Random Walk and Diffusion

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Abstract: Randomness plays important roles in the systems with a large number of degrees of freedom, especially in the multi-particle systems. Even though the underlying physics of the systems may be deterministic, our incomplete knowledge will force us to resort to a statistical, stochastic description. Random walk is an excellent way to describe the motion of a particle in complex systems.

Introduction:

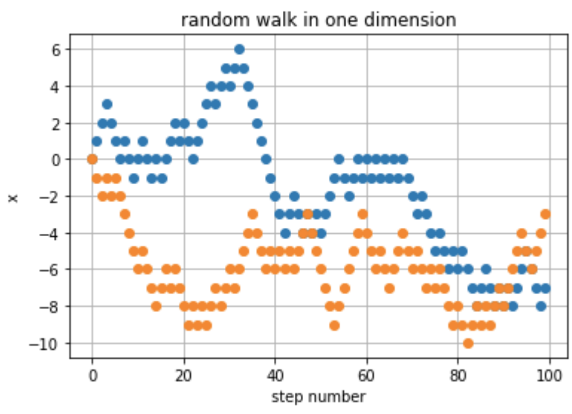
A random walk is a mathematical object, known as a stochastic or random process, that describes a path that consists of a succession of random steps on some mathematical space such as the integers. As we introduced before, the motion of a particle or molecule in solution is analogous to a random walk.

The simplest situation involves a walker that is able to take steps of length unity along a line, which is so called on dimensional random walk. Such description divides into the solution with fixed length of steps and the one with random length of steps. And then we talked about the SAW problem, which means the path followed by our polymer molecule must not be allowed to interest itself. At last, we will explore the connection between random walk and diffusion.

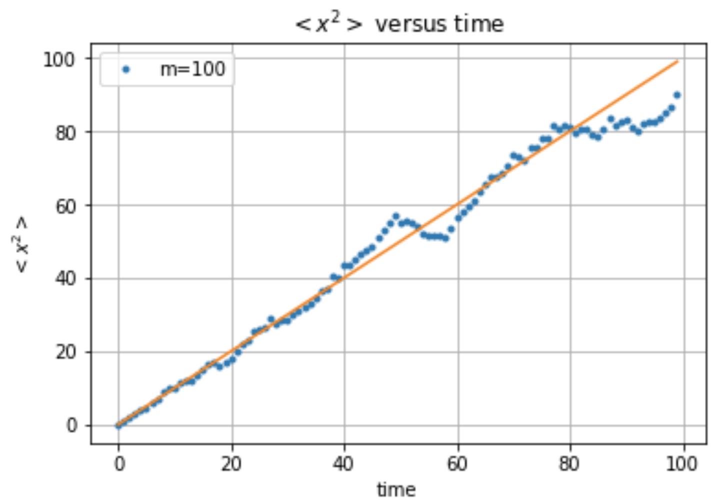
Random Walk:

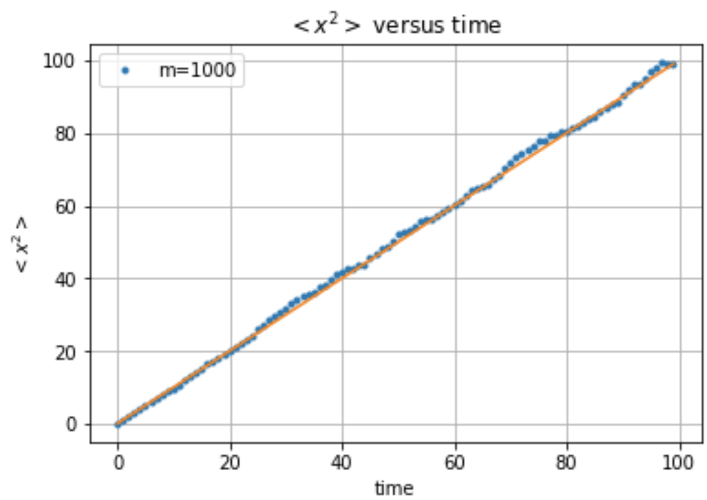
A routine that implements a random walk in one dimension is illustrated below. Here we generate a random value number in the range between 0 and 1 and compare its value to 1/2. If it is less than 1/2, then our walker moves right, otherwise it moves left. And we repeat this process to get x_n.

Random walk with a fixed step-length:



Since a walker is as likely to step left as right, this average which we denote by $\langle x_n \rangle$, must be zero. As a consequence, a more interesting and informative quantity is $\langle x_n^2 \rangle$, the average of the square of the displacement after n steps. To get the numerical solution, we generate a loop to compute the value.

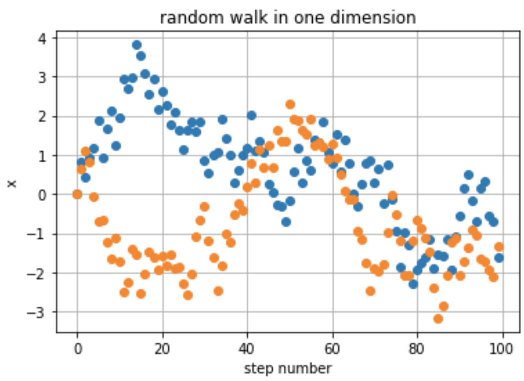


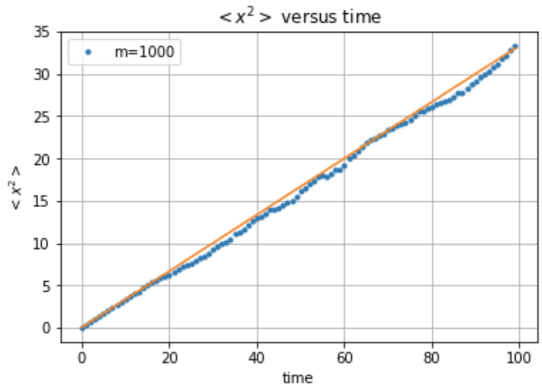


As the pictures show, the more times we compute, the closer the solution is to the ideal line, that is

$$\langle x^2 \rangle = 2Dt$$

The value of 2D is the slope of the $\langle x^2 \rangle$ versus t plot, as is shown above. So in the situation of fixed step-length, $D = 1/2$. While for the situation of random step-length, we will get

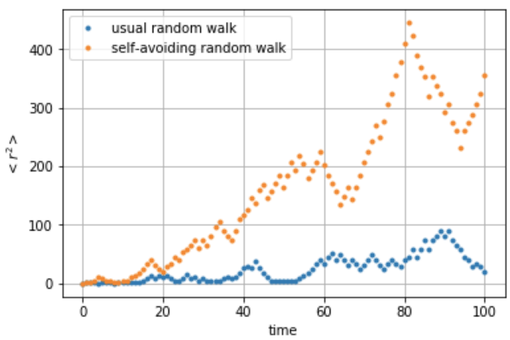


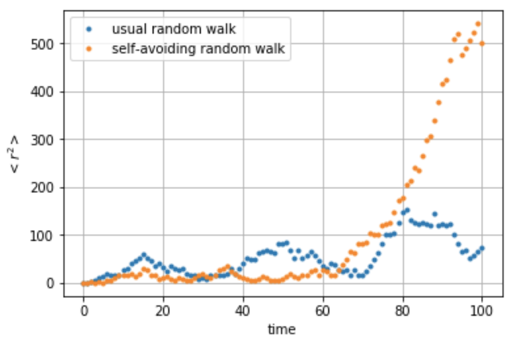


In such cases, we can see D=1/6 approximately.

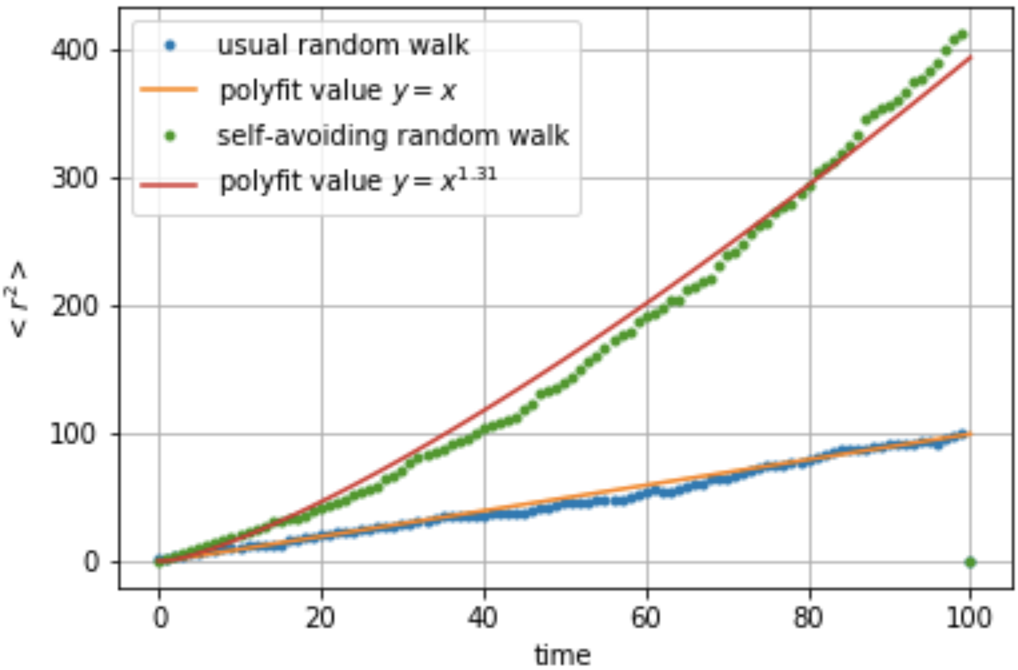
Self-Avoiding Walks:

A simulation of SAWs is similar to that of ordinary random walks, but with one very important difference: we must keep track of all prior steps and make sure that configuration that would revisit a previously tramped site are not included. It is known that for polymers in an equilibrium solution, all possible SAWs configuration will occur with equal probability. The self-avoidance constraint(often called the excluded-volume effect) also has an obvious effect on the size of SAW. As compared with an ordinary random walk, a self-avoiding walker will, on average, get further away from its starting point in a given number of steps. Avoidance of self-interactions forces a SAW to stretch out more rapidly into previously unvisited regions of space. Ordinary SAW solutions and a self-avoidance walk solution is shown below.





As is shown above, clearly the self-avoiding walks stretch out further than the ordinary ones. However, both of them are random process, which means to see, it is hard to see the trend in several numerical solutions. So we repeat the computation for a large number of times and compute the average values. Results are as follows:



It can be seen that two dimensional SAW the mean-square distance from the starting point, $\langle r^2 \rangle$, does not vary linearly with time as is the case for an ordinary random walk. We see that $\langle r^2 \rangle \sim t^{1.31}$ for the SAW, so the behavior intermediate that of a random walk(diffusion), for which $\langle r^2 \rangle \sim t$, and a free particle, for which $\langle r^2 \rangle \sim t^2$. Thus, if we define the exponent ν, (called the Flory exponent) by

$$\sqrt{\langle r^2 \rangle} \sim At^{\nu}$$

As for self-avoiding walks, $\nu = 1.5$. However, in order to decrease high attrition caused by the self-avoiding walks and improve the efficiency, here we choose the approach to grow the random walk, which just means no-heading-back. As a consequence, the ν here, 1.31, is less than the normal valve, 1.5.

Random Walk and Diffusion:

In order to explore more details in the connection between random walk and particle diffusion. The idea, as known as coarse graining, is to consider regions of space that are big enough to contain a large number of particles so that the density can be meaningfully defined. The density is then proportional to the probability per unit space per unit time.

As for a individual random walker, $P(i, j, k, n)$ is the probability to find the particle at the site (i, j, k) at time .Since we are on a simple cubic lattice, there are 6different nearest neighbor sites. If the walker is on one of these sites at time n-1, there is a probability of 1/6 that it will then move to site (i, j, k) at time n. Hence, the total probability to arrive at (i, j, k) is:

$$P(i,j,k,n) = \frac{1}{6}[P(i+1,j,k,n-1) + P(i-1,j,k,n-1) + P(i,j+1,k,n-1)$$
$$+ P(i,j-1,k,n-1) + p(i,j,k+1,n-1) + p(i,j,k-1,n-1)]$$

Rearranging the equation, and it suggests taking the continuum limit, which lead to

$$P(i,j,k,n) - P(i,j,k,n-1) =$$
$$\frac{1}{6}\{[P(i+1,j,k,n-1) - 2P(i,j,k,n-1) + P(i-1,j,k,n-1)]$$
$$+[P(i,j+1,k,n-1) - 2P(i,j,k,n-1) + P(i,j-1,k,n-1)]$$
$$+[P(i,j,k+1,n-1) - 2P(i,j,k,n-1) + P(i,j,k-1,n-1)]\}$$

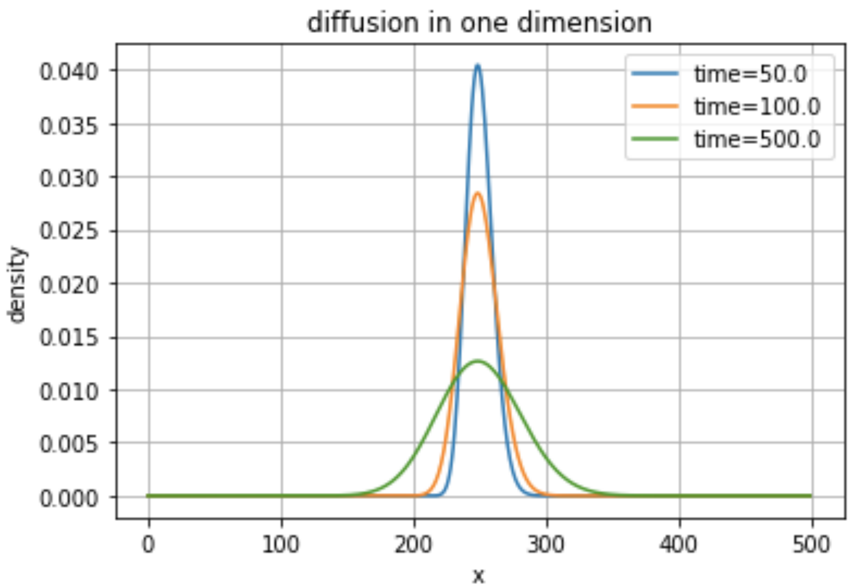
While taking the continuum limit will lead to

$$\frac{\partial P(x,y,z,t)}{\partial t} = D\nabla^2 P(x,y,z,t)$$

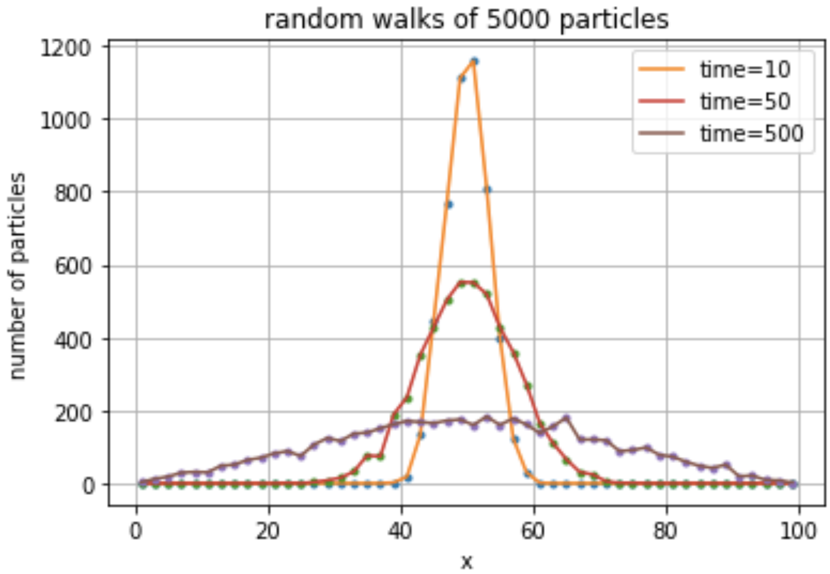
where $D = (\frac{1}{6})(\Delta x)/\Delta t$ in this approximation. This derivation shows the close connection between the random walks and diffusion. The density ρ obeys the same equation:

$$\frac{\partial \rho}{\partial t} = D\nabla^2 \rho$$

Using the equations above, we will get the distribution of particle diffusing after a certain time,



While in the random walk occasion, we set the initial condition of 5000 particles in a limiting location, x=50, and then plot their distribution after some time. And before depicting we could remove the dots where the density is zero, which is caused by fixed step-length. The result is as follows:



After all, both of approaches above exhibit the Gaussian spreading of the particle spreading as expected. All in all, It can be seen as two equivalent solutions to one problems.

Conclusion:

Random walk can be used to describe many random systems with many degrees of freedom, especially systems including a great amount of particles. And in a way the diffusion algorithm is equivalent to random walk.