Random Walks, the Diffusion Equation, and Cluster Growth

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Abstract

In this assignment we blah blah blah

1 Theory

1.1 Random Walks in 2D

Mean and squared displacement Distance from origin

1.2 Diffusion Equations and the Finite Difference Form

The diffusion equation in $1D$ is written,

$$\frac{\partial \rho(x,t)}{\partial t} = D\nabla^2 \rho(x,t), \tag{1}$$

where D is the diffusion constant. Equation 1 is turned into an iterable form by noting: $\rho(x,t) = \rho(i\Delta x, n\Delta t) = \rho(i,n)$. This is the finite difference form[1].

After using the formal definition of derivatives and algebraically manipulating Equation 1 in the finite difference form, we get

$$\rho(i,n+1) = \rho(i,n) + \frac{D\Delta t}{\Delta x^2}\left(\rho(i+1,n) + \rho(i-1,n) - 2\rho(i,n)\right), \tag{2}$$

where Δt and Δx are the step sizes in an iteration. This solution requires knowledge of initial conditions. We must assume that the x displacement is known at times prior to and including $t_n = n\Delta t$. Two consecutive steps prior to the first unknown step is sufficient to solve such an equation. Finally, to guarantee stability, the following criterion must be met

$$\Delta t \leq \frac{(\Delta x)^2}{2D}. \tag{3}$$

We will use an initial density profile that is sharply peaked around $x = 0$, but extends over a few grid sites to resemble a box. This is sufficient for generating the solution to the diffusion equation. Interestingly, after a couple iterations, the box profile will diffuse into a Gaussian normal distribution. The $1D$ Gaussian normal distribution has the form,

$$\rho(x,t) = \frac{1}{\sqrt{2\pi\sigma(t)^2}} \exp\left(-\frac{x^2}{2\sigma(t)^2}\right), \tag{4}$$

where $\sigma(t) = \sqrt{2Dt}$.

The spatial expectation value, $\langle x(t)^2 \rangle$, of Equation 4 is equal to $\sigma(t)^2$. Expectation values are calculated according to the equation

$$\langle x \rangle = \int_{-\infty}^{\infty} f(x) x dx, \tag{5}$$

where $f(x)$ is the Guassian normal distribution for our purposes. Because we are looking for $\langle x^2 \rangle$, Equation 5 becomes

$$\begin{aligned}\langle x^2 \rangle &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma(t)^2}} \exp\left(-\frac{x^2}{2\sigma(t)^2}\right) x^2 dx \\ &= 2\int_{0}^{\infty} \frac{1}{\sqrt{2\pi\sigma(t)^2}} \exp\left(-\frac{x^2}{2\sigma(t)^2}\right) x^2 dx.\end{aligned} \tag{6}$$

[1] The finite difference form must be used because the diffusion equation is time dependent. Therefore, a relaxation method cannot be used.

The last step can be done because the x^2 term makes it an even function being symmetrically integrated about zero. Now, we make a change of variable ($x = \sigma\sqrt{2}$) to obtain, after a couple steps of algebra,

$$\langle x^2 \rangle = \frac{4\sigma^2}{\sqrt{\pi}} \int_0^\infty x^2 \exp(-x^2) dx. \tag{7}$$

Integrating the above equation by parts yields

$$\langle x^2 \rangle = \sigma^2 \tag{8}$$

Typically, we call this equation the variance.

2 Computations

2.1 Random Walks in 2D

To code for the basic 2D walk, we assume that the probability to step in either direction left, right, up or down is the same. Then, for every step, we generate a random number. This is equivalent to drawing from Uniform (0,1). We assign every move to one of the segments of .25. If the random numbers falls within that value, we move in the assigned direction. The evidence for a successfully coded $2D$ walker program is given in Figure 1 and 2.

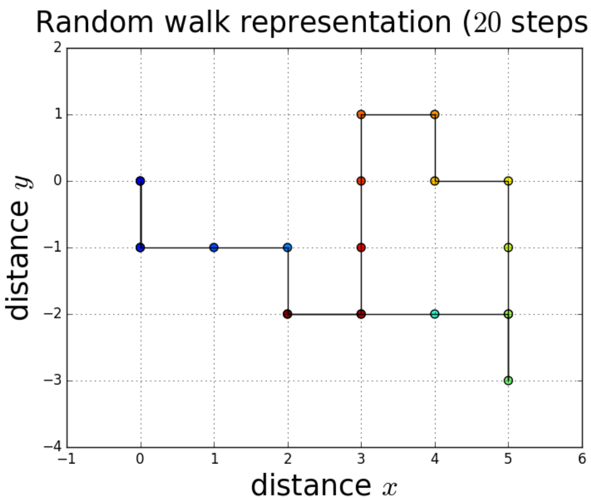

Figure 1: 20-step random walk

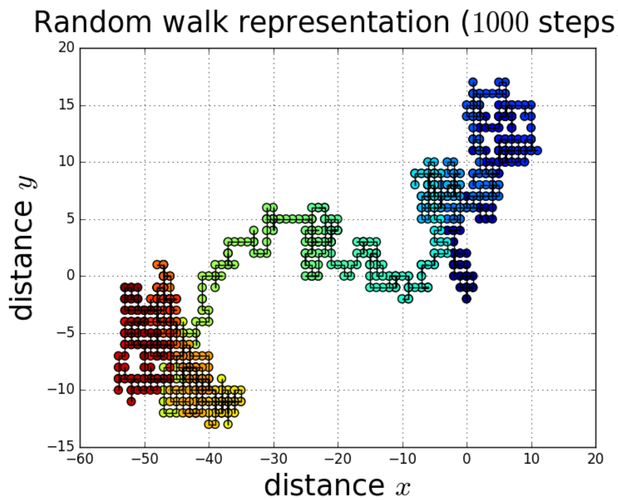

Figure 2: 1000-step random walk

2.2 Diffusion of a Box Density Distribution

Using the arguments in Section 1.2, we solve the $1D$ Diffusion Equation over a period of time. Five different snapshots in time were then fit against Equation 4 to show a box shaped density will eventually diffuse into a Gaussian normal distribution. This $1D$ diffusion solver was performed for an initial box shaped density, shown in Figure 3.

In Figures 4-8, we took snapshots of the $1D$ density equation and fit a Gaussian to the solution. A value of σ was then extracted and compared to the analytical solution, $\sigma = \sqrt{2Dt}$. As can be seen, the fit worked well during early time snapshots but got progressively worse.

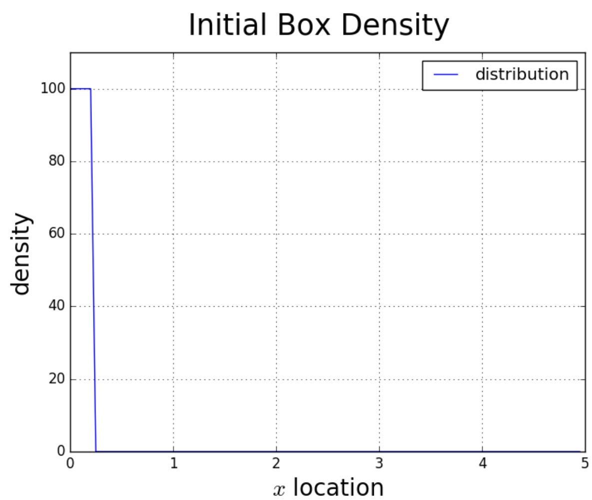

Figure 3: initial box-shaped density

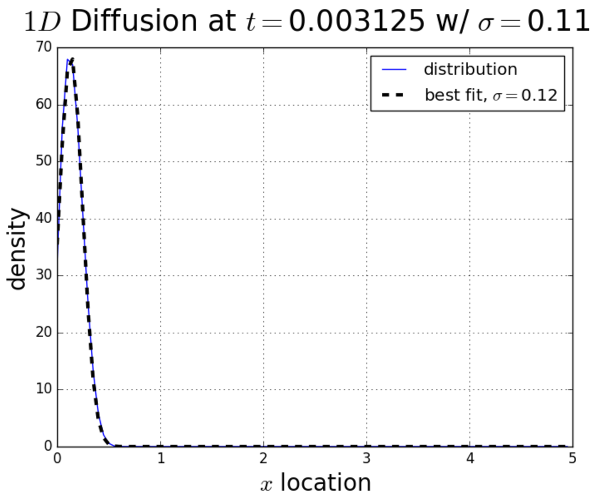

Figure 4: $1D$ density after time evolution

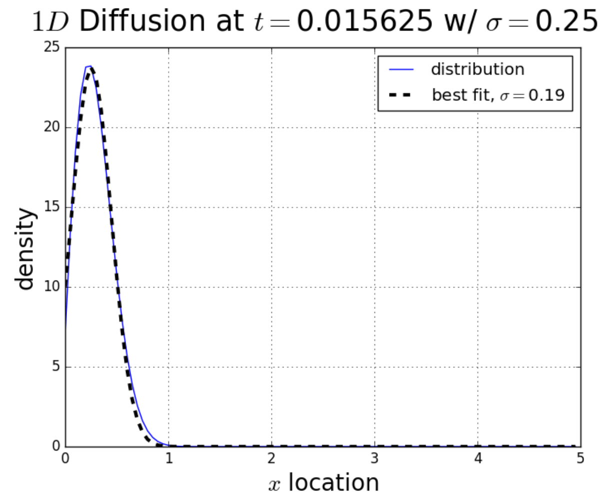

Figure 5: $1D$ density after time evolution

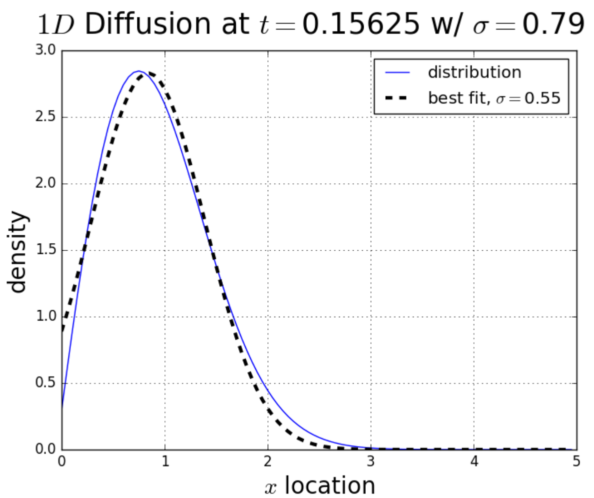

Figure 6: $1D$ density after time evolution

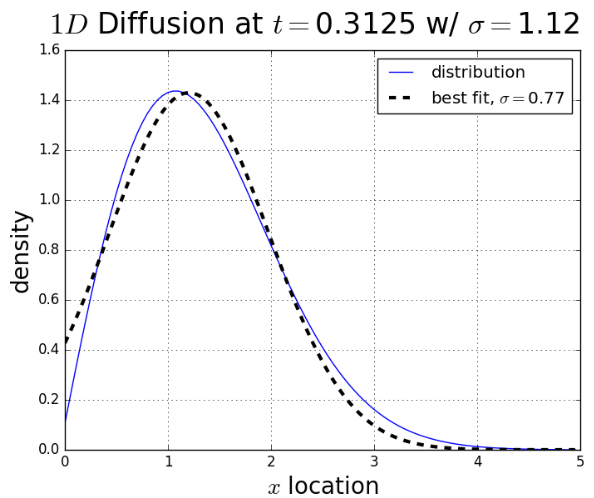

Figure 7: $1D$ density after time evolution

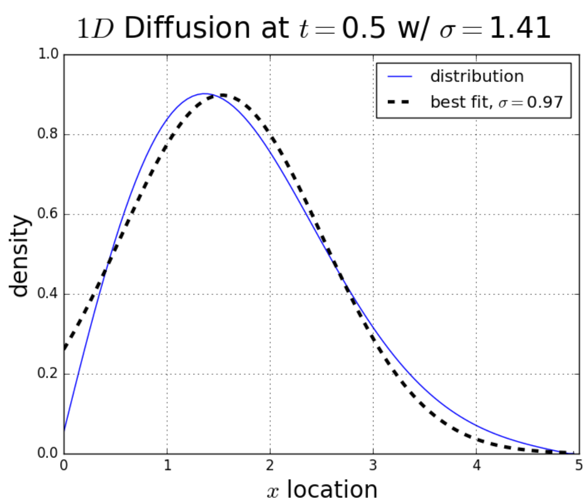

Figure 8: $1D$ density after time evolution