PROJECT THREE: Self-Avoiding Random Walk

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Abstract

- Modeling polymers with self-avoiding random walks
- Firstly with a simple SAW and finding the success rate of completed walks and the mean squared end-to end distances for step sizes.
- Implementing Rosenbluth and Rosenbluth
- Found Flory exponent, v experimentally

Background

- What are polymers?
- Why do they matter?
- How should they be modeled?

01

Basic 2D Walk

Base Method

In this method we are randomly choosing a direction and simply walking until we hit somewhere we have already been or completed N steps

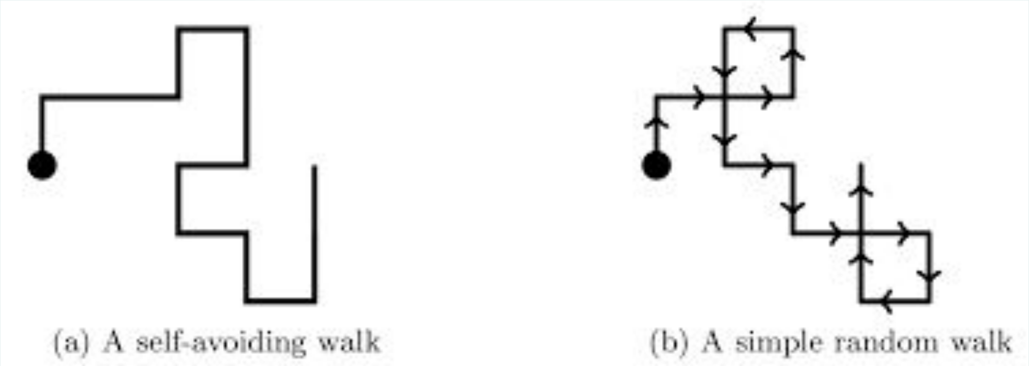
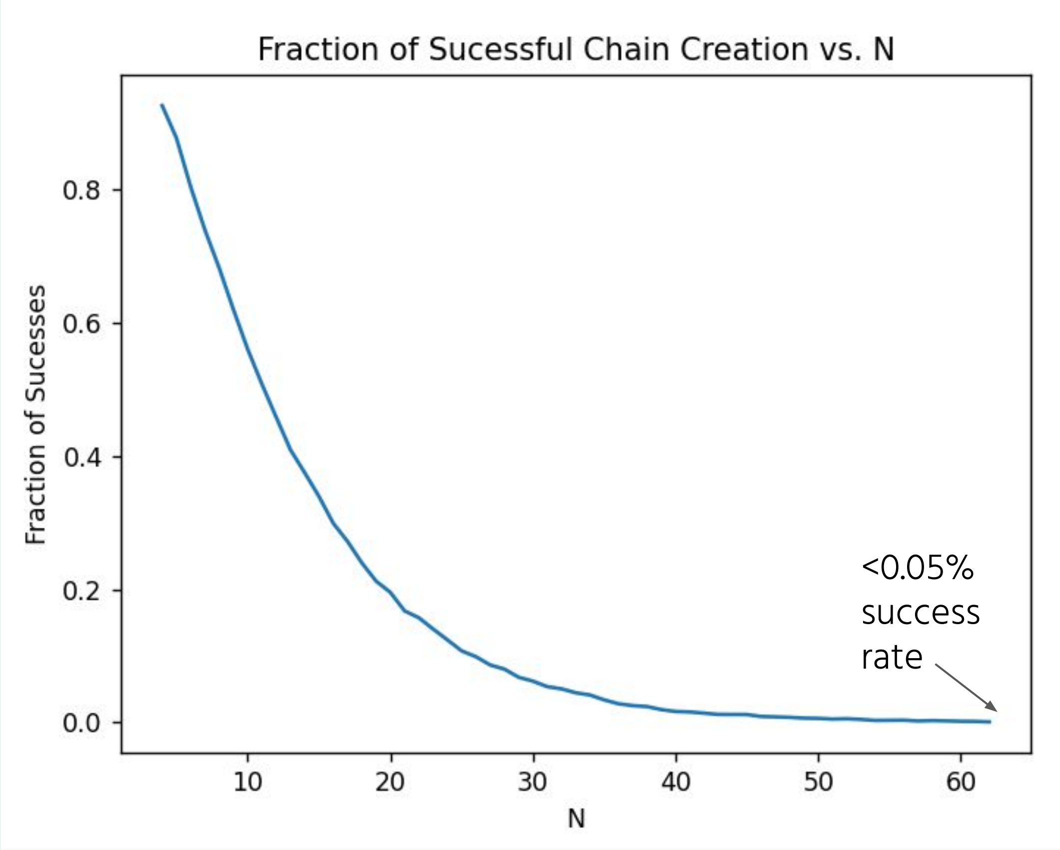


image: https://clisby.net/projects/saw_feature/

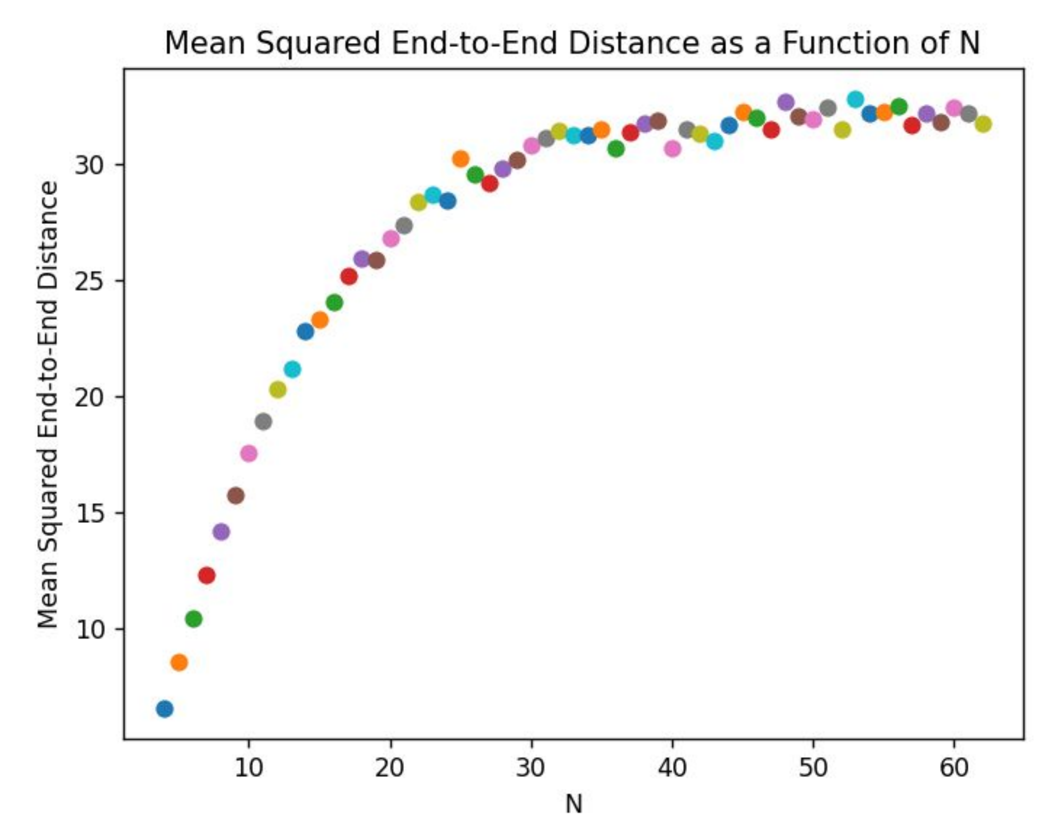
Successful Chain Creation



This graph depicts the fraction of walks that actually made it to step size N vs the N they were trying to achieve.

(it can be concluded from this graph that we can not expect any significant fraction of successful chains for step sizes of 63+)

Mean End-To-End Distances For Basic 2D Walk



This graph depicts the mean squared end-to-end distance (MSED) as a function of step size (N)

(it can be concluded from this graph that the MSED for this basic method can be expected to top out at approx 33)

Rosenbluth and Rosenbluth Method

02

Rosenbluth and Rosenbluth Method

In this method we are randomly choosing our step direction so that it DOES NOT cause termination.

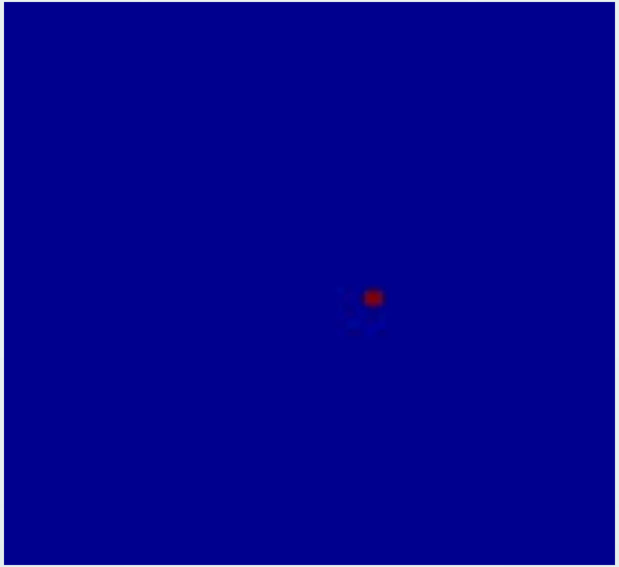
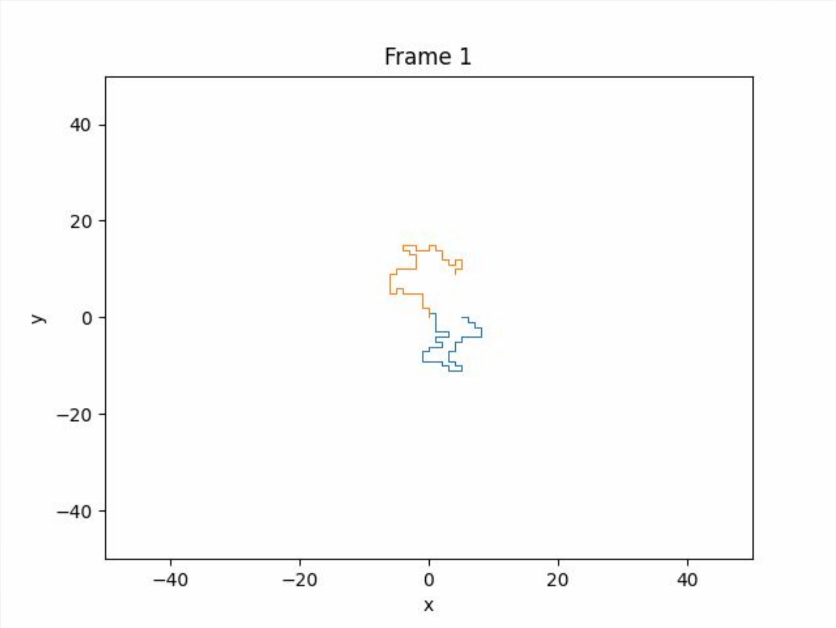


image: https://www.physicsforums.com/insights/fun-self-avoiding-walks/

Rosenbluth and Rosenbluth Method

This is what our walks look like for N = 50



Rosenbluth and Rosenbluth Method

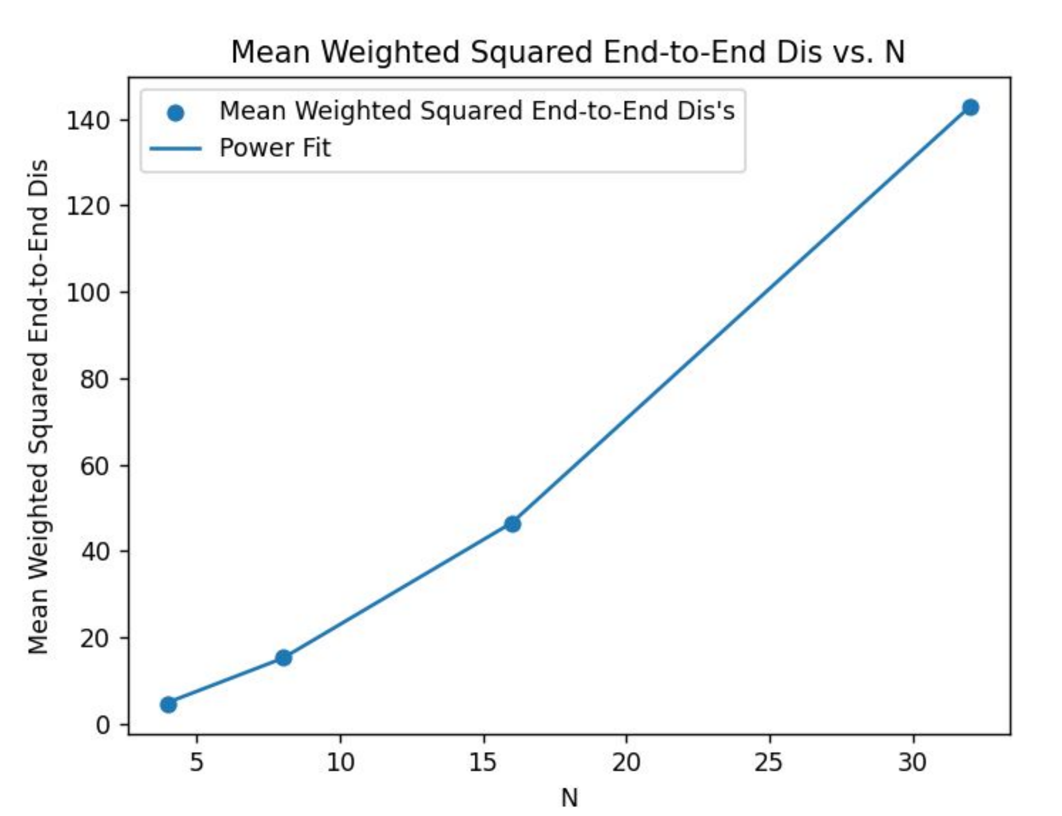
In this method we also continuously keep track of a weighting factor W at each step of the walk based off of S_n (3-the number of available steps)

$$
\begin{array}{lcl}
s_n = 0 & \rightarrow & W(N) = W(N-1) \\
s_n = 1 & \rightarrow & W(N) = \frac{2}{3} W(N-1) \\
s_n = 2 & \rightarrow & W(N) = \frac{1}{3} W(N-1) \\
s_n = 3 & \rightarrow & W(N) = 0
\end{array}
$$

This value can be used to calculate the weighted mean squared end-to-end distances for each walk

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

Mean End-To-End Distances For R



This graph depicts the weighted mean squared end-to-end distances for N = 4, 8, 16 and 32

This graph also shows a power law fit that can be used to estimate the Flory exponent, v from the equation:

$$\langle R^2(N)\rangle \approx N^{2\nu}$$

Conclusions

- Obtained the Flory exponent, v of 0.75 for Rosenbluth
- V for simple self avoiding random walk is 0.5
- Better scaling of the end-to-end distance
- Achieved better modeling of polymer chains