Problem Set 1a

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Problem 1.

The concentration $c(x, t+\tau)$ is given by the integral

$$c(x,t+\tau) = \int P(x,t+\tau|x',t)C(x',t)dx'.$$

Define the difference $y = x - x'$. The integrand may then be written in the form

$$P(x,t+\tau|x',t)C(x',t) = P(x+y-y,t+\tau|x-y,t)C(x-y,t).$$

A Taylor expansion for small y yields

$$P(x,t+\tau|x',t)C(x',t) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} y^n \left(\frac{\partial}{\partial x}\right)^n P(x+y,t+\tau|x,t)C(x,t).$$

Integration is now over y instead of x', where the negative sign may be adsorbed into the bounds of integration (as suggested by Risken, *The Fokker-Planck Equation*),

$$c(x,t+\tau) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-\partial}{\partial x}\right) C(x,t) \int y^n P(x+y,t+\tau|x,t)dy.$$

Noting the definition of the moments,

$$M_n(x,t,\tau) \stackrel{\text{def.}}{=} \int y^n P(x+y,t+\tau|x,t)dy,$$

and the fact that the zeroth first moment $M_0(x,t,\tau) = 1$,

$$c(x,t+\tau) - c(x,t) = \sum_{n=1}^{\infty} \frac{1}{n!} \left(\frac{-\partial}{\partial x}\right) C(x,t) M_n(x,t,\tau).$$

Divide by τ and note that the left hand side is non-stationary, so it may be expanded in a Taylor series for small τ,

$$\sum_{n=1}^{\infty} \frac{\tau^{n-1}}{n!} \frac{\partial^n c}{\partial t^n} = \sum_{n=1}^{\infty} \left(\frac{-\partial}{\partial x}\right) C(x,t) \frac{M_n(x,t,\tau)}{n! \cdot \tau}.$$

Finally, using the definition

$$D_n(x,t,\tau) \stackrel{\text{def.}}{=} \frac{M_n(x,t,\tau)}{n! \cdot \tau},$$

we recover the Kramers-Moyal forward expansion,

$$\frac{\partial c}{\partial t} + \sum_{n=2}^{\infty} \frac{\tau^{n-1}}{n!} \frac{\partial^n c}{\partial t^n} = \sum_{n=1}^{\infty} \left(\frac{-\partial}{\partial x} \right) C(x,t) D_n(x,t,\tau).$$

In the limit $\tau \to 0$, the sum on the left-hand-side vanishes. Assuming that the moments $D_n(x,t,\tau) \to D_n(x,t)$ for $n \leq 2$, then all terms except for the first two in the right-hand-side sum also vanish. The Kramers-Moyal expansion thereby reduces to the Fokker-Planck equation,

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x} (D_1(x,t)c) = \frac{\partial^2}{\partial x^2} (D_2(x,t)c).$$

Problem 2.

Define the dimensionless scales

$$\theta = \frac{c - c_0}{c_0}, \quad \eta = t \left(\frac{D}{l^2} \right), \quad \phi = \frac{x}{l},$$

where l is a length scale to be determined later. This is required so that the problem be rendered entirely dimensionless. The dimensionless equation then becomes

$$\frac{\partial \theta(\phi,\eta)}{\partial \eta} = \frac{\partial^2 \theta(\phi,\eta)}{\partial \phi^2},$$

subject to the boundary conditions

$$\begin{aligned} \theta(\phi, 0) &= 0, \\ \theta(\infty, \eta) &= 0, \\ \frac{\partial \theta(0,\eta)}{\partial \phi} &= -\alpha, \end{aligned}$$

where α is the dimensionless parameter,

$$\alpha = \frac{Jl}{Dc_0}.$$

Laplace transform the original equation into $\overline{\theta}(\phi, s)$,

$$\frac{\partial^2 \overline{\theta}}{\partial \phi^2} - s\overline{\theta} = 0.$$

The transformed boundary conditions are thereby

$$\overline{\theta}(\infty, s) = 0,$$
$$\frac{\partial \overline{\theta}}{\partial \phi} = \frac{-\alpha}{s}.$$

The solution of the transformed equation is,

$$\theta' = c_1(s)\exp(-\sqrt{s}\phi) + c_2(s)\exp(\sqrt{s}\phi),$$

where the boundary conditions are satisifed by the integration functions

$$c_1(s) = \alpha s^{-3/2}, \quad c_2(s) = 0.$$

Taking the inverse Laplace transform (Abramowitz and Stegun, *Handbook of Mathematical Functions*),

$$\theta(\phi, \eta) = \alpha\left[2\sqrt{\frac{\eta}{\pi}}\exp\left(\frac{-\phi^2}{4\eta}\right) - \phi\,\mathrm{erfc}\left(\frac{-\phi}{2\sqrt{\eta}}\right)\right].$$

Converting back to dimensional units,

$$\frac{c(x,t)}{c_0} = 1 + \frac{J}{Dc_0}\left[\sqrt{\frac{4Dt}{\pi}}\exp\left(\frac{-x^2}{4Dt}\right) - x\,\mathrm{erfc}\left(\frac{x}{\sqrt{4Dt}}\right)\right],$$

where the complementary error function is defined as

$$\mathrm{erfc}\left(\frac{x}{\sqrt{4Dt}}\right) = 1 - \frac{2}{\sqrt{\pi}}\int_{-\infty}^{x/\sqrt{4Dt}}\exp(-\eta^2)\,d\eta.$$

Notice that the length scale l, previously left undefined, does not appear in the final expression for the concentration.

When the flux is negative, then the Sands time occurs when the (dimensionless) concentration is zero,

$$t_s = \frac{\pi}{4}D\left(\frac{c_0}{J}\right)^2.$$

The Sands time is increased by increasing the initial concentration (since it takes more time to deplete the $x = 0$ concentration), while the Sands time is decreased by increasing the flux (since the $x = 0$ concentration is depleted more rapidly). The linear dependence on diffusivity represent the "ease" of drawing concentration from the $x = \infty$ boundary towards the $x = 0$ boundary.

After the Sands time, the boundary condition at $x = 0$ becomes $c = 0$, or $\theta = -1$. This makes the boundary conditions for the transformed equation

$$\overline{\theta}(0, s) = -1/s,$$

whereby the integration function $c_1(s)$ becomes

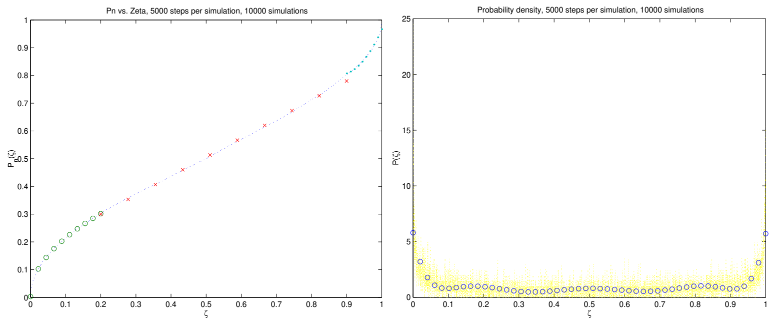
$$c_1(s) = -1/s.$$

Taking the inverse Laplace transform and converting to dimensional units,

$$c = c_0\,\mathrm{erfc}\left(\frac{x}{\sqrt{4Dt}}\right).$$

Problem 3.

The following two graphs illustrate the cumulative probability density, P_n, and the probability density P, for the indicated number of steps per simulation and the number of simulations used to effect the statistics.



In the first plot, the data was fit with three separate functions:

$$P_n(\zeta) = \begin{cases} 0.6684 + 0.0031\sqrt{\zeta} & \text{on} \quad 0 < \zeta < 0.2 \\ 0.6858\zeta + 0.1628 & \text{on} \quad 0.2 < \zeta < 0.9 \\ 11.7\zeta^2 - 20.7\zeta + 9.9 & \text{on} \quad 0.9 < \zeta < 1.0 \end{cases}$$

In the second plot, the data was fit globally with an eighth order polynomial since there was significant noise. Moreover, although the three piece fit for the cumulative probability density is qualitatively in good agreement with the simulations, the derivative of the fit does not agree well with the numerical differentiation, especially for $0.9 < \zeta < 1.0$, where the derivative of the fit is negative! The probability density $P(1/2)$ was found to be 0.8031 from the fit of the numerical differentiation, 0.6858 from the fit of the cumulative probability density, and 1.000 from the simulation data. One can see how an ensemble of walkers forms a Gaussian distribution from the symmetric nature of the probability density for a single walker.

Note: As mentioned by Prof. Bazant in office hours, the cumulative probability density P_n has an analytical solution which is proportional to $\arcsin(\zeta)$. The simulation data in the first plot is, in fact, an arcsin.

```
clear variables
steps=5000; trials= 10000; P = zeros(1,steps+1); Pd = zeros(1,steps+1);
spacing = 1/steps; zeta = linspace(0,1,steps+1);

for j=1:trials
   x = 0; Mn = 0; %initialize the simulation
   for i=1:steps
      a=rand(1);
    if a < 0.5
       x = x+1;
    else
       x = x-1;
    end
    if x > 0
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      Mn = Mn+1; %check if on the right
     end
   end
   M(j)=Mn; %Record the number of times on the right
   for L=1:steps+1
      if M(j) < L
         P(L) = P(L)+1; %Check if M is inside L
      end
   end
end
P = P/trials;
P1=P(1:1000); P2=P(1001:4500); P3=P(4501:5000);
zeta1=zeta(1:1000); zeta2=zeta(1001:4500); zeta3=zeta(4501:5000);
zeta1a=zeta1.^(0.5); a1=polyfit(zeta1a,P1,1); %a1(1)=B, a1(2)=A
z1 = linspace(min(zeta1),max(zeta1),10);
for n=1:10
   plot1(n)=a1(2)+a1(1)*sqrt(z1(n));
end
a2 = polyfit(zeta2,P2,1); z2 = linspace(min(zeta2),max(zeta2),10);
a3 = polyfit(zeta3,P3,2); z3= linspace(min(zeta3),max(zeta3),10);
plot(zeta,P,':',z1,plot1,'o',z2,polyval(a2,z2),'x',z3,polyval(a3,z3),'.');
title('Pn vs. Zeta, 5000 steps per simulation, 10000 simulations')
xlabel('\zeta'); ylabel('P_{n}(\zeta)')
Pd = zeros(1,steps);
for n=1:steps-1
   Pd(n)=(P(n+1)-P(n))*steps;
end
Pd(steps)=Pd(steps-1); b=polyfit(zeta,Pd,8); zd=linspace(0,1,50);
plot(zeta,Pd,'y:',zd,polyval(b,zd),'o')
title('Probability density, 5000 steps per simulation, 10000 simulations')
xlabel('\zeta'); ylabel('P(\zeta)')
phalf=polyval(b,0.5)
```

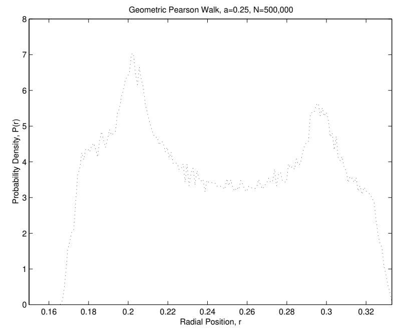
Problem 4.

The geometric Pearson walk was simulated for values of $a = 0.25, 0.5, 0.75$ with the infinite limiting number of steps $N = 5, 10, 20$, respectively. These values were chosen so the the resolution $\Delta r = 0.1$, used to calculate the probability density by the relationship

$$p(r) = \frac{\text{Prob}(r < r_N < r + \Delta r)}{2\pi r \Delta r},$$

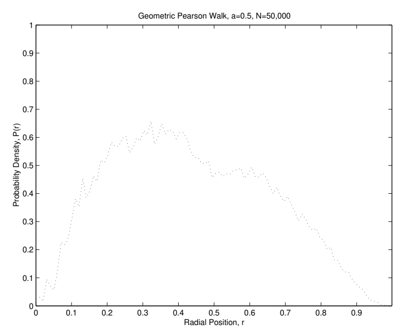
was not appreciably effected by the $N + 1$ step.

The first plot is of the probability density for $a = 0.25$, $N = 5$ over 500,000 simulations. The large number of simulations were used because the results seemed incorrect initially.



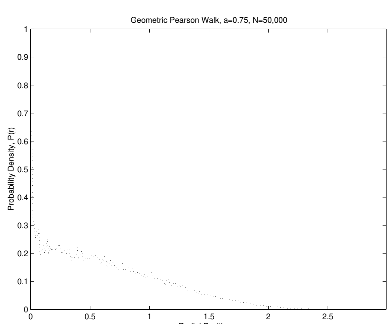
Since the second step has a small radius, 0.0625, then the probability density is primarily due to the random first step, which always is of a length $r = 0.25$. The second step represents a small correction to the first, hence the low probability density at $r = 0.25$ compared to its neighbors. The probability density reaches a sharp peak and then declines rapidly, since to be outside the sharp peak requires the remaining small steps to be in identical directions. Also, the probability density is zero for values $r \lesssim 0.15$, again owing to the fact that the last 4 steps are small.

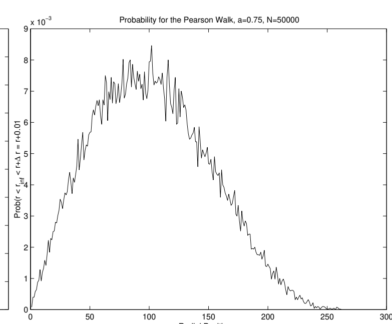
The second plot is for $a = 0.5$, $N = 10$ for 50,000 simulations.



Here the probability density still has a plateau at $r = 0.5$, but the remaining steps have more significant impact on the final radial position. The probability density extends closer to the origin, again owing to the impact of the later steps.

The final plots are the probability density $p(r)$ and the probability $\mathrm{Prob}(r < r_N < r + \Delta r)$ for $a = 0.75$, $N = 20$ from 50,000 simulations.





The probability density continues to extend towards zero since the influence of successive steps becomes even greater as a increases. The seemingly skewed probability density occurs due to the scaling $2\pi r$, which exaggerates the probability density near $r = 0$. The second plot is the probability for a value $\Delta r = 0.01$, which illustrates that the probability, rather than the probability density, is similar between $a = 0.5$ and $a = 0.75$.

```
clear variables
N = 20; a = 0.75; trials = 50000;
for i=1:trials
   x = 0; y = 0;
   for j=1:N
      theta=rand(1)*2*pi;
      x = x+a^j*cos(theta);
      y = y+a^j*sin(theta);
   end
   r(i)=sqrt(x^2+y^2);
end
maximum = 0;
for j=1:N
   maximum = maximum+a^j;
end
dr = 0.01; intervals = round(maximum/dr); P = zeros(intervals,1);
for i=1:trials
   spot=round(r(i)/maximum*intervals);
   P(spot) = P(spot)+1;
end
P = P/trials; xx=linspace(0,maximum,intervals); ending=intervals-1;
Pd = P(2:ending)/(2*pi*dr)./(xx(2:ending).');
plot(xx(2:ending),Pd,':')
axis([0 maximum 0 1])
title('Geometric Pearson Walk, a=0.75, N=50,000')
xlabel('Radial Position, r'); ylabel('Probability Density, P(r)')
```