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Problem Set 3

(1) **Order statistics**

(a) By symmetry, each X_i is equally likely to be the "splitting" value or the value that $Y_N^{(\alpha)}$ assumes. The conditional probability that $Y_N^{(\alpha)} = y$ given X_i is the splitting value is easy to calculate. We need $[\alpha N] - 1$ to fall to the left of y, $N - [\alpha N]$ values to fall to the right of y, and X_i to fall on y. Since the values of X_j for $j \neq i$ may be arranged in any order and are completely independent of each other we have

$$P\left(Y_N^\alpha = y | X_i \text{ "splits"}\right) = \overbrace{p(y)}^{X_i=y} \quad [P(y)]^{[\alpha N]-1} \left[1 - P(y)\right]^{N-[\alpha N]} \binom{N-1}{[\alpha N]-1}.$$

To get the unconditional probability, sum over all X_i with the probability that X_i is the splitting variable. Since each is equally likely and the value is the same for all X_i, we get the same result for the unconditional probability. This is the PDF we were looking for:

$$f_{N,\alpha}(y) = p(y) \left[P(y)\right]^{[\alpha N]-1} \left[1 - P(y)\right]^{N-[\alpha N]} \binom{N-1}{[\alpha N - 1]} = p(y) B(N-1, P(y), 2[\alpha N] - N - 1)$$

where $B(N, p, k)$ is the probability of ending up at $x = k$ after N steps of a Bernoulli walk with probability $P(y)$ of stepping to the right. For $\alpha \neq 0.5$, we are sampling at a location that scales approximately linearly with N. The width of the central region must scale at least this quickly, or we will quickly find ourselves outside the region where it holds. It was shown in an earlier lecture that the width of the central region for the Bernoulli walk with *symmetric* steps was $N^{3/4}$, and that for non-symmetric steps was even smaller. Thus we will always be outside of the central region for N large enough.

(b) Since the asymptotic expression should be globally valid, we shouldn't have to worry about removing the mean. This has the added advantage that we can follow almost exactly the derivation from lecture 16, save that we carry around the probability p of stepping to the right. We want to approximate $B(n, p, m)$, and will use this later to get an expression for $f_N(y)$. The distribution is

$$p\delta_{m,1} + (1-p)\delta_{m,-1}.$$

The DFT gives

$$\hat{p}(k) = pe^{ik} + (1-p)e^{-ik}.$$

The manipulations of lecture 16 may now be used in exactly the same way, save that we must show that

$$e^{-im(k'+\pi)}\hat{p}^n(k'+\pi) = (-1)^{n+m}e^{-imk'}\hat{p}^n(k').$$

Note that this is equivalent to showing $\hat{p}(k'+\pi) = (-1)^n\hat{p}(k')$ or

$$\hat{p}^n(k'+\pi) = \left(pe^{ik'+i\pi} + (1-p)e^{-ik'-i\pi}\right)^n = \left(-pe^{ik'} - (1-p)e^{-ik'}\right)^n = (-1)^n\hat{p}^n(k').$$

We are now reduced to evaluating $I(n,m)$ from equation (15) from lecture 16. Our $\psi(k)$ is different. In our case,

$$\psi(k,\xi) = ik\xi - \ln\left(pe^{ik} + (1-p)e^{-ik}\right).$$

Find k_s:

$$\begin{aligned}
\frac{\partial\psi}{\partial k} &= i\xi - \frac{ipe^{ik} - i(1-p)e^{-ik}}{pe^{ik} + (1-p)e^{-ik}} \\
\Rightarrow \qquad 0 &= -pe^{ik_s}(1-\xi) + (1-p)e^{-ik_s}(1+\xi) \\
\Rightarrow \quad e^{2ik_s} &= \frac{(1-p)}{p}\cdot\frac{1+\xi}{1-\xi} \\
\Rightarrow \qquad k_s &= \frac{i}{2}\ln\left(\frac{p}{1-p}\cdot\frac{1-\xi}{1+\xi}\right).
\end{aligned}$$

Find the second derivative of ψ at k_s:

$$\frac{\partial^2\psi}{\partial k^2} = \frac{pe^{ik} + (1-p)e^{-ik}}{pe^{ik} + (1-p)e^{-ik}} + \frac{\left(ipe^{ik} - i(1-p)e^{-ik}\right)^2}{\left(pe^{ik} + (1-p)e^{-ik}\right)^2} = 1 - \xi^2.$$

Now evaluate ψ at k_s:

$$\begin{aligned}
\psi(k_s) &= \frac{i^2\xi}{2}\ln\left(\frac{p}{1-p}\cdot\frac{1-\xi}{1+\xi}\right) - \ln\left(p\sqrt{\frac{1+\xi}{1-\xi}\cdot\frac{1-p}{p}} + (1-p)\sqrt{\frac{1-\xi}{1+\xi}\cdot\frac{p}{1-p}}\right) \\
&= \frac{\xi}{2}\ln\left(\frac{1-p}{p}\cdot\frac{1+\xi}{1-\xi}\right) + \frac{1}{2}\ln\left(\frac{1-\xi^2}{4p(1-p)}\right).
\end{aligned}$$

Since $\psi''(k_s)$ is the same as in lecture 16, the result we get is the same:

$$B(n,p,n\xi) \approx \frac{1+(-1)^{n+m}}{\sqrt{2\pi n(1-\xi^2)}}\,e^{-n\psi_s(\xi)}$$

where $\psi_s(\xi) = \psi(k_s)$ (evaluated above). It is only the exponent that is different for the non-symmetric walk.

This result may now be substituted into our expression for $f_N(y)$ as an approximation for the non-symmetric Bernoulli random walk. Since $n + m = (N-1) + (2[\alpha N] - N - 1) = 2([\alpha N] - 1)$, the $(-1)^{n+m}$ term in the numerator will always be 1. The rest of the approximation is not sensitive to the exact parity of n and m, and is a continuous function of these two quantiles. Thus as N gets large we can take large N approximations. In this limit $\xi = (2[\alpha N] - N - 1)/N \approx 2\alpha - 1$ and $N - 1 \approx N$. Thus

$$f_N(y) \approx \frac{2\,p(y)}{\sqrt{2\pi N(1-\xi^2)}}\,e^{-N\psi_s(\xi,P(y))}$$

where $\psi_s(\xi, P(y)) = \psi(k_s)$ with $p \to P(y)$ is given above (and we allow p to vary in addition to ξ) and $\xi = 2\alpha - 1$. It is possible to simplify this further. Clearly $1 + \xi = 2\alpha$ and $1 - \xi = 2(1-\alpha)$. Filling in these values into ψ_s yields

$$\psi_s(p) = \frac{2\alpha - 1}{2} \ln\left(\frac{1-p}{1-\alpha} \cdot \frac{\alpha}{p}\right) + \frac{1}{2} \ln\left(\frac{\alpha}{p} \cdot \frac{1-\alpha}{1-p}\right) = -(1-\alpha)\ln\left(\frac{1-p}{1-\alpha}\right) - \alpha \ln\left(\frac{p}{\alpha}\right).$$

Thus

$$f_N(y) \approx \frac{p(y)}{\sqrt{2\pi N\alpha(1-\alpha)}} \left(\frac{1-P(y)}{1-\alpha}\right)^{N(1-\alpha)} \left(\frac{P(y)}{\alpha}\right)^{N\alpha}.$$

(c) Expand the expression about y_α and let $\gamma = (y - y_\alpha) = \zeta\sqrt{N}$. (The derivatives are taken on the Maple page. It simplifies things a great deal.)

$$p(y)\left(\frac{1-P(y)}{1-\alpha}\right)^{N(1-\alpha)} \left(\frac{P(y)}{\alpha}\right)^{N\alpha} \approx p(y_\alpha)\left[1 + \gamma\frac{p'(y_\alpha)}{p(y_\alpha)} + \frac{\gamma^2}{2}\left(\frac{p''(y_\alpha)}{p(y_\alpha)} - \left(\frac{\alpha(1-\alpha)}{Np(y_\alpha)^2}\right)^{-1}\right)\right]$$

$$= p(y_\alpha)\left[1 + \zeta\sqrt{N}\frac{p'(y_\alpha)}{p(y_\alpha)} + \frac{N\zeta^2}{2}\left(\frac{p''(y_\alpha)}{p(y_\alpha)} - N\left(\frac{\alpha(1-\alpha)}{p(y_\alpha)^2}\right)^{-1}\right)\right].$$

At this point, we let $\gamma \to 0$ keeping ζ fixed and assume $p''(y)$ exists and is continuous at y_α. If we expanded $p(y)$ and and the other terms and took the limit separately, we would not need the second derivative to go zero and would only require that $p'(y)$ exists and is continuous at y_α. In any case, the lower power terms in N become negligible and we get the following approximation

$$p(y_\alpha)\left[1 - \frac{\gamma^2}{2}\left(\frac{\alpha(1-\alpha)}{Np(y_\alpha)^2}\right)^{-1}\right] \approx p(y_\alpha)\exp\left(-\frac{\gamma^2}{2\sigma_{Y_N}^2}\right)$$

Thus in the central region the pdf is well approximated by

$$\frac{1}{\sqrt{2\pi\sigma_{Y_N}^2}} \exp\left(-\frac{\gamma^2}{2\sigma_{Y_N}^2}\right)$$

which is a normal distribution centered on y_α with the variance suggested on the problem set. We are done.

(d) The variance of the mean is $1/N$ while the approximate variance of the median is

$$(1/2)^2/(Ne^{-0^2/2}) = 1/4N,$$

or about one fourth that of the mean.

(2) **A "Thin-Tailed" Random Walk**

(a) We want to calculate the following integral:

$$\hat{p}(k) = \int_{-\infty}^{\infty} \frac{2a\, e^{-ikx}\, \mathrm{d}x}{e^{bx} + e^{-bx}} = \frac{2a}{b}\int_{-\infty}^{\infty} \frac{e^{ik'y}\, \mathrm{d}y}{e^{y} + e^{-y}} = \frac{2a}{b} I(k')$$

where $k' = k/b$. To calculate $I(k')$ we must use contour integration. Integrate to the right along the x-axis and back to the left along the line parallel to the x-axis but shifted up a distance π. Poles of the integrand are where $e^y + e^{-y} = 0$ or $y = i(\pi/2 + \pi n)$. Thus the contour contains one pole with residue

$$\begin{aligned}\lim_{y\to i\pi/2} \frac{e^{-ik'y}(y - i\pi/2)}{e^y + e^{-y}} &= \lim_{y\to i\pi/2} \frac{-ik'e^{-ik'y}(y - i\pi/2) + e^{-ik'y}}{e^y - e^{-y}} \quad \text{by L'hôpital's rule}\\ &= \frac{e^{\pi k'/2}}{2i}.\end{aligned}$$

The integral along the bottom leg is $I(k')$ while the integral along the top leg (taking into account the reversed direction) is

$$\int_{-\infty}^{\infty} \frac{e^{-ik'(y+i\pi)}\,(-\mathrm{d}x)}{e^{y+i\pi} + e^{-y-i\pi}} = -\int_{-\infty}^{\infty} \frac{e^{-ik'y}e^{k'\pi}\,\mathrm{d}x}{-e^y - e^{-y}} = e^{k'\pi} I(k').$$

The vertical legs contribute exponentially little to the contour integral as $R \to \infty$ so the sum of the integrals around the contour is $(1 + e^{k'y})I(k')$. This must be equal to $2\pi i$ times the sum of the residues inside the integral, hence

$$(1 + e^{k'\pi})I(k') = 2\pi i\left(\frac{e^{\pi k'/2}}{2i}\right) \quad\Rightarrow\quad I(k') = \pi\frac{e^{\pi k'/2}}{1 + e^{k'\pi}} = \frac{\pi}{2}\cdot\frac{2}{e^{\pi k'/2} + e^{-\pi k'/2}} = \frac{\pi}{2}\mathrm{sech}(\pi k'/2).$$

Thus

$$\hat{p}(k) = \frac{a\pi}{b}\,\mathrm{sech}\left(\frac{k\pi}{2b}\right).$$

We need to know the function and it's second derivative at $k = 0$ to determine normalization and variance. These are simple evaluations if we note that $\mathrm{sech}(0) = 1$, $\tanh(0) = 1$, $\mathrm{d}\,\mathrm{sech}(x)/\mathrm{d}x = -\mathrm{sech}(x)\tanh(x)$, and $\mathrm{d}\tanh(x)/\mathrm{d}x = 1 - \tanh^2(x)$. Let $k' = k\pi/2b$ for notational convenience. The second derivative of $\hat{p}(k)$ is

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}k^2}\hat{p}(k) &= -\frac{\mathrm{d}}{\mathrm{d}k}\left(\frac{a\pi}{b}\right)\left(\frac{\pi}{2b}\right)\mathrm{sech}(k')\tanh(k')\\ &= -\left(\frac{a\pi}{b}\right)\left(\frac{\pi}{2b}\right)^2\left(-\mathrm{sech}(k')\tanh^2(k') + \mathrm{sech}(k')(1 - \tanh^2(k'))\right).\end{aligned}$$

Since $p(x)$ is an even function of x, the mean must be zero, so $\langle x^2\rangle = \sigma^2$. Now we can evaluate (note that at $k = k' = 0$, the tanh terms vanish from $\hat{p}''(k)$):

$$\begin{aligned}\hat{p}(0) &= a\pi/b\\ \hat{p}''(0) &= -\frac{a\pi^3}{4b^3} = -\sigma^2.\end{aligned}$$

Normalization requires that $a\pi/b = 1$ or $a = b/\pi$. The unit variance requirement requires $a\pi^3/4b^3 = (\pi/2b)^2 = 1$ or $b = \pi/2$. Thus $a = 1/2$ and $b = \pi/2$. Filling this into the initial distribution (and the structure function) yields

$$\begin{aligned}p(x) &= \mathrm{sech}(\pi x/2)/2\\ \hat{p}(k) &= \mathrm{sech}(k).\end{aligned}$$

(b) We want to find an expansion for the inverse transform

$$\int_{-\infty}^{\infty} \frac{2^N\, e^{ikx}\, \mathrm{d}k/2\pi}{(e^k + e^{-k})^N} = \frac{2^N}{2\pi} I(\xi, N)$$

where $\xi = x/N$.

The integrand has poles where $e^k + e^{-k} = 0$ or $k = i\pi/2 + i\pi t$ for $t \in \mathbf{Z}$. As the real part of x approaches $\pm\infty$, the magnitude of the integrand vanishes, hence we can deform the path of integration freely without changing the value of the integral, provided we do not cross any of the poles.

Now use the saddle point method to approximate $I(\xi, N)$. First rewrite I:

$$\begin{aligned} I(\xi, N) &= \int_{-\infty}^{\infty} e^{-N\psi(\xi,k)}\, \mathrm{d}k \\ \psi(\xi, k) &= -ik\xi + \ln\left(e^k + e^{-k}\right). \end{aligned}$$

Find the critical points.

$$\begin{aligned} \left.\frac{\partial \psi}{\partial k}\right|_{k_s} &= -i\xi + \frac{e^{k_s} - e^{-k_s}}{e^{k_s} + e^{-k_s}} = 0 \\ \Rightarrow \qquad 0 &= e^{k_s}(1 - i\xi) - e^{-k}(1 + i\xi) \\ \Rightarrow \qquad k_s &= \frac{1}{2}\ln\left(\frac{1 + i\xi}{1 - i\xi}\right). \end{aligned}$$

The magnitude of $(1 + i\xi)/(1 - i\xi)$ is clearly 1, but the argument is

$$\tan^{-1}(2\xi/(1 - \xi^2)) = \tan^{-1}(2/(1/\xi - \xi)).$$

This is only unique up to integer multiples of π of course, so

$$k_s = \frac{i}{2}\tan^{-1}\left(\frac{2}{1/\xi - \xi}\right) + i\,t\frac{\pi}{2}$$

for any $t \in \mathbf{Z}$. For continuity we need to pick $t = 1$ for $\xi > 1$ and $t = -1$ for $\xi < 1$. We will still remain away from the poles, so we can deform the contour from the real axis to a constant $\Im$ part (and in fact a vanishing $\Im$ part). The second derivative of ψ at any k_s is $1 - (i\xi)^2 = 1 + \xi^2$. If we let $A(\xi) = -ik_s$, then $\psi(k_s, \xi)$ is

$$\psi(k_s, \xi) = \xi A(\xi) + \ln(2\cos(A(\xi))) = \xi A(\xi) + \ln(\cos(A(\xi))) + \ln 2.$$

Thus the desired approximation for the integral is

$$I(\xi, N) \approx e^{-N\psi_s(\xi)}\sqrt{\frac{2\pi}{N(1 + \xi^2)}} = 2^{-N}\sqrt{\frac{2\pi}{N(1 + \xi^2)}}\exp\left(-N\xi A(\xi) - N\ln(\cos(A(\xi)))\right).$$

Filling this back into our original equation we get

$$P_N(N\xi) \approx \frac{1}{\sqrt{2\pi N(1 + \xi^2)}}\exp\left(-N\xi A(\xi) - N\ln(\cos(A(\xi)))\right).$$

(c) In the large ξ limit $A(\xi) \approx -1/\xi + \pi/2$ and so

$$-N\xi A(\xi) - N\ln(\cos(A(\xi))) \approx -N\xi(-1/\xi + \pi/2) - N\ln(-\sin(-1/\xi)) \approx N - N\xi\pi/2 - N\ln(1/\xi).$$

Filling this into our asymptotic approximation (and noting that $1+\xi^2 \approx \xi^2$ in this limit we get

$$P_N(N\xi) \approx \frac{\xi^N}{\sqrt{2\pi N\xi^2}} e^N e^{-N\xi\pi/2} = \frac{(x/N)^{N-1}}{\sqrt{2\pi N}} e^N e^{-x\pi/2}.$$

The exponential decay is correct, but the constants aren't perfect. In particular, we should have 1 but we have $e/\sqrt{2\pi} \approx 1.0844$ instead.

(d) In the small ξ limit, $A(\xi) \approx \xi$ so

$$-N\xi A(\xi) - N\ln(\cos(A(\xi))) \approx -N\xi^2 - N\ln(1-\xi^2/2) \approx -N\xi^2 + N\xi^2/2 = -N\xi^2/2 = -x^2/2N.$$

Filling this into our approximation and noting that $1+\xi^2 \approx 1$ we have

$$P_N(x) \approx \frac{1}{\sqrt{2\pi N}} e^{-x^2/2N}$$

which is clearly a standard normal distribution. The Central Limit Theorem holds. For $N=1$ the approximation is horrible. This gives us a value of $1/\sqrt{2\pi} \approx 0.3989$ at $x=0$ but the real value is $1/2$.

(3) **Slowly Draining Sand**

(a) It is worth noting that the void distribution is simply the binomial distribution, and we have a globally valid asymptotic approximation for this from lecture 16. However, I use a different approach: I derive continuum equations for the steady state void concentration and solve them.

Let $f(x,z)$ represent the density of voids at (x,z) in the steady state and normalized so that 1 is the maximum void density and 0 is the minimum. Since voids are introduced at a rate of $/k\tau$ voids per unit time, the integral of void density for a given z should always be $1/\tau$. Each lattice point receives half of the void density from each of the two lattice points below it during each unit of time. Thus (let h be the vertical distance between lattice layers)

$$f(x,z) = \frac{1}{2}\left[f(x-\sigma, z-h) + f(x+\sigma, z-h)\right].$$

Taylor expand about (x,z) (all function evaluations are at (x,z) below):

$$\begin{aligned}
2f &= \left(f - \sigma\partial_x f - h\partial_z f + \sigma^2\partial_{xx}f/2 + h\sigma\partial_{xz}f + h^2\partial_{zz}f/2 + \cdots\right) \\
&\quad + \left(f + \sigma\partial_x f - h\partial_z f + \sigma^2\partial_{xx}f/2 - h\sigma\partial_{xz}f + h^2\partial_{zz}f/2 + \cdots\right) \\
\Rightarrow \quad f &= f - h\partial_z f + \sigma^2\partial_{xx}f/2 + O(h^2, \sigma^3, h\sigma^2, h^2\sigma).
\end{aligned}$$

The void concentration should not be constant in either x or y to lowest order, so the lowest non-vanishing terms should balance each other. Thus

$$\partial_z f = (h/2\sigma^2)\partial_{xx}f + O(h, \sigma^3/h, \sigma^2, h\sigma) \quad \Rightarrow \quad \partial_z f \approx D\partial_{xx}f$$

where $D = h/2\sigma^2$. Since h should be of comparable size to σ, D is going to be comparable to $1/\sigma$, which will divergently large as $\sigma \to 0$. Thus $\partial_{xx} f$ will be exceedingly small wrt $\partial_z f$ in our solution. This is curious.

A solution to this (a very classic solution) is the standard Gaussian diffusion with z playing the role of time. Since we want the integral wrt x to be $1/k$, we simply multiply the standard distribution by $1/k$. Thus $f(x, z)$ should be well approximated by

$$f(x,z) \approx \frac{1}{k\sqrt{4\pi Dz}} e^{-x^2/4Dz}.$$

The mass profile is simply $1 - f(x, z)$. One may scale by c_{max} to get appropriate units if one so desires.

Now consider that the velocity of the mass is equal and opposite to the velocity of the voids. The void flowing out of lattice point upwards produces no x component, but the void flowing in from below may be unbalanced in this respect. Let u_x be the x-component of the mass velocity. Noting the direction of flow of the two incoming components (and that flow takes place at time scale τ) we get

$$u_x = \frac{\sigma}{2\tau\sqrt{\sigma^2 + 4h^2}} \left(f(x + \sigma, z - h) - f(x - \sigma, z - h)\right).$$

(The $\sigma/\sqrt{\sigma^2 + 4h^2}$ is the appropriate $\cos(\theta)$ term.) Taylor expanding about x, z gives (all evaluations are at (x, z) below):

$$\begin{aligned}
u_x &= \frac{\sigma}{2\sqrt{\sigma^2+4h^2}} \Big[\big(f + \sigma\partial_x f - h\partial_z f + \sigma^2\partial_{xx} f/2 - h\sigma\partial_{xz} f + h^2\partial_{hh} f/2 + \cdots\big) \\
&\quad - \big(f - \sigma\partial_x f - h\partial_z f + \sigma^2\partial_{xx} f/2 + h\sigma\partial_{xz} f + h^2\partial_{hh} f/2 + \cdots\big)\Big] \\
&= \frac{\sigma}{\tau\sqrt{\sigma^2+4h^2}} \left(\sigma\partial_x f + O(h^\infty, \sigma^3, \sigma h^2, \sigma^3 h)\right) \approx \frac{\sigma^2}{\tau\sqrt{\sigma^2+4h^2}}\partial_x f \\
&= \frac{D}{\sqrt{1+\sigma^2/4h^2}}\partial_x f = \frac{-x/2z}{\tau\sqrt{1+(\sigma/2h)^2}} f
\end{aligned}$$

There is flow $f(x, z)$ coming into and out of the lattice point at (x, z). Taking the vertical components of the incoming and outgoing vectors (and making the sign flip to get *mass* velocity) yields

$$u_z = -\frac{2h}{\tau\sqrt{\sigma^2+4h^2}} f = -\frac{1}{\tau\sqrt{1+s^2/4h^2}} f.$$

The magnitude of $\mathbf{u}$ is

$$\begin{aligned}
\|\mathbf{u}\| &= \left(\frac{(-x/2z)^2}{\tau^2(1+(\sigma/2h)^2)} f^2 + \frac{(-1)^2}{\tau^2(1+(\sigma/2h)^2)}\right)^{1/2} \\
&= \frac{f}{\tau\sqrt{1+(\sigma/2h)^2}}\sqrt{1+(x/2z)^2}.
\end{aligned}$$

Clearly f dominates the behavior, so "significant movement" could be taken to be within one "decay length" of f, or where $x^2/4Dz \le 1$. This describes the parabola $z = 4Dx^2$, so "significant movement" is within a very wide parabola. The direction of movement at (x, z) has "slope"

$$\frac{u_z}{u_x} = \frac{2z}{x}.$$

This gives a diffeq for the stream lines:

$$\frac{dz}{dx} = \frac{2z}{x} \quad \Rightarrow \quad z = Ax^2.$$

Thus the stream lines are parabolas.

I don't know the solution for a flow field in a fluid (and I don't want to calculate it right now), but fluid does flow differently. The motion of the marbles is due entirely to the flow of voids upwards. There are no effects due to pressure or kinetic energy of the particles. In fluid (water for example), however, pressure and momentum play very important roles. I'm sorry I cannot say more (a bit of time pressure unfortunately).

(b) Since the stream lines are parabolas, if we can show that the integral of f wrt x in the container is invariant wrt z, the solution above should work modulo some normalization. To check let f be as for part (a) and let $x_c = \sqrt{z/k}$:

$$\begin{aligned}
\partial_z \int_{-x_c}^{x_c} f(x', z)\,\mathrm{d}x' &= \partial_z 2 \int_0^{x_c} f(x', z)\,\mathrm{d}x' = 2f(x_c, z)\partial_z x_c + 2\int_0^{x_c} \partial_z f(x', z)\,\mathrm{d}x' \\
&= f(x_c, z)\frac{1}{\sqrt{kz}} + 2D\int_0^{x_c} \partial_{xx} f(x', z)\,\mathrm{d}x' \\
&= f(x_c, z)\frac{1}{\sqrt{kz}} + 2D\partial_x f(x_c, z) = f(x_c, z)\left(\frac{1}{\sqrt{kz}} - \frac{x_c}{z}\right) = 0.
\end{aligned}$$

We need the integral $\int_{-x_c}^{x_c} f(x', z)\,\mathrm{d}x'$ to be $1/k$ for appropriate normalization. Let f be as for part (a). Our solution for the void concentration (and everything else) for this part can be obtained by replacing f in part (A) with f/C where

$$\begin{aligned}
C/k &= \int_{-x_c}^{x_c} f(x', z)\,\mathrm{d}x = \frac{2}{k\sqrt{2\pi}} \int_0^{x_c/\sqrt{2Dz}} e^{-y^2}\,\mathrm{d}y \\
&= \frac{1}{k\sqrt{2}} \frac{2}{\sqrt{\pi}} \int_0^{x_c/\sqrt{2Dz}} e^{-y^2}\,\mathrm{d}y = \frac{1}{k\sqrt{2}}\,\mathrm{erf}\left(\frac{x_c}{\sqrt{2Dz}}\right) \\
\Rightarrow \quad C &= \frac{1}{\sqrt{2}}\,\mathrm{erf}\left(\frac{1}{\sqrt{2Dk}}\right).
\end{aligned}$$

(4) **Sorption and Desorption from a Lattice**

We've seen the arguments so many times, I'll just summarize what is going on. We know that $\partial_t c = -\partial_x v$ where v is the number of walkers passing to the right through a given x per unit time. For the usual random walk, $v = -D_0 \partial_x c$ which yields the standard diffusion equation with. In this case, however, there are only $(c_0 - c)$ voids available to the walkers, so only a fraction $(1 - c/c_0)$ of them can participate in the "walking" per unit time. This leads to a reduction in v by this factor and we get the result stated in the homework set.

First non-dimensionalize the equation by setting $\bar{c} = c/c_0$, $\bar{t} = t/\tau$ and $\bar{x} = x/\sigma$. After making these substitutions (and omitting the bars henceforth) we get

$$\partial_t c = \frac{\tau D_0}{\sigma^2} \partial_x ((1 - c)\partial_x c)$$

where $0 \leq c \leq 1$ and we can pick τ, σ so that $D_0\tau/\sigma^2 = 1$. Thus we want to solve

$$\partial_t c = \partial_x((1-c)\partial_x c).$$

Consider the case of desorption. Let $d = (1-c)$ and hypothesize a solution of the form $d = f(\zeta)$ where $\zeta = x/\sqrt{2t}$. Filling in d to our differential equation yields

$$-\partial_t d = \partial_x(-d\partial_x d) \quad \Rightarrow \quad \partial_t d = \partial_x(d\partial_x d) = (\partial_x d)^2 + d\partial_{xx} d.$$

Filling in our similarity guess for the solution yields

$$-\frac{\zeta}{2t}f'(\zeta) = \frac{1}{2t}(f'(\zeta))^2 + \frac{1}{2t}f(\zeta)f''(\zeta) \quad \Rightarrow \quad ff'' + (f')^2 + \zeta f' = 0.$$

The boundary conditions on f stipulate that $f \to 1$ as $x \to 0$ or $t \to \infty$ which translates to $f \to 1$ as $\zeta \to 0$. In addition we need $f \to 0$ as $x \to \infty$ or $t \to 0$ which translates to $f \to 0$ as $\zeta \to \infty$. Thus a similarity solution is possible if we can solve this ordinary differential equation (which I, for one, cannot do in closed form).

Now consider the case of sorption. We use the same form of similarity solution but we have a different differential equation. In particular we have

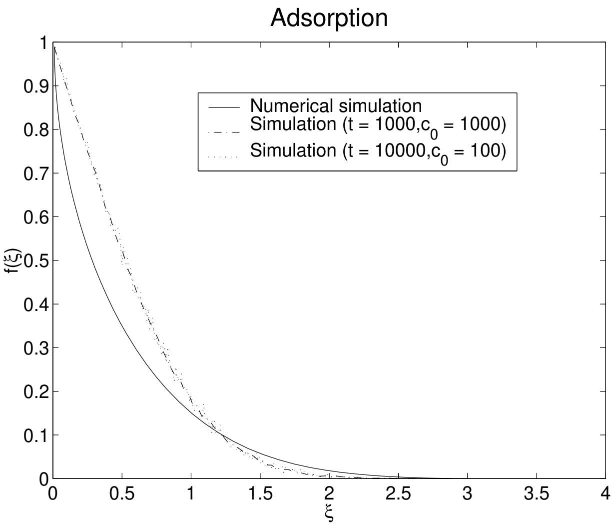
$$\partial_t c = -(\partial_x c)^2 + (1-c)\partial_{xx} c.$$

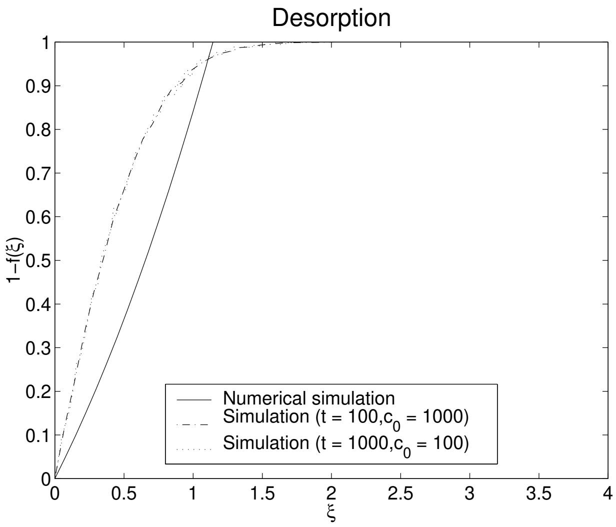
Fill in our similarity guess to get

$$-\frac{\zeta}{2t}f'(\zeta) = -\frac{1}{2t}(f'(\zeta))^2 + (1-f(\zeta))\frac{1}{2t}f''(\zeta) \quad \Rightarrow \quad (1-f)f'' - (f')^2 + \zeta f' = 0.$$

The boundary conditions are the same as for the similarity solution above so a similarity solution is again possible but I don't know how to solve it. Again, numerical results are possible.

(b) We can find numerical results for both adsorption and desorption, however. The following plots show both the numerical integration an walker simulation results for both cases:





(The simulation results are averaged over ten trials.)

For desorption the initial conditions for $f(\xi)/$ were $f(0) = 0$ and $f'(0) = -0.6275$. It is not perfect as the leveling off near $1 - f(\xi) = 1$ is not precisely 1, but experiments suggest that tweaking $f'(0)$ will put it there eventually, save with a discontinuity in $f'(\xi)$ where $1 - f(\xi^*) = 1$. The incipient singularity in $f'(\xi)$ appears to be around $\xi \approx 1.144$.

For adsorption, initial conditions are $y(0.01) = 0.99$ and $f'(0.01) = -4.75$. There are no cusps.

The simulation results do not fit the numerical integrations well. They have no cusps in the case of desorption. This makes sense as there is always some probability (very small) at each step that a single void could diffuse arbitrarily far into the body: a walker at the edge could step left, followed by its previous neighbor to the right and so forth. Nevertheless the desorption solution moves from 0 to 1 more sharply than the solution for adsorption moves from 1 to 0. This makes sense: the higher density of walkers in the case of desorption hinders comparatively rapid diffusion away from the "interaction" edge.

The most reassuring result, however, is that the scaling of the simulated solutions is almost exactly what we expected: plotting them a function of $x/\sqrt{2t}$ places them on top of each other.