

Solutions to Problem Set 1

Edited by Chris H. Rycroft*

February 17, 2005

1 Rayleigh's Random Walk

We consider an isotropic random walk in 3 dimensions with independent identical displacements of length a , given by the PDF

$$p(\vec{x}) = \frac{\delta(r - a)}{4\pi a^2} \quad (r = |\vec{x}|)$$

for which we verify

$$\iiint p(\vec{x}) d\vec{x} = \int_0^{2\pi} \int_0^\pi \int_0^\infty \frac{\delta(r - a)}{4\pi a^2} r^2 \sin \theta dr d\theta d\phi = 1.$$

1.1 PDF of the position after n steps

The characteristic function is given by

$$\hat{p}(\vec{k}) = \langle e^{i\vec{k} \cdot \vec{x}} \rangle = \iiint p(\vec{x}) e^{i\vec{k} \cdot \vec{x}} d\vec{x}.$$

If we choose the spherical coordinate system such that ϕ is the rotation angle around \vec{k} (fixed in this integration), then $\vec{k} \cdot \vec{x} = kr \cos \theta$ and

$$\begin{aligned} \hat{p}(\vec{k}) &= \frac{2\pi}{4\pi a^2} \int_0^\pi \int_0^\infty e^{ikr \cos \theta} \delta(r - a) r^2 \sin \theta dr d\theta \\ &= \frac{1}{2} \int_0^\pi e^{ika \cos \theta} \sin \theta d\theta \\ &= \frac{1}{2} \int_{-1}^1 e^{ikas} ds \quad (\text{with } s = \cos \theta) \\ &= \frac{\sin(ka)}{ka} \quad (k = |\vec{k}|) \end{aligned}$$

for which we verify again the normalization condition $\hat{p}(\vec{0}) = 1$. We know from the lecture that the PDF of the position after n steps is given by

$$P_n(\vec{x}) = \iiint [\hat{p}(\vec{k})]^n e^{-i\vec{k} \cdot \vec{x}} \frac{d\vec{k}}{(2\pi)^3}.$$

*Based on solutions for problems 1 and 2 by Thierry Savin (2003), and for problem 3 by Chris H. Rycroft (2005).

Using the spherical coordinates system such that ϕ is now the rotation angle around \vec{x} (fixed in this integration), we can write (again using $\vec{k} \cdot \vec{x} = kr \cos \theta$)

$$\begin{aligned} P_n(\vec{x}) &= \frac{1}{(2\pi)^2} \int_0^\pi \int_0^\infty e^{-ikr \cos \theta} \left[\frac{\sin(ka)}{ka} \right]^n k^2 \sin \theta \, dk d\theta \\ &= \frac{1}{(2\pi)^2} \int_0^\infty \left[\frac{\sin(ka)}{ka} \right]^n k^2 \left[\int_{-1}^1 e^{-ikrs} ds \right] dk \quad \text{with } s = \cos \theta. \end{aligned}$$

Therefore

$$P_n(\vec{x}) = \frac{1}{2\pi^2 r} \int_0^\infty k \sin(kr) \left[\frac{\sin(ka)}{ka} \right]^n dk.$$

1.2 Asymptotic formula

We can write

$$P_n(\vec{x}) = \frac{1}{2\pi^2 r} \int_0^\infty k \sin(kr) e^{n\psi(k)} dk$$

where

$$\psi(k) = \log \left[\frac{\sin(ka)}{ka} \right].$$

In the limit $n \rightarrow \infty$, we are interested in the region around $k = 0$, where $\psi(k)$ is a maximum. Taylor expanding $\psi(k)$ at $k = 0$ gives

$$\begin{aligned} \frac{\sin(ka)}{ka} &= 1 - \frac{(ka)^2}{3!} + \frac{(ka)^4}{5!} + O(k^6) \\ \psi(k) &= -\frac{(ka)^2}{6} - \frac{(ka)^4}{180} + O(k^6). \end{aligned}$$

For this part, we are just interested in the first term. We write

$$P_n(\vec{x}) \sim \frac{1}{2\pi^2 r} \int_0^\infty k \sin(kr) e^{-n(ka)^2/6} dk$$

and using relation (1) shown in appendix A, we obtain

$$P_n(\vec{x}) \sim \left(\frac{3}{2\pi a^2 n} \right)^{3/2} \exp \left(-\frac{3r^2}{2a^2 n} \right).$$

1.3 Second Term

Taking into account the next term in the Taylor expansion of $\psi(k)$, and writing

$$e^{n\psi(k)} = e^{-n(ka)^2/6} e^{-n(ka)^4/180} = e^{-n(ka)^2/6} - \frac{n(ka)^4}{180} e^{-n(ka)^2/6}$$

we get

$$P_n(\vec{x}) \sim \frac{1}{2\pi^2 r} \left[\int_0^\infty k \sin(kr) e^{-n(ka)^2/6} dk - \frac{na^4}{180} \int_0^\infty k^5 \sin(kr) e^{-n(ka)^2/6} dk \right].$$

After simplification, and using relations (1) and (2), we obtain

$$P_n(\vec{x}) \sim \left(\frac{3}{2\pi a^2 n} \right)^{3/2} \exp\left(-\frac{3r^2}{2a^2 n} \right) \left[1 - \frac{3}{4n} + \frac{3}{2a^2} \frac{r^2}{n^2} - \frac{9}{20a^4} \frac{r^4}{n^3} \right].$$

By introducing the scaling variable $\xi = r\sqrt{\frac{3}{2a^2 n}}$ we can write

$$\frac{a^3 P_n(\vec{x})}{(2\pi/3)^{-3/2}} \sim \frac{e^{-\xi^2}}{n^{3/2}} \left[1 - \frac{1}{n} \left(\frac{3}{4} - \xi^2 + \frac{\xi^4}{5} \right) \right]$$

and we see that the Central Limit Theorem holds as long as

$$\frac{1}{n} \left(\frac{3}{4} - \xi^2 + \frac{\xi^4}{5} \right) = O(1) \quad \Leftrightarrow \quad \xi^4 = O(n).$$

We conclude that the width of the central region is given by $r = O(n^{3/4})$.

2 Cauchy's Random Walk

We consider a random walk in one dimension with independent, nonidentical displacements, given by the PDF

$$p_n(x) = \frac{A_n}{x_n^2 + x^2}$$

where $x_n > 0$ for every n .

2.1 Characteristic function

The characteristic function for this PDF is given by

$$\hat{p}_n(k) = \langle e^{ikx} \rangle = \int_{-\infty}^{+\infty} p_n(x) e^{ikx} dx = A_n \int_{-\infty}^{+\infty} \frac{e^{ikx}}{x_n^2 + x^2} dx.$$

To evaluate this we consider the complex integral

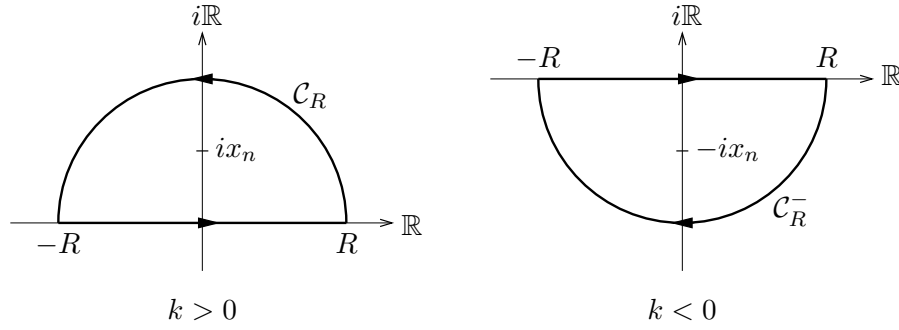
$$\oint_{\mathcal{C}_R} \frac{e^{ikz}}{z^2 + x_n^2} dz$$

in which the integrand exhibits 2 poles at $z = \pm ix_n$, and where \mathcal{C}_R is one of the contours defined in figure 1, depending on the sign of k . For the first case where $k > 0$, the Residue Theorem gives us

$$\oint_{\mathcal{C}_R^+} \frac{e^{ikz}}{z^2 + x_n^2} dz = 2i\pi \operatorname{Res}_{z=ix_n} \left(\frac{e^{ikz}}{z^2 + x_n^2} \right).$$

The left-hand side can be expressed as

$$\oint_{\mathcal{C}_R^+} \frac{e^{ikz}}{z^2 + x_n^2} dz = \int_{-R}^{+R} \frac{e^{ikx}}{x_n^2 + x^2} dx + \int_{\Gamma_R^+} \frac{e^{ikz}}{z^2 + x_n^2} dz$$

Figure 1: Contour \mathcal{C}_R . R is sufficiently big so that \mathcal{C}_R runs around the pole.

where Γ_R^+ is the open contour over which z is imaginary (with $|z| = R$). On this contour, we have

$$\left| \int_{\Gamma_R^+} \frac{e^{ikz}}{z^2 + x_n^2} dz \right| < \pi R \frac{e^{-kR}}{R^2 - x_n^2} \xrightarrow{R \rightarrow \infty} 0.$$

We conclude that when $R \rightarrow \infty$, we have

$$\oint_{\mathcal{C}_\infty^+} \frac{e^{ikz}}{z^2 + x_n^2} dz = \int_{-\infty}^{+\infty} \frac{e^{ikx}}{x_n^2 + x^2} dx.$$

The residue can be calculated as

$$\text{Res}_{z=ix_n} \left(\frac{e^{ikz}}{z^2 + x_n^2} \right) = \lim_{z \rightarrow ix_n} (z - ix_n) \frac{e^{ikz}}{z^2 + x_n^2} = \frac{e^{-kx_n}}{2ix_n}$$

and hence we obtain

$$\int_{-\infty}^{+\infty} \frac{e^{ikx}}{x_n^2 + x^2} dx = \frac{\pi}{x_n} e^{-kx_n} \quad \text{for } k > 0.$$

Using the other contour for $k < 0$, we show similarly that

$$\int_{-\infty}^{+\infty} \frac{e^{ikx}}{x_n^2 + x^2} dx = \frac{\pi}{x_n} e^{kx_n} \quad \text{for } k < 0.$$

Thus we can write¹

$$\hat{p}_n(k) = \frac{\pi A_n}{x_n} e^{-|k|x_n};$$

the normalization condition gives us

$$\hat{p}_n(0) = 1 \quad \Leftrightarrow \quad A_n = \frac{x_n}{\pi}$$

and therefore

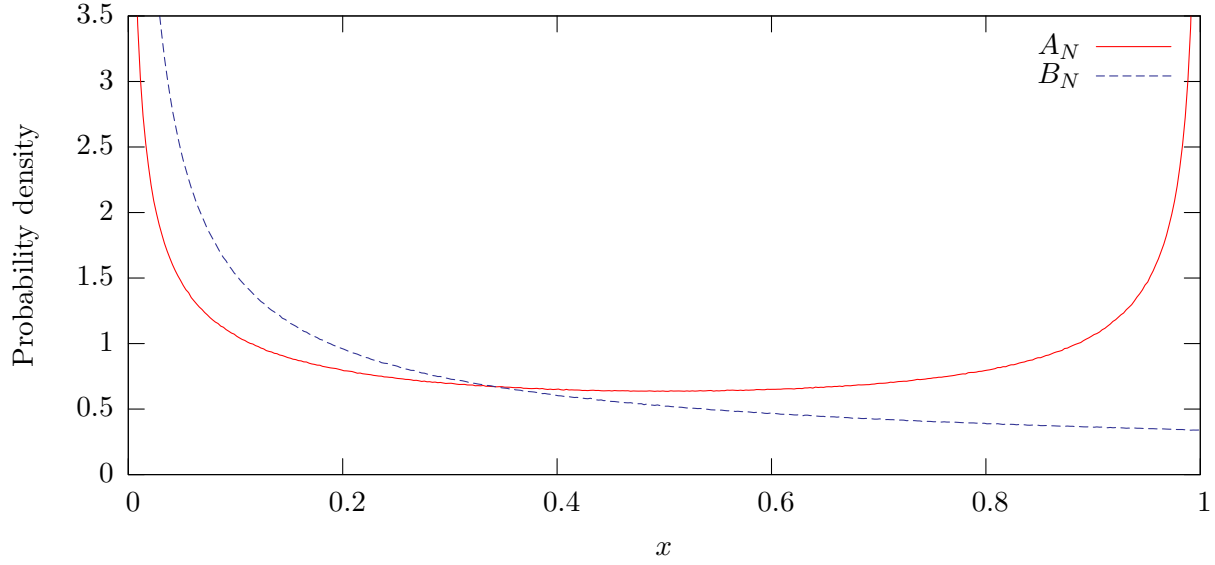
$$\boxed{\hat{p}_n(k) = e^{-x_n|k|}.$$

We see that $\hat{p}_n(k)$ is continuous at $k = 0$, but $\hat{p}'_n(k)$ is not, since it doesn't have the same value at $k = 0^+$ and $k = 0^-$. In terms of $p(x)$, this is because $\langle x \rangle_n = -i \hat{p}'_n(k = 0)$ is not defined.

¹Another rigorous way to prove this formula is to calculate the integral

$$\int_{-\infty}^{+\infty} e^{-ikx} e^{-|k|x_n} \frac{dk}{2\pi} = \frac{1}{\pi} \frac{x_n}{x_n^2 + x^2}$$

as it is shown in paragraph 2.2, and then use the Inverse Fourier Transform Theorem.

Figure 2: Computed probability density functions for A_N and B_N .

2.2 PDF of the position after n steps

From class, we know

$$\begin{aligned}
 P_n(x) &= \int_{-\infty}^{+\infty} e^{-ikx} \left[\prod_{j=1}^n \hat{p}_j(k) \right] \frac{dk}{2\pi} \\
 &= \int_{-\infty}^{+\infty} e^{-ikx} e^{-|k|X_n} \frac{dk}{2\pi} \quad \text{where } X_n = \sum_{j=1}^n x_j \\
 &= \int_0^{+\infty} e^{-(ix+X_n)k} \frac{dk}{2\pi} + \int_{-\infty}^0 e^{-(ix-X_n)k} \frac{dk}{2\pi} \\
 &= \frac{1}{2\pi} \left(\frac{1}{ix+X_n} - \frac{1}{ix-X_n} \right) \quad \text{since } X_n > 0.
 \end{aligned}$$

Thus we obtain

$$\boxed{P_n(x) = \frac{1}{\pi} \frac{X_n}{X_n^2 + x^2}} \quad \text{with } X_n = \sum_{j=1}^n x_j.$$

As noticed earlier, the variance of the PDF is infinite. Since one of the assumptions of the CLT was violated, we can not apply the CLT to this problem and the resulting PDF is not in the form of the gaussian distribution.

For the case of identical steps $x_n = a$ we get

$$p(x) = \frac{a}{\pi} \frac{1}{a^2 + x^2} \quad \text{and} \quad P_n(x) = \frac{na}{\pi} \frac{1}{n^2 a^2 + x^2}.$$

It is not surprising to not observe a gaussian behavior for the PDF after n steps. That is, the scaling $\xi = \frac{x}{a\sqrt{n}}$ is not appropriate. However, by scaling $\xi = \frac{x}{na}$, the normalized PDF for the variable ξ is written

$$\tilde{P}_n(\xi) = naP_n(x) = \frac{1}{\pi} \frac{1}{1 + \xi^2} \quad \text{independent of } n.$$

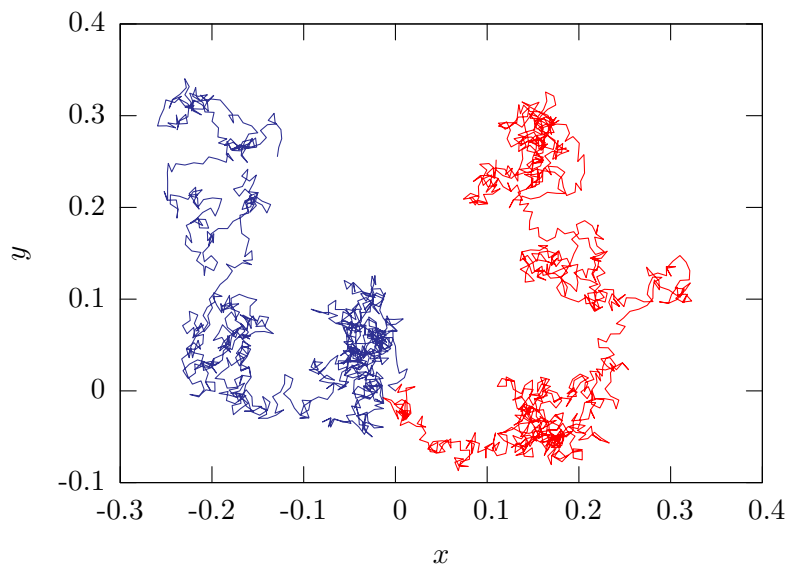


Figure 3: Two typical Pearson random walks of length 1000.

3 Pearson's random walk

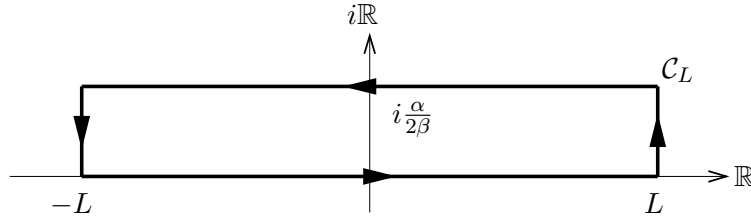
Appendix B shows an example C++ code for simulating a Pearson random walk. The code calculates the distribution of A_N , the proportion of steps that the walker is in the half plane $x > 0$, and of B_N , the proportion of steps that the walker is in the upper-right quadrant $x > 0, y > 0$.

Figure 2 shows the computed probability density functions for A_N and B_N , based on simulations of 10^8 random walks of length $N = 10^5$. Since the walk is isotropic, it is clear that the expected value of A_N should be $\frac{1}{2}$. However, it is clear from the plot that the most likely values for A_N are 0 and 1 – the walker is most likely to spend all of its time in the left or right half plane. The probability density function is an extremely good match to

$$p(x) = \frac{1}{\pi\sqrt{x(1-x)}}.$$

and in subsequent lectures we shall examine this more carefully.

Similarly, we know that the expected value of B_N is $\frac{1}{4}$. However, it is clear from figure 2, that the most probable value is 0. Interestingly, we do not see a peak close to 1. Figure 3 shows two typical random Pearson random walks of length 1000. We see that one of the walkers spends almost all the time in the left half plane (hence $A_N \approx 0$) while the other spends almost all the time in the right half plane (hence $A_N \approx 1$).

Figure 4: Contour \mathcal{C}_L .

A Appendix

We consider the integral

$$\begin{aligned}
 \int_0^\infty \cos(k\alpha) e^{-\beta k^2} dk &= \frac{1}{2} \int_{-\infty}^\infty \cos(k\alpha) e^{-\beta k^2} dk \\
 &= \frac{1}{4} \left[\int_{-\infty}^\infty e^{-ik\alpha - \beta k^2} dk + \int_{-\infty}^\infty e^{ik\alpha - \beta k^2} dk \right] \\
 &= \frac{e^{-\frac{\alpha^2}{4\beta}}}{4} \left[\int_{-\infty}^\infty e^{-\beta \left(k + i\frac{\alpha}{2\beta}\right)^2} dk + \int_{-\infty}^\infty e^{-\beta \left(k - i\frac{\alpha}{2\beta}\right)^2} dk \right].
 \end{aligned}$$

To calculate the first integral, let us now consider the complex integral

$$\oint_{\mathcal{C}_L} e^{-\beta z^2} dz$$

where \mathcal{C}_L is the contour defined in figure 4.

Cauchy's Theorem implies that this integral vanishes. Expanding the integration on each side of the contour \mathcal{C}_L gives

$$\begin{aligned}
 \oint_{\mathcal{C}_L} e^{-\beta z^2} dz &= \int_{-L}^L e^{-\beta x^2} dx + \int_0^{\frac{\alpha}{2\beta}} e^{-\beta(L+iy)^2} dy \\
 &\quad + \int_L^{-L} e^{-\beta \left(x + i\frac{\alpha}{2\beta}\right)^2} dx + \int_{\frac{\alpha}{2\beta}}^0 e^{-\beta(-L+iy)^2} dy \\
 &= 0
 \end{aligned}$$

We see immediately to see that the second and fourth term in this expansion vanish as $L \rightarrow \infty$. In this limit, we can conclude

$$\int_{-\infty}^\infty e^{-\beta \left(x + i\frac{\alpha}{2\beta}\right)^2} dx = \int_{-\infty}^\infty e^{-\beta x^2} dx = \sqrt{\frac{\pi}{\beta}}.$$

Similarly, we can also prove

$$\int_{-\infty}^\infty e^{-\beta \left(x - i\frac{\alpha}{2\beta}\right)^2} dx = \int_{-\infty}^\infty e^{-\beta x^2} dx = \sqrt{\frac{\pi}{\beta}}.$$

Thus we obtain

$$\int_0^\infty \cos(k\alpha) e^{-\beta k^2} dk = \frac{\sqrt{\pi}}{2\sqrt{\beta}} e^{-\frac{\alpha^2}{4\beta}}.$$

Using the equalities

$$\begin{aligned}\int_0^\infty k \sin(k\alpha) e^{-\beta k^2} dk &= -\frac{d}{d\alpha} \int_0^\infty \cos(k\alpha) e^{-\beta k^2} dk \\ \int_0^\infty k^5 \sin(k\alpha) e^{-\beta k^2} dk &= -\frac{d^5}{d\alpha^5} \int_0^\infty \cos(k\alpha) e^{-\beta k^2} dk\end{aligned}$$

we obtain the useful relations

$$\int_0^\infty k \sin(k\alpha) e^{-\beta k^2} dk = \frac{\alpha\sqrt{\pi}}{4\beta^{3/2}} e^{-\frac{\alpha^2}{4\beta}}, \quad (1)$$

$$\int_0^\infty k^5 \sin(k\alpha) e^{-\beta k^2} dk = \frac{\alpha\sqrt{\pi}}{64\beta^{11/2}} e^{-\frac{\alpha^2}{4\beta}} (\alpha^4 - 20\alpha^2\beta + 60\beta^2). \quad (2)$$

B C++ code for simulating Pearson's Random Walk

```
#include <string>
#include <iostream>
#include <cstdio>
#include <cmath>
using namespace std;

const double p=6.283185307179586476925286766559;
const long n=2000; //Number of steps in a walk
const long w=200000; //Number of walkers

int main () {
    long i,j,c,d,a[n+1],b[n+1];
    for(i=0;i<=n;i++) a[i]=b[i]=0;
    double r,t,x,y;
    for(j=0;j<w;j++) {
        x=y=0;c=d=0;
        for(i=0;i<n;i++) {
            x+=cos(t=double(rand())/RAND_MAX*p);
            y+=sin(t);
            if (x>0) {c++;if(y>0) d++;}
        }
        a[c]++;b[d]++;
    }
    for(i=0;i<=n;i++) {
        x=double(i)/n;
        cout << i << "_" << x << "_"
              << a[i] << "_" << b[i] << endl;
    }
}
```