Solution exercise set 3

Problem 1

The diffusion of the water tracing solution in the pipe follows the solution of the diffusion equation in one dimension

$$\rho(x,t) = \frac{\text{Cste}}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}} \tag{1}$$

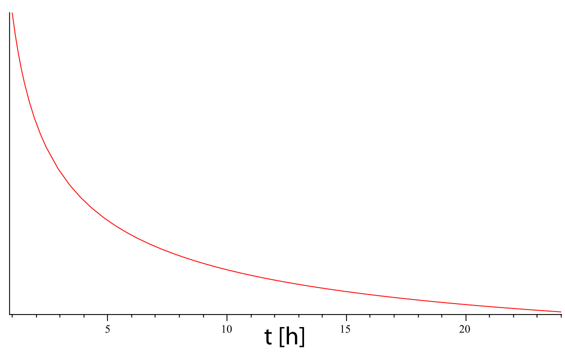
with $\rho(x)$ the density assumed to be constant over the radial coordinates in the pipe (narrow pipe), D the diffusion coefficient and $\text{Cste} = \frac{M}{A}$. This solution is valid for a point source (infinite concentration at a point at $t = 0$). In Problem 2 we will show that the integral of the solution (1) over the space variable x does not change in time (in other words the mass of water tracing solution remains constant). However, we see from (1) that $\rho(x = 0) \to \infty$ and $\rho(x \neq 0) \to 0$ when $t \to 0$. This means that when the time goes to zero, we model the ideal injection of mass by an infinite peak of concentration centered at $x = 0$, however, since the peak is infinitely narrow, the total mass is finite (integral of the concentration over x).

- Using (1) we see that the concentration at $x = 0$ diverges when $t \to 0$. In the next exercise set we will see a more realistic description of the intitial state taking into account the volume of the solution injected. The point source approximation is a good approximation for some problems but would fail when the volume of the injected solution needs to be taken into account.
- The standard deviation after one second σ is given by

$$\sigma = \sqrt{2Dt} \approx 0.005cm \tag{2}$$

- The maximal concentration is always at x=0 and is given by the simple expression

$$\frac{\text{Cste}}{\sqrt{4\pi Dt}} \tag{3}$$



- Here we compare the solution at $x = 0\ cm$ (where the maximum is) and at $x = 100\ cm$. As a result we get that $\frac{\rho(x=0,t)}{\rho(x=100,t)} = \frac{100}{95}$ for $t \approx 119$ years !! Molecular diffusion is not sufficient to effectively reach a state with a homogeneous concentration.

Problem 2

Using the change of variables $\alpha = \frac{x}{2\sqrt{Dt}}$ we get that the total mass is given by

$$A \cdot \frac{\text{Cste}}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\alpha^2} d\alpha \tag{4}$$

and the variance is given by

$$\frac{4Dt}{\sqrt{\pi}} \int_{-\infty}^{\infty} \alpha^2 e^{-\alpha^2} d\alpha. \tag{5}$$

Recall that D is the diffusion coefficient and $\text{Cste} = \frac{M}{A}$. Now we need to compute the two integrals $I = \int_{-\infty}^{\infty} e^{-\alpha^2} d\alpha$ and $J = \int_{-\infty}^{\infty} \alpha^2 e^{-\alpha^2} d\alpha$.

- To compute the integral $I = \int_{-\infty}^{\infty} e^{-\alpha^2} d\alpha$ we will compute instead $I^2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\left(\alpha^2+\beta^2\right)} d\alpha d\beta$. Going to polar coordinates ($\alpha = r\cos\theta, \beta = r\sin\theta$) and using the Pythagoras theorem we get

$$I^2 = \int_0^{\infty} 2\pi r e^{-r^2} dr = -\pi e^{-r^2}\Big|_0^{\infty} = \pi \tag{6}$$

  And therefore the initial integral $I = \sqrt{\pi}$. Using this result in (4) we get the total mass $A \cdot \text{Cste} = M$ as expected.

- To compute the integral $J = \int_{-\infty}^{\infty} \alpha^2 e^{-\alpha^2} d\alpha$ we introduce the other integral $K(T) = \int_{-\infty}^{\infty} e^{-T\alpha^2} d\alpha$. We have that $K(T) = \sqrt{\frac{\pi}{T}}$ from the previous point (to see this make the change of variable to $\sqrt{T}\alpha$). But we also see that the initial integral we wanted to compute is related to the derivative of $K(T)$ evaluated at $T = 1$

$$J = -\left.\frac{\partial K(T)}{\partial T}\right|_{T=1} = -\left.\frac{\partial(\sqrt{\pi/T})}{\partial T}\right|_{T=1} = \frac{\sqrt{\pi}}{2} \tag{7}$$

  Using this result in (5) we get the variance $\sigma^2 = 2Dt$.

Problem 3

- It is interesting to remark (see Figure 1) that in one dimension, if we take a sufficient number of steps, the random walk will alway return to the origin after some time. For the random walk in two dimensions this fact is still true. In three dimensions, however, there is a probability that the walk does not return to the origin even after an infinite number of steps. In other words: "A drunk man will find his way home but a drunk bird may get lost forever"!

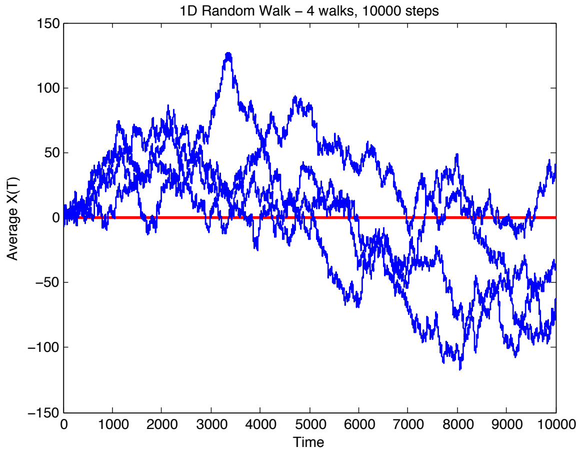


Figure 1: realizations of the random walk in one dimension

- The law of large numbers tells us that if we take the average over a sufficient number of realizations we will converge to the real expectation value. From Figure 2 we see that the average distance squared is proportional (actually even equals for the case we consider !) to the number of steps (in accordance with the result of the lecture since the number of steps is itself proportional to the time).
- The maximal distance squared is proportional to the number of steps squared if we take a sufficient number of realizations (i.e. much larger than the number of steps, see how it begins to fail on Figure 3 when the number of steps is too large). The distance $d_{max} = n^2$ with n the number of steps corresponds to a trajectory where all the steps go in the same direction ($+1$ or -1).

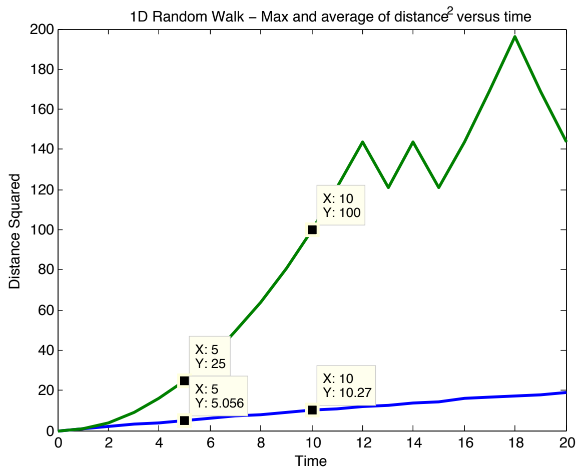


Figure 2: average and maximal distance squared over several simulated realizations of the random walk

- The central limit theorem tells us that the distribution of the sum of a large number of independent and identically distributed random variables follows a Gaussian distribution (also called Normal distribution). This can be observed from Figure 3. It is necessary to take a sufficient number of walkers to get a "nice" Gaussian shape.

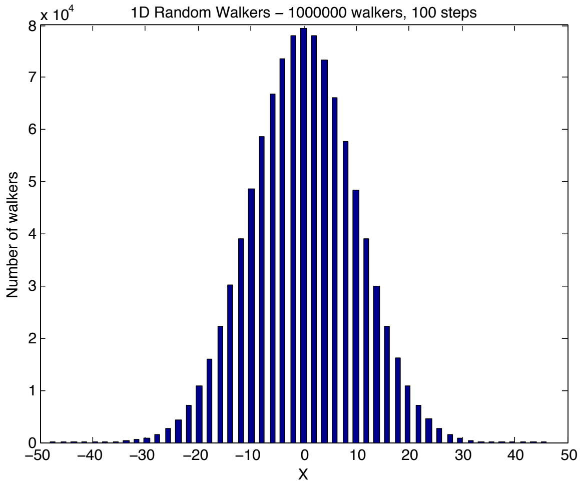


Figure 3: histograms of the positions computed for several realizations of the random walk