cases}$$

A natural approach to solving the equation is to take the Fourier transform in x of both sides of the diffusion equation to get

$$\hat{c}(s, t) = -Ds^2\hat{c}, \quad \hat{c}(s, 0) = \mathcal{F}(c(x, 0)) = \frac{2K}{is}\,.$$

(The transform of the step function giving the initial condition is not trivial to derive.) Solving this IVP gives:

$$is\,\hat{c}(s,t) = 2K\,e^{-Ds^2t}, \quad \Rightarrow \quad \mathcal{F}(c_x(x,t)) = 2K\,e^{-Ds^2t}.$$

From tables of inverses, we get

$$c_x(x,t) = 2K\sqrt{\frac{1}{4Dt\pi}}e^{-x^2/(4Dt)} \quad \Rightarrow \quad c(x,t) = 2K\sqrt{\frac{1}{4Dt\pi}}\int_0^x e^{-u^2/(4Dt)}\,du\,.$$

Setting $y = u/\sqrt{4Dt}$, we get

$$c(x,t) = \frac{2K}{\sqrt{4Dt\pi}}\int_0^{x/\sqrt{4Dt}} e^{-y^2}\sqrt{4Dt}\,dy = \frac{2K}{\sqrt{\pi}}\int_0^{x/\sqrt{4Dt}} e^{-y^2}\,dy = K\,\mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right),$$

where, as usual $\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-s^2}\,ds$. Note that, for any fixed x, $\lim_{t\to\infty} p(x,t) = 0$, i.e., there is no nontrivial stationary distribution.

First passage times. Without doing extra work, we can now make some claims about first passage times for a particle with initial position $y > 0$ evolving according to the SDE above (namely, $dX = \sqrt{2D}\,dW, \quad X(0) = y > 0$). In particular, we show that the half-time to absorption (i.e., the time until the particle has been absorbed with probability 1/2) grows like y^2.

Let $T(y)$ be the first passage time to 0 and $h(y,t) := \mathbb{P}(T(y) > t)$. We know what h satisfies the BKE, which is, in this case,

$$h_t = Dh_{yy}\,.$$

Moreover we must have $h(y,0) = 1$ for all $y > 0$, $h(0,t) = 0$ for all $t \geq 0$, and $h(y,t) \in [0,1]$ for all $y > 0$ and $t > 0$ (being a probability). From the working above, we have immediately that

$$h(y,t) = \mathrm{erf}\left(\frac{y}{2\sqrt{Dt}}\right) = \frac{2}{\sqrt{\pi}}\int_0^{y/(2\sqrt{Dt})} e^{-s^2}\,ds\,.$$

In particular, for any fixed t, $h(y,t)$ rapidly approaches 1 as y becomes large. The half-time to absorption, namely the value of t which solves $h(y,t) = 1/2$, grows like y^2.

If we only want to obtain the *mean* first passage time (MFPT) to 0, say $\tau(y)$ where y is the initial position of the particle, this is simpler, we can consider the MFPT equation

$$-1 = D\tau_{yy}$$

on the *bounded* interval $[0,a]$ with absorption at 0 and a and then let $a \to \infty$. Solving gives

$$\tau(y) = \frac{y}{2D}(a-y)\,.$$

We now observe that for any fixed $y > 0$, $\tau(y) \to \infty$ as $a \to \infty$, i.e., the mean first passage time becomes infinite. It is also possible (but more challenging) to check directly that

$$\int_0^\infty h(y,t)\,dt = \frac{2}{\sqrt{\pi}}\int_0^\infty\int_0^{y/(2\sqrt{Dt})} e^{-s^2}\,ds\,dt = \infty\,.$$

(Consider swapping the order of integration and note that $\int_0^\infty e^{-s^2}/s^2\,ds$ is divergent.) Note that the MFPT to 0 is infinite, even though the probability that the particles "escapes to infinity" is zero as we will see in the next example.

4.2 Brownian particle on an interval

Let $a > 0$ and consider a Brownian particle evolving in $[0, a]$ according to the stochastic differential equation

$$dX = \sqrt{2D}\,dW, \quad X(0) = y \in (0, a)\,.$$

Our goal is to find the probability that it reaches a before it reaches 0: if, for example, arriving at a represents "escape", while arriving at 0 represents annihilation, we may refer to this probability as the *survival probability* of the particle.

Intuition from the symmetric random walk. To get some intuition about the survival probability, consider a symmetric random walk with state space $\{0, \ldots, n\}$, absorbing states 0 and n, and transition probabilities $p_{i,i+1} = p_{i,i-1} = \frac{1}{2}$ for $i \in \{1, \ldots, n-1\}$. We know such a walk has probability i/n of reaching state n given starting point i (make sure you recall how to prove this using techniques from Part A probability!) Considering the motion of the Brownian particle to be the continuous analogue of this discrete random walk, we might guess that the survival probability is y/a. Let us now prove this, and in the process develop some ideas which are useful in several situations.

Continuous production of particles at y. Instead of considering a single particle, we consider particles produced continuously at y, evolving according to the SDE, and subject to absorption at 0 and b. We assume that this system reaches a steady state, and consider the steady state probability density of the corresponding particles at (x, t) as a *concentration* of particles at (x, t). In order to estimate the probabilities of absorption at each end point we consider the *fluxes* of particles through the "walls" at 0 and a.

The Fokker-Planck equation corresponding to the SDE above is

$$p_t = Dp_{xx}\,.$$

The production of particles at $x = y$ can be treated as a Dirac delta function input on the RHS, and since the exact rate of production will not matter, we can write:

$$c_t = Dc_{xx} + D\delta(x - y)\,.$$

We have renamed the dependent variable c to remind us that we are interpreting the probability density as a *concentration* of particles. At steady state we have

$$c_{xx} + \delta(x - y) = 0 \quad \text{subject to} \quad c(0) = c(a) = 0\,.$$

This boundary value problem can be solved in various ways. It is clear that the solution is continuous and piecewise linear on $[0, a]$ with a jump discontinuity of magnitude -1 in the derivative at $x = y$ (as $c_{xx} = 0$ for $x \neq y$). It must thus take the form

$$x = \begin{cases} \frac{c_0}{y}x & \text{if } x \in [0, y) \\ \frac{c_0}{y-a}(x - a) & \text{if } x \in [y, a] \end{cases}\,,$$

where the constant c_0 is to be determined. The change in slope at $x = y$ gives $c_0 = \frac{y(a-y)}{a}$. We quickly find that the flux outwards at 0, namely $c_x(0) = 1 - \frac{y}{a}$, while the flux outwards at a, namely $-c_x(a) = \frac{y}{a}$. The desired probability is thus the flux ratio:

$$\frac{-c_x(a)}{c_x(0) - c_x(a)} = \frac{y}{a}\,.$$

Note that for any fixed $y > 0$, as $a \to \infty$, the probability of eventual absorption at 0 approaches 1, while the probability of escape to infinity approaches 0, showing that Brownian motion in 1D is recurrent. However, in our calculations of the MFPT in the previous example, we found that the MFPT to 0 is infinite. Putting together these calculations confirms that Brownian motion in 1D is, in fact, *null recurrent*.

The method above suggest an even simpler approach. Since the value of c_0 is clearly not relevant to the probabilities of eventual absorption, we can instead of a delta function input consider a new boundary condition. In other words, we consider the boundary value problem

$$c_{xx} = 0, \quad c(0) = c(a) = 0,\ c(y) = c_0\,,$$

for some arbitrary constant c_0, and then solve separately on the domains $[0, y]$ and $[y, a]$ to obtain the same fluxes upto a constant of proportionality. We will return to this idea below.

A more complicated, but flexible, Fourier series approach. Although the approach we took above is intuitive and natural, we now consider a more complicated, but more flexible, point of view for solving $c_{xx} + \delta(x-y) = 0,\ c(0) = c(a) = 0$, which gives us the solution as a Fourier series.

We set $\mathcal{D} = \frac{\partial^2}{\partial x^2}$ and first solve the eigenvalue problem

$$\mathcal{D}u = \lambda u,\ u(0) = u(a) = 0, \quad \text{giving} \quad \lambda_n = -\frac{n\pi}{a},\ u_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}\,.$$

(Note that the eigenfunctions are orthogonal to each other, and have been normalised.) We now try to represent the solution to $\mathcal{D}c(x) = -\delta(x-y)$, $c(0) = c(a) = 0$, as a linear combination of eigenfunctions, say

$$c(x) = \sum_{n=1}^{\infty} C_n(y) u_n(x)\,,$$

with unknown coefficients $C_n(y)$ dependent on y. Applying $\mathcal{D}$ gives

$$\mathcal{D}c(x) = \sum_{n=1}^{\infty} C_n(y)\mathcal{D}u_n(x) = \sum_{n=1}^{\infty} C_n(y)\lambda_n u_n(x) = -\delta(x-y)\,.$$

Multiplying through by $u_m(x)$ and integrating from 0 to a gives

$$\sum_{n=1}^{\infty} C_n(y)\lambda_n \delta_{n,m} = C_m(y)\lambda_m = -u_m(y)\,.$$

We thus have the solution

$$c(x) = \sum_{n=1}^{\infty} \frac{u_n(x)u_n(y)}{-\lambda_n} = \sum_{n=1}^{\infty} \frac{2\sin(n\pi x/a)\,\sin(n\pi y/a)}{n^2\pi^2/a}\,.$$

(It may not be immediately obvious that $c(y) = \frac{y(a-y)}{a}$, but this can be confirmed if we write $2\sin^2(n\pi y/a) = \cos(2n\pi y/a) - 1$, and write $\frac{y(a-y)}{a} = \sum_{n=0}^{\infty} a_n \cos(2n\pi y/a)$, not forgetting the constant term at the start.) Finally, we compute the outward fluxes at 0 and a, namely $c_x(0)$ and $-c_x(a)$, giving

$$c_x(0) = \sum_{n=1}^{\infty} \frac{2\sin(n\pi y/a)}{n\pi}, \quad -c_x(a) = \sum_{n=1}^{\infty} \frac{2(-1)^{n+1}\sin(n\pi y/a)}{n\pi}.$$

Adding together we can confirm that we get the total flux

$$c_x(0) - c_x(a) = \sum_{n=1}^{\infty} \frac{2(1-(-1)^n)\sin(n\pi y/a)}{n\pi} = 1.$$

(We can check that the LHS is, indeed the Fourier sine series for the constant function 1 on $[0, a]$.) The desired probability is thus the flux ratio:

$$\frac{-c_x(a)}{c_x(0) - c_x(a)} = \sum_{n=1}^{\infty} \frac{2(-1)^{n+1}\sin(n\pi y/a)}{n\pi} = \frac{y}{a},$$

as expected. (To check the last equality we can simply compute the Fourier sine series for y/a on $[0, a]$.)

While the Fourier series approach appears considerably more complicated, it does allow us to approach problems in higher dimensions and more complicated geomtries where the intuitive approach might fail.

4.3 Brownian particle in 1D with drift

We now consider a Brownian particle which, apart from diffusing, experiences a deterministic "force" as well. The SDE we consider is very simple, with *constant* drift and diffusion:

$$dX = -\alpha\, dt + \sqrt{2D}\, dW.$$

Here α and D are positive constants – we can think of the drift term as a constant "breeze" blowing the particle to the left, while at the same it is subject to the random diffusive force.

Probability of arriving at one end point before the other. We let $0 < a$, and consider the probability that a particle initially at $y \in (0, a)$ reaches a before reaching 0. Using our experience from the previous examples, we treat an auxiliary problem, and consider the stationary Fokker-Planck equation

$$0 = \frac{d}{dx}\left(\alpha c + D\frac{dc}{dx}\right).$$

on the two domains $[0, y]$ and $[y, a]$, subject to the boundary conditions $c(0) = c(a) = 0$, $c(y) = c_0$, where $c_0 > 0$ is arbitrary. Defining $h = \alpha/D$, we find

$$c(x) = \frac{c_0(1-e^{-hx})}{1-e^{-hy}} \quad (x \in [0, y]), \qquad c(x) = \frac{c_0(e^{h(a-x)}-1)}{e^{h(a-y)}-1} \quad (x \in (y, a]).$$

The fluxes outwards at 0 and a are, respectively,

$$Dc_x(0) = \frac{Dc_0 h}{1 - e^{-hy}}, \qquad -Dc_x(a) = \frac{Dc_0 h}{e^{h(a-y)} - 1}$$

The probability that the particle arrives at a before arriving at the origin is

$$\frac{-c_x(a)}{-c_x(a) + c_x(0)} = \frac{e^{hy} - 1}{e^{ha} - 1} \to \frac{y}{a} \quad (\text{as } h \to 0)\,.$$

Note that this is consistent with the case of zero drift.

Mean first passage time to zero. Let us now consider the mean first passage time to zero, $\tau(y)$, which satisfies the boundary value problem

$$-1 = \frac{d}{dy}(-\alpha\tau + D\tau_y)\,, \quad \tau(0) = \tau(a) = 0\,.$$

We solve easily to get

$$\tau(y) = \frac{y}{\alpha} - \frac{a}{e^{ha} - 1}\,\frac{e^{hy} - 1}{\alpha}\,.$$

We can check that $\lim_{\alpha\to 0}\tau(y) = y(a-y)/(2D)$ as expected from our analysis of the case without drift (we can see this by writing the expression as a single fraction, and applying l'Hôpital's rule twice). On the other hand, if we fix $\alpha, D > 0$, $\lim_{a\to\infty}\tau(y) \to \frac{y}{\alpha}$, namely the mean first passage time remains *finite* in the limit of an unbounded interval. Note that this is true however small $\alpha > 0$ may be.

A more interesting drift term. We now consider a problem where the drift "force" decreases in magnitude away from the origin where it takes its maximum value. It is not immediately obvious whether we expect the MFPT to 0 to be finite or not in the limit where we allow the interval to become unbounded.

We consider the SDE:

$$dX = -\frac{2DX}{1 + X^2}\,dt + \sqrt{2D}dW\,.$$

(The particular choice of drift term is to make the problem tractable.) The MFPT satisfies

$$\frac{-1}{D} = \frac{-2y}{1 + y^2}\tau_y + \tau_{yy}\,, \quad \tau(0) = \tau(a) = 0\,.$$

Multiplying by the integrating factor $(1 + y^2)^{-1}$ and integrating once gives

$$\tau_y = -\frac{1}{D}(1 + y^2)\tan^{-1}(y) + C\,(1 + y^2)$$

for some constant C. Integrating again from 0 to y (with the help of a computer algebra package!), and noting that $\tau(0) = 0$, gives

$$\tau(y) = \frac{2\ln(y^2 + 1) + y^2 - (2y^3 + 6y)\tan^{-1}(y)}{6D} + C(y + y^3/3)\,.$$

Setting $\tau(a) = 0$ gives

$$C = \frac{2(a^3 + 3a)\tan^{-1}(a) - 2\ln(a^2 + 1) - a^2}{2D(a^3 + 3a)} \to \frac{\pi}{2D} \;\text{ as } a \to \infty\,.$$

Thus for each fixed y, $\tau(y)$ remains bounded as $a \to \infty$ (i.e., zero is positive recurrent).

4.4 Brownian particle between two concentric spheres

We now consider a 3-dimensional problem where, however, the symmetry allows us effectively to reduce the problem to a one-dimensional one. We start with a problem involving only diffusion (and no drift). The example will highlight some fundamental differences between the behaviour of a Brownian particle in 3 dimensions and the one-dimensional situation.

Our Brownian particle evolves in $\mathbb{R}^3$ according to the SDE

$$\mathrm{d}X = \sqrt{2\mathrm{D}}\,\mathrm{d}W_x,\ \mathrm{d}Y = \sqrt{2\mathrm{D}}\,\mathrm{d}W_y\,,\ \mathrm{d}Z = \sqrt{2\mathrm{D}}\,\mathrm{d}W_z\,,\ (X(0), Y(0), Z(0)) = (x_0, y_0, z_0)\,,$$

where D is a positive constant, and W_x, W_y and W_z are independent Brownian motions. Consider two concentric absorbing spheres of radii a and b centred at the origin in $\mathbb{R}^3$, and suppose that

$$a < r_0 := \sqrt{x_0^2 + y_0^2 + z_0^2} < b\,.$$

Probability that the particle first reaches one of the spheres. The Fokker-Planck equation is

$$c_t = D\nabla^2 c.$$

With the experience of the 1D problem, we consider the auxiliary steady state problem where the concentration of particles is held at a constant value c_0 on the sphere of raidus r_0. Spherical symmetry of the problem means that we can assume that $c = c(r)$, giving

$$0 = \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2\frac{\mathrm{d}c}{\mathrm{d}r})\,, \quad \text{subject to} \quad c(a) = c(b) = 0,\ c(r_0) = c_0\,,$$

where c_0 is arbitrary. The general solution of the ODE is $A + B/r$ with constants A and B. On $r \in [a, r_0]$ we have $A + B/a = 0, A + B/r_0 = c_0$, giving

$$c(r) = \frac{c_0}{1 - a/r_0}(1 - a/r),$$

and similarly, for $r \in [r_0, b]$, we have

$$c(r) = \frac{c_0}{1 - b/r_0}(1 - b/r)\,.$$

To complete the problem, we note that the outward fluxes at $r = a$ and $r = b$ are, respectively,

$$4\pi D a^2 c_r(a) = \frac{4\pi D a c_0 r_0}{r_0 - a}\,, \quad \text{and} \quad -4\pi D b^2 c_r(b) = \frac{4\pi D b c_0 r_0}{b - r_0}\,.$$

The desired probability is thus

$$\frac{a^2 c_r(a)}{a^2 c_r(a) - b^2 c_r(b)} = \frac{a}{r_0}\,\frac{b - r_0}{b - a}\,.$$

In the limit $b \to \infty$, the outward flux at b approaches $4\pi D c_0 r_0 > 0$, and the probability of absorption at $r = a$ approaches $\frac{a}{r_0}$. This indicates a fundamental difference from the one-dimensional situation, where the probability of the particle "escaping to infinity" was zero, while here it is $1 - a/r_0$. In fact, Brownian motion is *transient* in dimensions 3 or higher.

The limit where $b \to \infty$ and $r_0 \to \infty$. Recall that the steady state concentration of particles in $[a, r_0]$ is $c(r) = \frac{c_0}{1-a/r_0}(1 - a/r)$. In the limit that $r_0 \to \infty$ (which also implies that $b \to \infty$), we get the steady state concentration

$$c(r) = c_0(1 - \frac{a}{r}).$$

In this case the flux through the sphere with radius a is equal to:

$$\lim_{r_0 \to \infty} 4\pi D a^2 c_r(a) = 4\pi D a c_0 \,.$$

This expression will be important when we consider models of second order reactions below.

Mean first passage time. We can also, if desired, work out the mean time τ to absorption of the particle. By spherical symmetry, $\tau = \tau(r)$. For $r \in (a, b)$, τ satisfies

$$-1 = D\nabla^2\tau = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\tau}{dr}\right), \quad \tau(a) = \tau(b) = 0\,.$$

We solve to get

$$\tau(r) = \frac{(r-a)(b-r)(a+b+r)}{6Dr}\,.$$

The fact that $\lim_{b\to\infty}\tau(r) = \infty$ should come as no surprise since the particle has a finite probability of escaping to infinity.

You are asked to do compute the first passage time for a particle between two absorbing spheres in *general dimensions* on Exercise Sheet 4.

4.5 Brownian particle between two spheres with "gravity"

Let us now consider a modification of the previous two-concentric-spheres problem where in addition to diffusion we have an advective gravity-like inverse square force acting on the particles, directed towards the origin. Our goal is to examine how this affects the probability of absorption at each of the spheres, and the probability of escape to infinity in the limit that the radius of the larger sphere becomes infinite.

Letting $R^2 = X^2 + Y^2 + Z^2$, a particle evolves according to

$$dX = \sqrt{2D}\,dW_x - \alpha\frac{X\,dt}{R^3}, \quad dY = \sqrt{2D}\,dW_y - \alpha\frac{Y\,dt}{R^3}, \quad dZ = \sqrt{2D}\,dW_z - \alpha\frac{Z\,dt}{R^3},$$

with $(X(0), Y(0), Z(0)) = (x_0, y_0, z_0)$. Here $\alpha > 0$ measures the strength of the gravitational force. As before we assume that the particle has initial position in between two concentric absorbing spheres with centre zero, and radii a and b, with $a < r_0 := \sqrt{x_0^2 + y_0^2 + z_0^2} < b$. The corresponding Fokker-Planck equation is now

$$c_t = D\nabla^2 c + \alpha\nabla \cdot (c\boldsymbol{e}_r/r^2)\,,$$

where we have written $\boldsymbol{e}_r$ for the unit vector in the radial direction (namely, $(x/r, y/r, z/r)^t$). By the spherical symmetry of the problem, we can search for radial solutions (i.e., $c = c(r)$).

Namely, writing $\nabla^2(\ )$ and $\nabla\cdot(\ )$ in spherical coordinates and keeping only the radial terms, we have,

$$\frac{\partial c}{\partial t} = \frac{D}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial c}{\partial r}) + \frac{\alpha}{r^2}\frac{\partial}{\partial r}(r^2\frac{c}{r^2}), \quad \text{so, at steady state,} \quad \frac{d}{dr}\left(r^2\frac{dc}{dr} + hc\right) = 0\,,$$

where $h := \alpha/D$. In order to find the probabilities of absorption at $r = a$ and at $r = b$, we set up the auxiliary problem as before, i.e., set $c(a) = c(b) = 0$, $c(r_0) = c_0 > 0$ and solve the steady state ODE on the domains $[a, r_0]$ and $[r_0, b]$ one at a time to get

$$c = c_0\left(1 - \frac{e^{h/r_0} - e^{h/r}}{e^{h/r_0} - e^{h/a}}\right)\ (r \in [a, r_0]), \quad c = c_0\left(1 - \frac{e^{h/r_0} - e^{h/r}}{e^{h/r_0} - e^{h/b}}\right)\ (r \in [r_0, b])\,.$$

The fluxes at $r = a$ and $r = b$ are, respectively

$$4\pi D a^2 c_r(a) = \frac{4\pi D h c_0 e^{h/a}}{e^{h/a} - e^{h/r_0}}, \quad \text{and} \quad -4\pi D b^2 c_r(b) = \frac{4\pi D h c_0 e^{h/b}}{e^{h/r_0} - e^{h/b}}\,.$$

In the limit as $h \to 0$ (the gravitational force is absent), we get the fluxes computed in the previous example, namely

$$\lim_{h\to 0} 4\pi D a^2 c_r(a) = \frac{4\pi D a c_0 r_0}{r_0 - a}, \quad \lim_{h\to 0}(-4\pi D b^2 c_r(b)) = \frac{4\pi D b c_0 r_0}{b - r_0}\,.$$

For fixed h, but letting $b \to \infty$ we get the outward flux at b,

$$-\lim_{b\to\infty} 4\pi D b^2 c_r(b) = \frac{4\pi D h c_0}{e^{h/r_0} - 1}\,.$$

The probability of escape to infinity is thus

$$\left(\frac{4\pi D h c_0}{e^{h/r_0} - 1}\right)\left(\frac{4\pi D h c_0}{e^{h/r_0} - 1} + \frac{4\pi D h c_0 e^{h/a}}{e^{h/a} - e^{h/r_0}}\right)^{-1} = \frac{e^{-h/r_0} - e^{-h/a}}{1 - e^{-h/a}}\,.$$

This approaches $1 - a/r_0$ as $h \to 0$ (no gravity), and approaches 0 as $h \to \infty$ (very strong gravity), as we woud expect.

In the limit that both b and r_0 tend to infinity, we have the flux through a being:

$$\lim_{r_0\to\infty} 4\pi D a^2 c_r(a) = \frac{4\pi D h c_0 e^{h/a}}{e^{h/a} - 1} = \frac{4\pi D h c_0}{1 - e^{-h/a}}\,,$$

which approaches, as expected, $4\pi D a c_0$ as $h \to 0$ (no gravity).

Mean first passage time. In this case the equation for the MFPT τ can be written

$$-1 = -\frac{\alpha}{r^2}\mathbf{e}_r\cdot\nabla\tau + D\nabla^2\tau\,.$$

Writing $\tau = \tau(r)$ and using expressions for $\nabla(\ )$ and $\nabla^2(\ )$ in sherical polar coordinates we get

$$-1 = -\frac{\alpha}{r^2}\frac{d\tau}{dr} + \frac{D}{r^2}\frac{d}{dr}(r^2\frac{d\tau}{dr}) \quad \Rightarrow \quad -r^2 = \frac{d}{dr}\left(-\alpha\tau + Dr^2\frac{d\tau}{dr}\right)\,.$$

Integrating gives

$$\frac{d\tau}{dr} - \frac{\alpha}{Dr^2}\tau = \frac{-r}{3D} + \frac{C_1}{Dr^2}$$

for some constant C_1. Multiplying by an integrating factor and integrating from a to r gives

$$\tau(r) = \frac{e^{-h/r}}{D}\left[\int_a^r \frac{-se^{h/s}}{3}\,ds + \frac{C_1}{h}(e^{h/a} - e^{h/r})\right],$$

where we have written $h := \alpha/D$. From the boundary condition $\tau(b) = 0$, we can calculate

$$C_1 = \frac{h}{3}\left(\int_a^b se^{h/s}\,ds\right)(e^{h/a} - e^{h/b})^{-1},$$

i.e.,

$$\tau(r) = \frac{e^{-h/r}}{3D}\left[\left(\int_a^b se^{h/s}\,ds\right)\frac{(e^{h/a} - e^{h/r})}{(e^{h/a} - e^{h/b})} - \int_a^r se^{h/s}\,ds\right],$$

We can, if desired, evaluate the MFPT numerically.

4.6 Reaction-diffusion: zeroth order production in 1D

Consider molecules of a single species A where each molecule diffuses in a thin tube, modelled as the interval $[0, 1]$ with position $X \in [0, 1]$ determined by the SDE

$$dX = \sqrt{2D}\,dW.$$

We assume that molecules are absorbed at 0 and 1. Additionally molecules are produced in $(0, 1)$ by some reaction.

Let us suppose that the molecules are produced according to the reaction

$$0 \xrightarrow{k} \mathsf{A}.$$

Here k is a deterministic mass action constant. We combine the reaction and diffusion processes by first considering the Fokker-Planck equation corresponding to the diffusion SDE, and then adding in the reaction terms to get the standard reaction diffusion PDE for the concentration, which in this case reads:

$$c_t = Dc_{xx} + k.$$

Steady state concentration. We easily find the steady state concentration of A subject to $c(0) = c(1) = 0$: we get

$$c(x) = \frac{k}{2D}x(1 - x).$$

Mean first passage time. We can also compute the mean first passage time of the molecules to the boundaries of the interval. For a molecule with initial position $y \in (0,1)$, this is computed in the usual way (do it!) to be

$$\tau(y) = \frac{y}{2D}(1-y)\,.$$

As molecules are produced uniformly at random throughout $(0,1)$, we simply average over all initial positions to get the expected time any individual molecules stays in $(0,1)$ before absorption at the boundary, namely,

$$\int_0^1 \tau(y)\,\mathrm{d}y = \int_0^1 \frac{y}{2D}(1-y)\,\mathrm{d}y = \frac{1}{12D}\,.$$

Time-dependent distribution. It is a little trickier to compute the full time-dependent distribution of molecules. For this, we need to specify an initial condition, which, for simplicity, we take to be $c(x,0) = 0$. As usual we first consider the homogeneous problem subject to the boundary conditions, namely

$$c_t - Dc_{xx} = 0\,.$$

We compute the (normalised) eigenfunctions and eigenvalues of $\frac{\partial^2}{\partial x^2}$ as usual, giving

$$u_n = \sqrt{2}\sin(n\pi x), \quad \lambda_n = -n^2\pi^2\,,$$

and write the solution in the form

$$c(x,t) = \sum_{n=1}^{\infty} a_n(t)u_n(x)\,, \quad \Rightarrow \quad c_t - Dc_{xx} = \sum_{n=1}^{\infty}(a_n'(t) - Da_n(t)\lambda_n)u_n(x) = k\,.$$

Multiplying the latter equation through by $u_m(x)$ and integrating from 0 to 1 gives the ODE for $a_n(t)$

$$a_n'(t) - D\lambda_n a_n = \frac{k}{n\pi}(1-(-1)^n)\,,$$

which solves, subject to $a_n(0) = 0$, to give

$$a_n(t) = \frac{k}{Dn^3\pi^3}(1-(-1)^n)[1-\exp(-Dn^2\pi^2 t)]\,.$$

The solution is thus

$$c(x,t) = \sum_{n=1}^{\infty} \frac{\sqrt{2}\,k}{Dn^3\pi^3}(1-(-1)^n)\,\sin(n\pi x)\,\left(1-e^{-Dn^2\pi^2 t}\right)\,.$$

We have

$$\lim_{t\to\infty} c(x,t) = \sum_{n=1}^{\infty} \frac{\sqrt{2}\,k}{Dn^3\pi^3}(1-(-1)^n)\,\sin(n\pi x)\,,$$

which is, indeed, the Fourier sine expansion of $\frac{k}{2D}x(1-x)$ as expected.

4.7 Reaction-diffusion: a point source and first order reproduction in 1D

Consider a slightly more complex model where the particles evolve as before on $(0, 1)$ according to $\mathrm{d}X = \sqrt{2D}\,\mathrm{d}W$, but now reproduce according to the first order reaction

$$A \xrightarrow{k} 2A\,.$$

Additionally, we have a point source of particles at $y \in (0, 1)$, a reflecting boundary at 0 and an absorbing boundary at 1. This time we get the reaction-diffusion equation

$$c_t = Dc_{xx} + kc + \delta(x - y)\,, \quad c_x(0) = 0 = c(1)\,.$$

We are interested in the steady state solution.

The Fourier approach. We first consider solutions to the eigenvalue problem

$$Dc_{xx} + kc = \lambda c$$

subject to the given boundary conditions. Assuming that $\lambda < 0$, we compute the normalised eigenfunctions

$$u_n(x) = \sqrt{2}\cos((n + 1/2)\pi x)\,, \quad \text{with eigenvectors} \quad \lambda_n = k - D(n + 1/2)^2\pi^2\,.$$

Note that the assumption that $\lambda_n < 0$ implies, in particular, that $\lambda_0 < 0$, i.e., $k < D\pi^2/4$. We now look for solutions to $Dc_{xx} + kc + \delta(x - y) = 0$ with the same boundary conditions in the form $c(x) = \sum_{n=0}^{\infty} a_n(y)u_n(x)$. Substituting in gives

$$\sum_{n=0}^{\infty} a_n(y)\lambda_n u_n(x) = -\delta(x - y)\,.$$

Multiplying by $u_m(x)$ and integrating from 0 to 1, we get

$$a_n(y)\lambda_n = -u_n(y) \quad \Rightarrow \quad c(x) = \sum_{n=0}^{\infty} \frac{u_n(x)u_n(y)}{-\lambda_n} = \sum_{n=0}^{\infty} \frac{2\cos((n + 1/2)\pi x)\,\cos((n + 1/2)\pi y)}{D(n + 1/2)^2\pi^2 - k}\,.$$

A simpler approach giving an explicit solution. Let us now consider a slightly simpler approach, which gives the solution in explicit form, and also highlights that the condition $k < D\pi^2/4$ is necessary and sufficient for physically meaningful solutions. Clearly solutions to the steady state equation

$$Dc_{xx} + kc = -\delta(x - y)$$

satisfy $Dc_{xx} + kc = 0$ on $[0, y)$ and $(y, 1]$, with the derivative of c decreasing by $1/D$ as we pass through y (i.e., $\lim_{x\to y+} c'(x) - \lim_{x\to y-} c'(x) = -1/D$). Let us suppose a solution exists, and satisfies $c(y) = c_0$. Defining $\omega = \sqrt{k/D}$, we can then solve on $[0, y]$ and $[y, 1]$ to get

$$c(x) = \begin{cases} \dfrac{c_0\cos(\omega x)}{\cos(\omega y)} & (x \in [0, y])\,, \\ \dfrac{c_0\sin(\omega(1 - x))}{\sin(\omega(1 - y))} & (x \in [y, 1])\,. \end{cases}$$

The derivative-jump condition amounts to

$$c_0\omega(\cot(\omega(1-y)) - \tan(\omega y)) = \frac{1}{D},$$

giving $c_0 = (D\omega(\cot(\omega(1-y)) - \tan(\omega y)))^{-1} > 0$, provided $\cot(\omega(1-y)) - \tan(\omega y)) > 0$. We can confirm that a physically meaningful solution exists if and only if $\omega < \pi/2$, namely $k < D\pi^2/4$. On the one hand, if $\omega < \pi/2$, then by observation c is positive on $[0,1)$ and zero at $x = 1$. Moreover, the derivative-jump condition, which is equivalent to

$$\frac{\tan(\omega(1-y)) + \tan(\omega y)}{\tan\,\omega} > 0,$$

clearly holds for any $y \in (0,1)$. On the other hand, suppose $\omega > \pi/2$. Then $c \geq 0$ on $[0,y)$ implies that $\omega y < \pi/2$ (if $\omega y = \pi/2$, the solution is undefined, and if $\omega y > \pi/2$, then $\cos(\omega x)$ can take all signs on $[0,y)$). This implies that $\lim_{x\to y+} c'(x) < 0$, and hence $\lim_{x\to y+} c'(x) < 0$. But $c > 0$ on $[y,1)$ and $\lim_{x\to y+} c'(x) < 0$ together imply that $\omega(1-y) < \pi/2$. Together $\omega y < \pi/2$ and $\omega(1-y) < \pi/2$ imply that $\omega < \pi$; consequently $\tan\,\omega < 0$, but $\tan(\omega(1-y)) + \tan(\omega y) > 0$, and the derivative-jump condition cannot be satisfied.

The limit $y \to 0$. It is interesting to consider the limit $y \to 0$. In this case, comparing the two forms of the solution, we get

$$c(x) = \sum_{n=0}^{\infty} \frac{2\cos((n+1/2)\pi x)}{D(n+1/2)^2\pi^2 - k} = \frac{\sin(\omega(1-x))}{D\omega\cos\,\omega} = \frac{1}{D\omega}(\tan(\omega)\,\cos(\omega x) - \sin(\omega x)).$$

(You can check by Fourier expanding the latter solution that these expressions are, in fact, equivalent.) Intuition tells us that in the limit, moving a delta source to a reflecting boundary is equivalent to insisting on unit flux through through this boundary, corresponding to a Neumann boundary condition at 0; i.e., to the problem:

$$Dc_{xx} + kc = 0, \quad c(1) = 0, \;\; c_x(0) = -1/D.$$

The above boundary value problem indeed solves to give

$$c(x) = \frac{1}{D\omega}(\tan(\omega)\,\cos(\omega x) - \sin(\omega x)),$$

as expected.

4.8 Reaction-diffusion: a naive model of second order reactions

[See Erban and Chapman for more details.] Consider a second-order reaction where molecules of two species A and B diffuse in some chamber in $\mathbb{R}^3$ of volume V, and react when they come sufficiently close to each other. In other words, we have the reaction

$$\mathsf{A} + \mathsf{B} \overset{k}{\to} *$$

where, the product $*$ may be any complex.

Let us suppose that A and B have diffusion coefficients D_A and D_B respectively. With mass action kinetics, the reaction intensity would be $\frac{k}{V}A(t)B(t)$ for some constant k. We could consider this as the rate at which reactions occurs in unit time given molecule numbers $A(t)$ and $B(t)$.

We could aim to model the situation at a molecular level by working in the frame of reference of some molecule of A and asking about the probability per unity time of this molecule reacting with a molecule of B. We suppose that the concentration of molecules of B sufficiently far from the chosen molecule of A at time t is $\frac{B(t)}{V}$. Working in the frame of reference of our molecule of A (i.e., we take its centre to be the origin), we assume that the reaction occurs when a molecule of B comes "sufficiently close" to A, i.e., comes within some distance, say R, of the molecule of A. We refer to R as the "reaction radius". Working in the frame of reference of a molecule of A amounts to setting the diffusion coefficient of B to be $D_A + D_B$.

To calculate the probability per unit time of a reaction occurring, we now recall the case of a sphere with centre at the origin, and radius a, with a Brownian particle diffusing outside the sphere. Holding the concentration of particles to be c_0 at $r = r_0 > a$, and letting $r_0 \to \infty$, we ended up with a steady state concentration, and flux through the sphere of radius a of, respectively

$$c(r) = c_0(1 - \frac{a}{r}), \quad \text{and} \quad \lim_{r_0 \to \infty} 4\pi D a^2 c_r(a) = 4\pi D a c_0\,.$$

In this case, $D = D_A + D_B$, $c_0 = B(t)/V$ and $a = R$ (the reaction radius). The probability per unit time of a molecule of B being absorbed at R (i.e., a reaction occurring with this particular molecule of A) is then $4\pi(D_A + D_B)R\frac{B(t)}{V}$. If there are $A(t)$ molecules of A in the chamber, the total probability per unit time of reactions occurring – i.e., the reaction intensity – should be $4\pi(D_A + D_B)R\frac{B(t)}{V}A(t)$.

Matching up this expression with the standard mass action intensity gives

$$\frac{k}{V}A(t)B(t) = 4\pi(D_A + D_B)RA(t)\frac{B(t)}{V} \quad \Rightarrow \quad R = \frac{k}{4\pi(D_A + D_B)}\,.$$

We can thus, in theory compute the reaction radius, given knowledge of the rate constant of the reaction, and diffusion coefficients of the reactants.

4.9 Reaction-diffusion: a more sophisticated model of second order reactions

In the naive model in the previous subsection, we modelled a reaction of the form

$$A + B \xrightarrow{k} *$$

(where, the product $*$ is not relevant). In that model, a reaction occurred for certain when a molecule of B came within a distance of R from a molecule of A. This model leads, however, to tiny values of the reaction radius R, suggesting that reactions do not occur unless molecules come unphysically close to each other (details in Erban and Chapman). This also leads to practical consequences where, in order to simulate a system with second order reactions, we need to take tiny time-steps Δt, for otherwise we are very likely to "miss" the reaction events, by simply not observing that two molecules came within a distance of R from each other.

An alternative is to suppose that a reaction occurs *with some fixed probability* λ per unit time whenever a molecule of B comes within some distance R of a molecule of A. For $r > R$, molecules of B simply diffuse; but for $r < R$, they are consumed with intensity λ, equivalent to the occurrence of the first order reaction

$$B \xrightarrow{\lambda} 0 .$$

We now expect R, which we can all the *influence radius* of the reaction to be larger than the reaction radius computed with the previous naive model. In Exercise Sheet 4, you are asked to set up the corresponding reaction-diffusion problem, solve it, and derive the relationship

$$k = 4\pi D \left(R - \sqrt{\frac{D}{\lambda}} \tanh\left(R\sqrt{\frac{\lambda}{D}} \right) \right) ,$$

between the mass action rate constant k, the influence radius R, the diffusion coefficient $D = D_A + D_B$, and λ, the intensity of consumption of molecules once they are within the influence radius. Note that we can "tune" this model, i.e., choose λ smaller so that R is larger. In simulations, this reduces the probability of missing reaction events simply because of our discretised Brownian motion. Taylor expanding for small λ gives

$$R \approx \left(\frac{3k}{4\pi\lambda} \right)^{1/3} ,$$

In simulations, we now choose our time-step Δt to that the mean distance covered in one step is much smaller than R, namely $\sqrt{2D\,\Delta t} \ll R$, equivalently, $\Delta t \ll R^2/(2D)$. For accurate capture of reaction events, we also require that time-steps Δt satisfy $\lambda\Delta t \ll 1$, or equivalently (by the approximation above)

$$\Delta t \ll \frac{4\pi R^3}{3k} .$$

(An alternative, related, model also appears in the 2023 Exam.)