Exercise 08 Sthavishtha Bhopalam Rajakumar December 27, 2017

1 Introduction

This work attempts to use Monte Carlo method to obtain configurational averages of a random walk system, in a systematic manner. For this purpose, two tasks are carried out :

1. **Simple Random walk** - This two dimensional random walk comprises of N positions with fixed step size of unity.
2. **Chains of Spherical Particles** - This three dimensional random walk comprises of N hard spherical particles which do not touch each other (self-avoiding random walk)

2 Algorithm Description

2.1 Simple Random Walk

The two-dimensional random walk is generated by keeping the step size fixed and by varying the angle θ, where the angle is chosen randomly (with `drand48()`) as seeded by `srand48()` function. Then, the updated positions of the random walk can be generated by :

$$x_{new} \; = \; x_{old} \; + \; \cos(\theta) \tag{1}$$

$$y_{new} \; = \; y_{old} \; + \; \sin(\theta) \tag{2}$$

where, the subscripts *new* and *old* refer to the updated and previous positions of the random walk.

These updated positions can later be used to compute end-to-end distance R^2 of the final position from the initial position of the random walk (taken to be the origin). This process can be repeated for several samples (or configurations M) of these positions.

The end-to-end distance can be computed as :

$$\langle R^2 \rangle \; = \; \frac{1}{M} \sum_{k=1}^{M} R_k^2 \tag{3}$$

The estimated error Δ to keep a track of the required number of samples (till Δ attains 1% of the average value) can be computed as :

$$\Delta \; = \; \sqrt{\frac{1}{M}[\langle (R^2)^2 \rangle \; - \; \langle R^2 \rangle^2]} \tag{4}$$

where $\langle (R^2)^2 \rangle$ is :

$$\langle (R^2)^2 \rangle \; = \; \frac{1}{M} \sum_{k=1}^{M} (R_k^2)^2 \tag{5}$$

2.2 Chains of Spherical Particles

In this task, three-dimensional particles touching each other (self-avoiding random walks with no overlap) have been considered. For this purpose, two angles (along the spherical coordinates) have been randomly varied as :

$$\theta \; = \; 2\pi \texttt{drand48()}, \qquad \phi \; = \; \pi \texttt{drand48()} \tag{6}$$

The updated positions of the random walk can now be computed as :

$$x_{new} = x_{old} + \sin(\phi)\cos(\theta) \tag{7}$$

$$y_{new} = y_{old} + \sin(\phi)\sin(\theta) \tag{8}$$

$$z_{new} = z_{old} + \cos(\phi) \tag{9}$$

Equations 3, 4 and 5 hold the same for this case too.

2.3 Algorithm

The outline of the general algorithm for the aforementioned tasks can be written as follows:

while $N \leq N_{max}$ **do**
  $r_{sq} \leftarrow 0$
  $r_{sq,sq} \leftarrow 0$
  $j \leftarrow 0$ //Increment variable to update samples/configurations M
  $M \leftarrow 1000$
  while $j \leq M$ **do**
    $x, y \leftarrow 0$ //Initial position is origin
    for $i \leftarrow 0; i \leq N$ **do**
      Calculate the updated positions from Equations 1, 2 or 7 - 9 depending on the case
    end for
    Calculate the distance from origin
    Update M till Δ/R^2 is less than 1% of the average distance according to Equation 4.
  end while
  Print the necessary variables into a file
end while

3 Results

3.1 Simple Random Walk

To keep a track of the necessary number of samples required to capture the random walk, a criterion of attaining 1% error of the average of $\langle R^2 \rangle$ has been chosen. This is seen in the Figure 1. To capture an approximate slope of this curve, a log-log graph of the same plot has been made with a linear fit as seen in Figure 2. To determine the relation of $\langle R^2 \rangle$ with N, a graph along with its corresponding linear fit curve has also been plotted as seen in Figure 3.

3.2 Chains of Spherical Particles

Similar to the previous section concerning **Simple Random Walk**, plots for determining the relationship between the average of $\langle R^2 \rangle$ and N were determined in this case too as seen in Figures 4 and 5.

4 Discussion

4.1 Simple Random Walk

As seen in Figure 1, it requires close to 20000 samples to satisfy the 1% criterion as described earlier, necessitating the need for higher number of samples. From Figure 2, the variation of $\Delta/\langle R^2 \rangle$ with $\log(M)$ is determined to have a theoretical slope of -0.5. However, the actual slope obtained after curve fitting is -0.5057, quite consistent with the theoretical observations. After fitting, the correlation can be thus determined as : $\log(\Delta/\langle R^2 \rangle) = 1.4535e^{-0.5057}$. Additionally, $\langle R^2 \rangle$ can be seen to be linearly related with N, with an actual slope of 1.00042 in Figure 3.

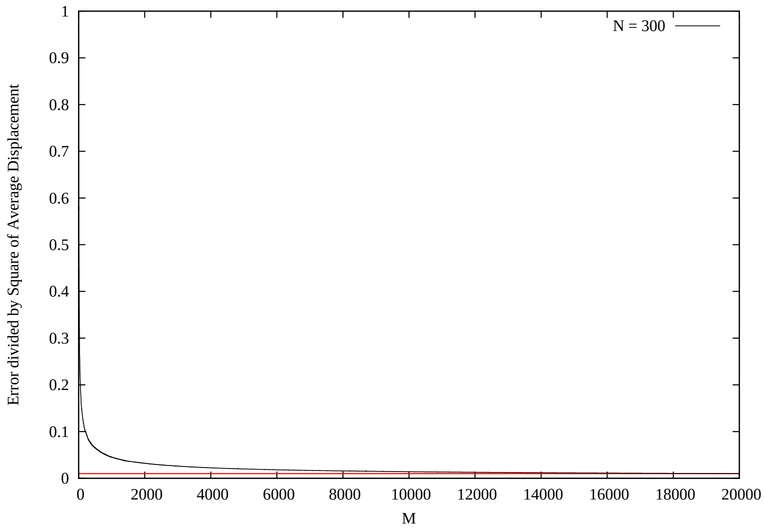

Figure 1: Graph of $\Delta/\langle R^2\rangle$ vs M for fixed $N = 300$: *Simple Random Walk*

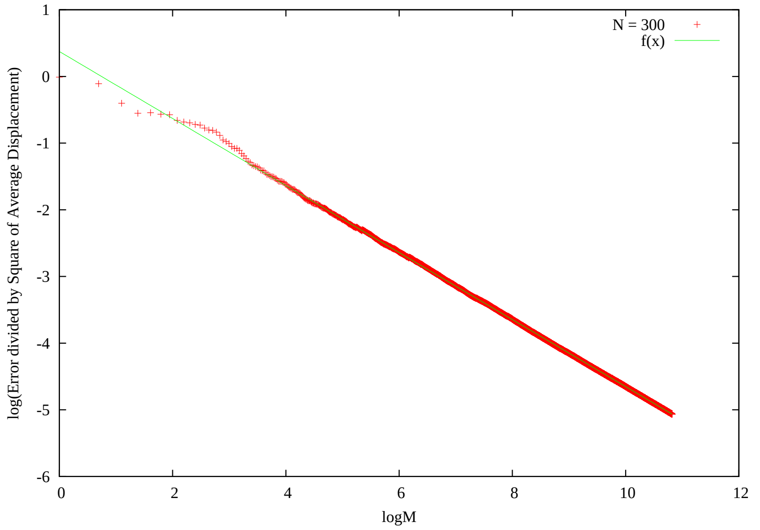

Figure 2: Graph of $\log(\Delta/\langle R^2\rangle)$ vs $\log(M)$ for fixed $N = 300$: *Simple Random Walk*

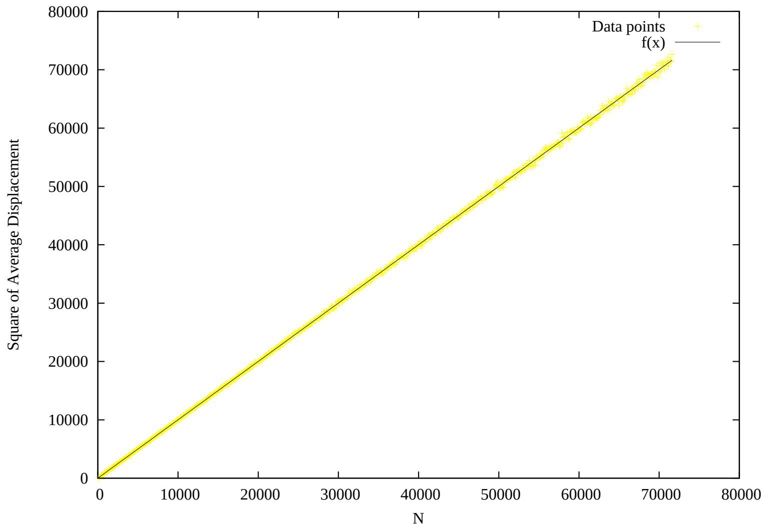

Figure 3: Graph of $\langle R^2\rangle$ vs N - note the linearity of this plot in accordance with the fit line : *Simple Random Walk*

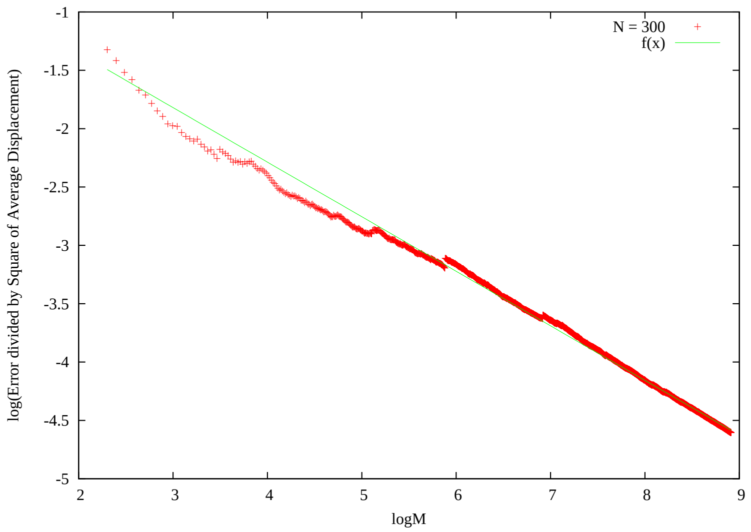

Figure 4: Graph of $\log(\Delta/\langle R^2\rangle)$ vs $\log(M)$ for fixed $N = 300$: *Chains of Spherical Particles*

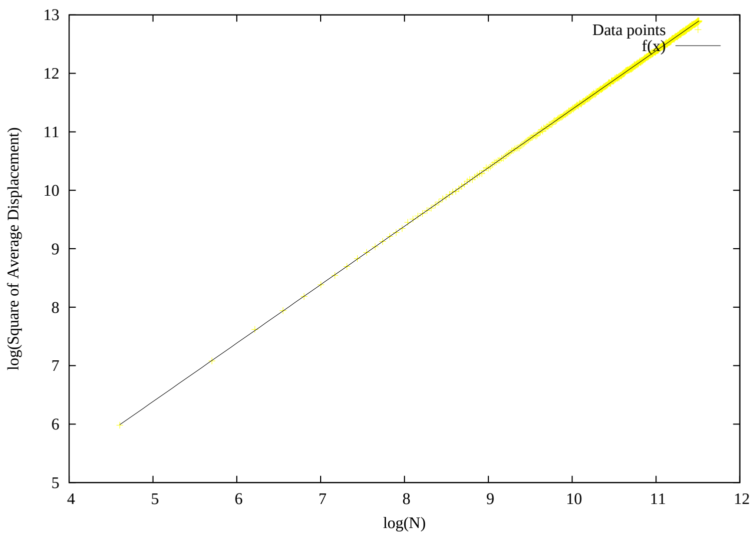

Figure 5: Graph of $\langle R^2\rangle$ vs N - note the linearity of this plot in accordance with the fit line : *Chains of Spherical Particles*

4.2 Chains of Spherical Particles

In this three-dimensional case, the variation of $\log(\Delta/\langle R^2\rangle)$ with $\log(M)$ is determined to have an actual slope of -0.4675 as seen in Figure 4, which gives a fitting correlation as $\Delta/\langle R^2\rangle = 0.6590e^{-0.4675}$. Additionally, $\langle R^2\rangle$ can be seen to be linearly related with N, with an actual slope of 1.00017 as seen in the log-log plot in Figure 5.

References

[1] Hermann, Hans J., *Lecture notes on introduction to computational physics*, Institute for Building Materials, ETH Zürich, 2017.