Project 3

Statistical Modeling of Polymers: A Weighted Random Walk via the Rosenbluth and Rosenbluth Method

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1 Abstract

Through a static statistical Monte Carlo modeling approach known as the Rosenbluth and Rosenbluth method, weighting is incorporated into a self avoiding random walk. Through this, physical properties of polymer chains are shown such that the success rate of completed walks and mean squared end-to-end distances were analyzed for different step sizes, and a fall-off point was identified for the basic self avoiding random walk. An exponent value of v was experimentally found to be approximately 0.75, indicating a departure from the square root dependence observed in simple random walks. The findings underscore the effectiveness of the Rosenbluth and Rosenbluth method in accurately capturing the self-avoiding nature of polymer chains and providing a more realistic portrayal of their physical properties.

2 Introduction

A polymer is typically a large molecule composed of a series of monomers, which join or break apart through polymerization, often assuming complex, coiled formations. Polymers are integral to numerous facets of our daily lives, finding applications in the production of plastics, drug delivery systems, electronic devices like phones, and much more. Comprehending the properties and behaviors of polymers is crucial, not only for advancing technological developments but also for exploring innovative approaches to mitigate the environmental impact of persistent polymers, such as those found in plastic waste.

Given the intrinsic coiling behavior of polymers, it is apt to model them using statistical physics through a random walk approach. This model enables us to estimate several physical characteristics such as size and shape. It also provides a platform to validate through empirical observations that the behavior of polymers aligns with the power law.

To accurately emulate the physical properties of polymers, we'll employ a self-avoiding walk model. This model, similar to a random walk, terminates when it attempts to retrace its steps, reflecting the behavior of real-world polymer chains that cannot overlap due to the physical space

each monomer occupies. This limitation results in the characteristic coiled configuration of polymers. Through this simulation, we aim to delve deeper into and better comprehend the fascinating and complex behavior of polymers, as well as determine the average length of the polymer chain.

Initially, we'll employ a straightforward algorithm with no directional weighting chosen at random. Subsequently, we'll introduce a weighting approach through the Rosenbluth and Rosenbluth algorithm. The Rosenbluth and Rosenbluth method is a type of static Monte Carlo algorithm where states are sampled independently, facilitating the calculation of a weighted average. To implement this, we'll continuously select a neighboring vertex from some V_i, a free neighbor of V_{i-1}. If there are no free neighbors, the walk ends. If there is a choice of neighbors, the weighting is updated, and the walk continues until i equals the total number of steps, n. This process can be repeated for as many walks as required. The weighted mean will be calculated as follows:

$$\langle R^2(N)\rangle = \frac{\sum_i W_i(N) R_i^2(N)}{\sum_i W_i(N)}$$

Where W is a weighting factor derived from the number of available steps (signifyed by $3 - s_n$) at each point in a walk as shown below:

$$s_n = \begin{cases} 0, & W(N) = W(N-1) \\ 1, & W(N) = \frac{2}{3} W(N-1) \\ 2, & W(N) = \frac{1}{3} W(N-1) \\ 3, & W(N) = 0 \end{cases}$$

3 Results

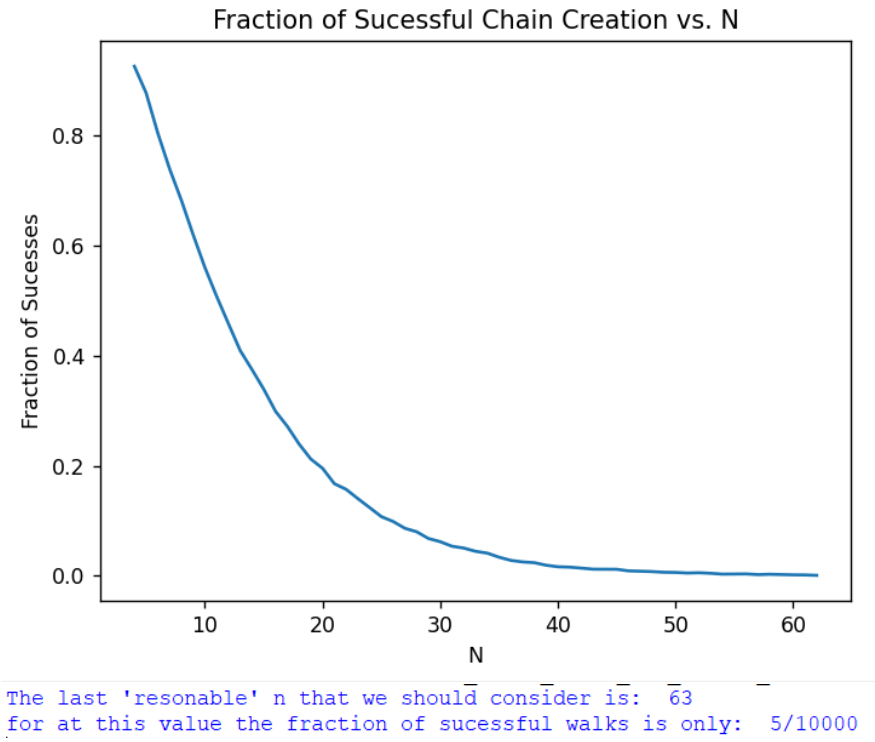


Figure 1: Sucessful chain creation vs number of steps goes to 63

The provided graph illustrates the qualitative relationship between $f(N)$ and N, representing the success rate of completed walks out of 1000 trials for a given step size, N. From this graphical representation, it can be inferred that the maximum ”reasonable” N value to consider for further exploration is approximately N = 63. This inference is based on the observation that the success rate of completed walks at N = 63 is a meager 0.05%. Any increase in N beyond this point would result in a progressively smaller success fraction, rendering further analysis less meaningful or practical.

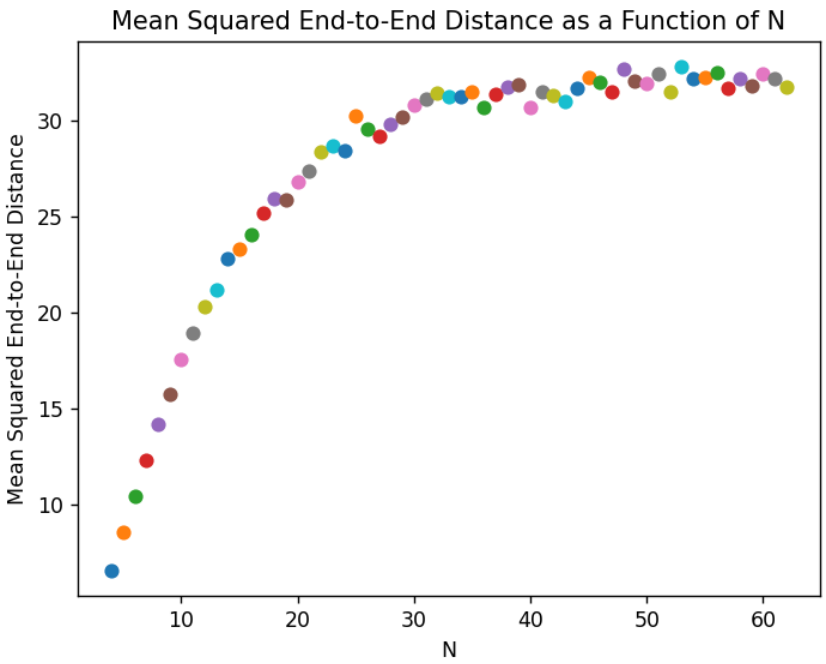
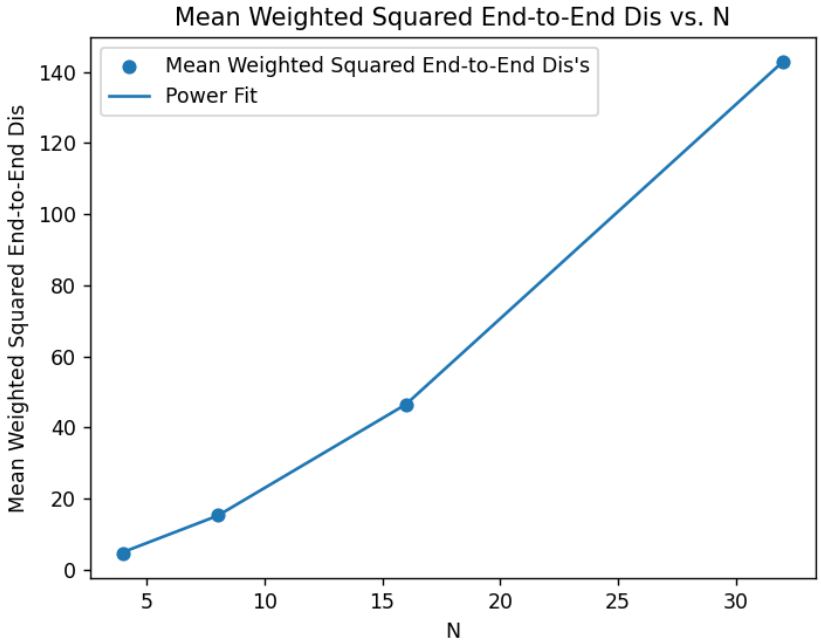


Figure 2: Unweighted Random Walk Mean Squared Distance

The graph above represents the average mean square end-to-end distance calculated over 1000 walks, plotted as a function of N, using the fundamental 2D walk method.

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Estimate for v: 0.7487441899289523
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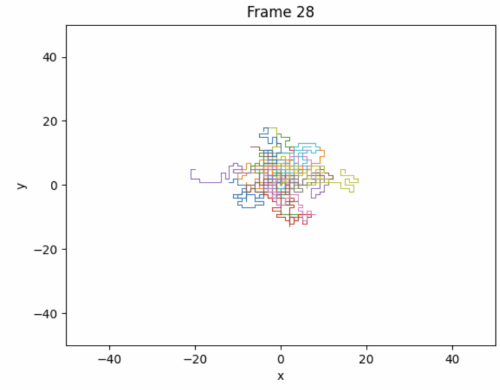
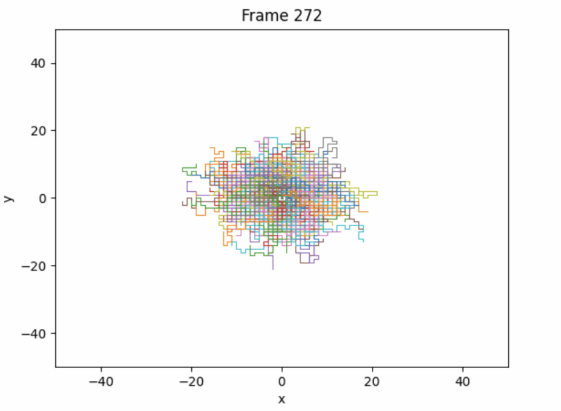
Figure 3: Rosenbluth and Rosenbluth method Weighted Mean Squared End-to-End Distances

This graph above illustrates the average mean square end-to-end distance, calculated over 1000 walks, as a function of N, employing the Rosenbluth and Rosenbluth method for $N = 4, 8, 16,$ and 32. Additionally, it includes a power law curve fit to the data, which is utilized to provide an estimate for the exponent v from the equation: $\langle R^2(N) \rangle = N^{2v}$ Which describes the mean squared end-to-end distance's scaling as N increases.

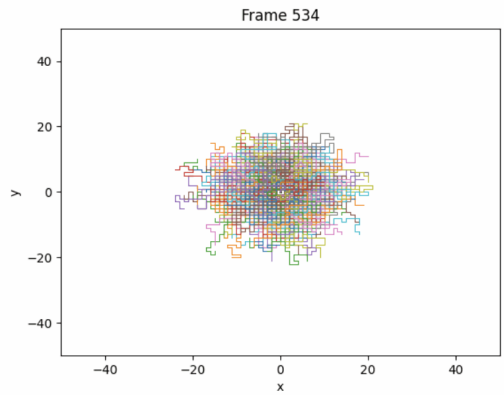
Attached will be an animated gif of one thousand random walks where each walker attempts a total of fifty steps, but below are a couple of images to also display the results.



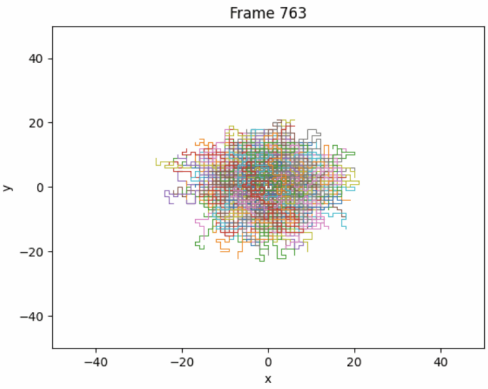
(a) 28 Random Walks



(b) 272 Random Walks



(c) 534 Random Walks



(d) 763 Random Walks

Figure 4: Weighted Random Walk behavior for up to 1000 walks when N = 50.

4 Conclusions

Initially, it was crucial to establish a relationship between the fraction of successful chain creations and N. This facilitated the identification of a fall-off point for the basic random walk. On a broader scale, it offered an understanding of the probabilities that a walker would reach a specific distance, N steps away, before self-intersecting and subsequently terminating the walk. Additionally, the mean squared end-to-end distances, as shown in Figure 2, began to stabilize around 33 as N increased to values beyond 63. These findings underscored the need for a more effective method to model polymers, such as the Rosenbluth and Rosenbluth method.

By implementing the Rosenbluth and Rosenbluth method and plotting the weighted mean end-to-end distances, we obtained an estimate of v through applying power fit, of approximately 0.75. This value is significant as it indicates that the polymer chain's end-to-end distance scales with N to the power of 0.75, which is a departure from the square root dependence observed in simple random walks. The scaling of the weighted mean end-to-end distances also illustrates how much more effective this method is over basic 2D self avoiding random walk at creating long polymer chains. These findings underscore the effectiveness of the Rosenbluth and Rosenbluth method in accurately capturing the self-avoiding nature of polymer chains and, thus, providing a more realistic portrayal of their physical properties.