Solutions to Problem Set 1b

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1 Intermediate asymptotics of a random walk

1.1 Derivation

Using the Kramers-Moyal expansion,

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - D_3\frac{\partial^3 c}{\partial x^3} + O(\tau) \tag{1}$$

and defining $\mathcal{D}_3 = D_3/\tau^{1/2}$, then

$$\frac{\partial c}{\partial t} \approx D\frac{\partial^2 c}{\partial x^2} - \tau^{1/2}\mathcal{D}_3\frac{\partial^3 c}{\partial x^3} \tag{2}$$

Expressing $c(x,t)$ as a function of the dimensionless groups $\zeta = \frac{x}{\sqrt{2Dt}}$, $\xi = \left(\frac{t}{\tau}\right)^{1/2}$ and $\eta = \frac{\mathcal{D}_3}{D^{3/2}}$, i.e.

$$\frac{c(x,t)}{M_0/\sqrt{2DT}} = \Phi(\zeta,\xi,\eta) \tag{3}$$

then, in the limit $\xi \to 0$ with finite ζ and constant η,

$$\frac{c(x,t)}{M_0/\sqrt{2DT}} = \phi(\zeta) + \xi\phi_1(\zeta) + O(\xi^2) \tag{4}$$

where $\phi_0(\zeta)$ is the zeroth-order solution

$$\phi_0 = \frac{e^{-\frac{\zeta^2}{2}}}{\sqrt{2\pi}} \tag{5}$$

Expecting that $\phi_1(\zeta) = \phi_0(\zeta)f(\zeta)$, then the first-order approximation to $c(x,t) = c_0(x,t) + c_1(x,t)$ may be written as

$$c_1(x,t) = \xi\frac{f(\zeta)\phi_0(\zeta)}{\sqrt{2Dt}} \tag{6}$$

which can be inserted into the first-order equation

$$\left[\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2}\right] c_1 = -\tau^{1/2}\mathcal{D}_3\frac{\partial^3 c_0}{\partial x^3} \tag{7}$$

giving

$$\left[\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2}\right] \frac{f(\zeta)\phi_0(\zeta)}{t^{1/2}\sqrt{2Dt}} = -\mathcal{D}_3\frac{\partial^3}{\partial x^3}\frac{\phi_0(\zeta)}{\sqrt{2Dt}} \tag{8}$$

Expanding the LHS,

$$\left[\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2}\right] \frac{f(\zeta)\phi_0(\zeta)}{t^{1/2}\sqrt{2Dt}} = -\frac{\phi_0}{2t^{3/2}\sqrt{2Dt}}[f''(\zeta) - \zeta f'(\zeta) + f(\zeta)] \tag{9}$$

and similarly the RHS,

$$-\mathcal{D}_3\frac{\partial^3}{\partial x^3}\frac{\phi_0(\zeta)}{\sqrt{2Dt}} = -\frac{\mathcal{D}_3}{(2Dt)^2}\phi_0(\zeta)(3\zeta - \zeta^3) \tag{10}$$

therefore

$$\frac{\phi_0}{2t^{3/2}\sqrt{2Dt}}[f''(\zeta) - \zeta f'(\zeta) + f(\zeta)] = \frac{\mathcal{D}_3}{(2Dt)^2}\phi_0(\zeta)(3\zeta - \zeta^3) \tag{11}$$

or

$$f''(\zeta) - \zeta f'(\zeta) + f(\zeta) = \frac{\mathcal{D}_3}{2^{1/2}D^{3/2}}(3\zeta - \zeta^3) = \frac{\eta}{\sqrt{2}}(3\zeta - \zeta^3) \tag{12}$$

A solution of this ODE has the form

$$f(\zeta) = \frac{\eta}{2\sqrt{2}}\zeta^3 + C\zeta \tag{13}$$

where C is a coefficient to be determined from additional considerations. Since the zeroth-order solution already has the right first and second moments, the same moments of the correction should be null, which is obviouly true for even moments. For the first moment:

$$\int xc_1(x,t)\,dx = \int \zeta\sqrt{2Dt}\xi\frac{f(\zeta)\phi_0(\zeta)}{\sqrt{2Dt}}\,dx = \int \zeta\left(\frac{\eta}{2\sqrt{2}}\zeta^3 + C\zeta\right)\xi\phi_0(\zeta)\,dx = 0 \tag{14}$$

which can be simplified, using the moments of the Gaussian $\phi_0(\zeta)$, to

$$3\frac{\eta}{2\sqrt{2}} + C = 0 \tag{15}$$

$$C = -3\frac{\eta}{2\sqrt{2}} \tag{16}$$

Therefore,

$$f(\zeta) = \frac{\eta}{2\sqrt{2}}\zeta^3 - 3\frac{\eta}{2\sqrt{2}}\zeta \tag{17}$$

$$c_1(x,t) = \left(\frac{\eta}{2\sqrt{2}}\zeta^3 - 3\frac{\eta}{2\sqrt{2}}\zeta\right)\xi\frac{\phi_0(\zeta)}{\sqrt{2Dt}} \tag{18}$$

1.2 Application to an asymmetric walk

First, the mean D_1 (drift v) will be calculated:

$$v = D_1 = \frac{M_1}{\tau} = pa - qa = \frac{a}{\tau}(2p-1) \tag{19}$$

then, the variable $\bar{x} = x - vt = x - a(2p-1)n$ must be used instead of x. In this new frame of reference, the transition probability reads

$$p_\tau(x) = p\delta(\bar{x} + a(2p-1) - a) + q\delta(\bar{x} + a(2p-1) + a) = p\delta(\bar{x} - 2aq) + q\delta(\bar{x} + 2ap) \tag{20}$$

and the next moments are

$$D = \frac{M_2}{2\tau} = \frac{1}{2\tau}(p(2aq)^2 + q(2ap)^2) = \frac{2}{\tau}a^2pq(p+q) \tag{21}$$

$$D_3 = \frac{M_3}{6\tau} = \frac{1}{6\tau}(p(2aq)^3 - q(2ap)^3) = \frac{4}{3\tau}a^3pq(q^2-p^2) \tag{22}$$

$$\mathcal{D}_3 = \frac{D_3}{\tau^{1/2}} = \frac{4}{3\tau^{3/2}}a^3pq(q^2-p^2) \tag{23}$$

$$\eta = \frac{\mathcal{D}_3}{D^{3/2}} = \frac{\sqrt{2}}{3\sqrt{pq}}\frac{q^2-p^2}{(p+q)^{3/2}} = \frac{\sqrt{2}(q-p)}{3\sqrt{pq(p+q)}} \tag{24}$$

And, from (18),

$$c_1(x,t) = \left(\frac{\eta}{2\sqrt{2}}\zeta^3 - 3\frac{\eta}{2\sqrt{2}}\zeta\right)\xi\frac{\phi_0(\zeta)}{\sqrt{2Dt}} = \frac{1}{12}\frac{q-p}{pq(p+q)a}\zeta(\zeta^2-3)\phi_0(\zeta) \tag{25}$$

which can be added to c_0 giving $c(x,t) = c_0(x,t) + c_1(x,t)$ to the order $O(\xi) = O(\tau/t)^{1/2}$.

For example, calculating this approximate solution for $p = 2/3$, $q = 2/3$, $n = t/\tau = 2$, as a function of $\zeta = x/\sqrt{2Dt}$, the graph at Figure 1 is obtained.

2 Similarity solution of a diffusion problem

The relevant quantities for the problem are the concentration $c - c_0$, the initial concentration c_0, the diffusion coefficient D ($[D] = L^2T^{-1}$), the flux at the boundary J ($[J] = [c]LT^{-1}$), the position x (L) and the time t (T). From a simple dimensional analysis, three dimensionless groups may be found:

$$\Pi = \frac{c - c_0}{c_0}; \quad \Pi_1 = \xi = \frac{x}{\sqrt{4Dt}}; \quad \Pi_2 = \eta = \frac{2J}{c_0\sqrt{D/t}} \tag{26}$$

and the relation between them may be written as

$$\Pi = \frac{c-c_0}{c_0} = \Phi(\xi,\eta) = \Phi\left(\frac{x}{\sqrt{4Dt}}, \frac{2J}{c_0\sqrt{D/t}}\right) \tag{27}$$

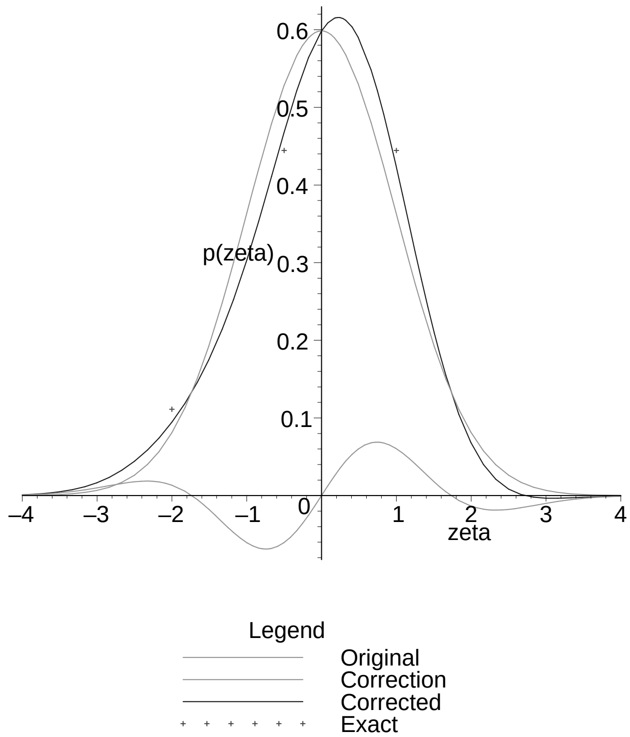

Figure 1: Approximation to a biased random walk.

Introducing this dimensionless function in the diffusion equation, via $c = c_0\Phi + c_0$,

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \tag{28}$$

$$\frac{\partial \Phi}{\partial t} = D\frac{\partial^2 \Phi}{\partial x^2} \tag{29}$$

where

$$\frac{\partial \Phi}{\partial t} = \frac{\partial \Phi}{\partial \xi}\frac{\partial \xi}{\partial t} + \frac{\partial \Phi}{\partial \eta}\frac{\partial \eta}{\partial t} = -\frac{\xi}{2}t\frac{\partial \Phi}{\partial \xi} + \frac{\eta}{2t}\frac{\partial \Phi}{\partial \eta} \tag{30}$$

and

$$\frac{\partial \Phi}{\partial x} = \frac{\partial \Phi}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial \Phi}{\partial \eta}\frac{\partial \eta}{\partial x} = \frac{1}{\sqrt{4Dt}}\frac{\partial \Phi}{\partial \xi}\frac{\partial^2 \Phi}{\partial x^2} = \frac{1}{4Dt}\frac{\partial^2 \Phi}{\partial \xi^2} \tag{31}$$

so that (29) may be rewritten as

$$-\frac{\xi}{2}t\frac{\partial \Phi}{\partial \xi} + \frac{\eta}{2t}\frac{\partial \Phi}{\partial \eta} = \frac{1}{4t}\frac{\partial^2 \Phi}{\partial \xi^2} \tag{32}$$

$$-\xi\frac{\partial \Phi}{\partial \xi} + \eta\frac{\partial \Phi}{\partial \eta} = \frac{1}{2}\frac{\partial^2 \Phi}{\partial \xi^2} \tag{33}$$

and the cancellation of the t factor hints that the dimensionless groups are adequate. The boundary conditions may be similarly translated, giving

$$\Phi(\infty, \eta) = 0 \tag{34}$$

for the initial and long-range behavior, and

$$-D\frac{1}{\sqrt{4Dt}}c_0\frac{\partial\Phi}{\partial\xi} = J \tag{35}$$

$$\frac{\partial\Phi}{\partial\xi} = -\eta, \quad \text{at } \xi = 0 \tag{36}$$

for the boundary, where again only dimensionless quantities appear.

One can proceed with the solution of this equation as usual, but since it was already done in the last Problem Set, the solution will be only checked.

The solution found previously was

$$c(x,t) = 2J\sqrt{\frac{t}{D\pi}}\exp\left(-\frac{x^2}{4Dt}\right) + \frac{Jx}{D}\left[\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) - 1\right] + c_0 \tag{37}$$

which can be translated as

$$\Phi(\xi,\eta) = \frac{1}{\sqrt{\pi}}\eta e^{-\xi^2} + \eta\xi(\operatorname{erf}(\xi) - 1) \tag{38}$$

Substituting this formula into the dimensionless diffusion equation, one has

$$-\xi\frac{\partial\Phi}{\partial\xi} + \eta\frac{\partial\Phi}{\partial\eta} = \frac{1}{2}\frac{\partial^2\Phi}{\partial\xi^2} \tag{39}$$

$$-\xi\eta(\operatorname{erf}(\xi) - 1) + \frac{\eta}{\sqrt{\pi}}e^{-\xi^2} + \xi\eta(\operatorname{erf}(\xi) - 1) = \frac{\eta}{\sqrt{\pi}}e^{-\xi^2} \tag{40}$$

which is clearly an identity, showing that the equations are indeed equivalent. Moreover,

$$\Phi(\infty,\eta) = \lim_{\xi\to\infty}\eta\xi(\operatorname{erf}(\xi) - 1) = 0 \tag{41}$$

and

$$\left.\frac{\partial\Phi}{\partial\xi}\right|_{\xi=0} = \eta(\operatorname{erf}(0) - 1) = -\eta \tag{42}$$

showing that the boundary conditions are also adequate.