POLYTECHNIC UNIVERSITY
Department of Computer and Information Science

A Model of a Flexible Polymer

K. Ming Leung

Abstract: A flexible polymer is modeled as a chain of rigid links connected by flexible joints.

Directory

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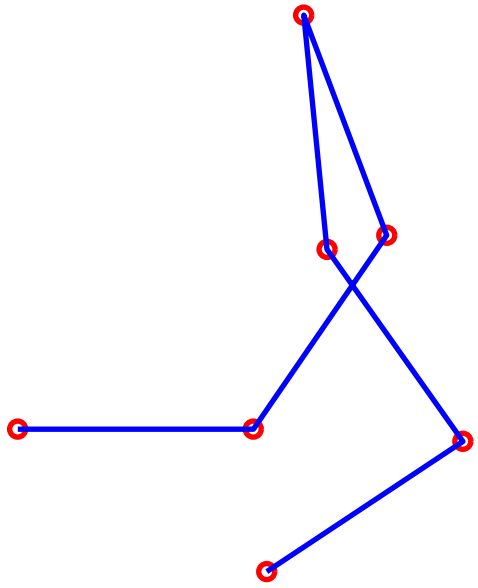


A polymer can be modeled as a sequence of n segments (monomers) of fixed length joined by $n-1$ flexible joints, so that each angle between adjacent segments can take any value from 0 to 360 degrees with equal probability. One can study this model using a random number generator to produce the angles. We can measure all lengths in units of the length of each segment. Therefore by definition each segment has unit length.

Let one end of the polymer to be at the origin. We can always

rotate the polymer (or equivalently rotate the coordinate system) so that the first segment (monomer 0) lies on the positive x-axis, and its end is located at position $(0, 1)$. The next segment (monomer 1) is oriented at an angle θ_1 measured with respect to the x-axis. This angle is randomly and uniformly distributed in the interval $[0, 2\pi]$. The end point of monomer 1 is then located at $(0, 1) + (\cos(\theta), \sin(\theta))$. We can continue this way until we build up an entire polymer consisting of a total of n monomers. Therefore the other end of the polymer is located at

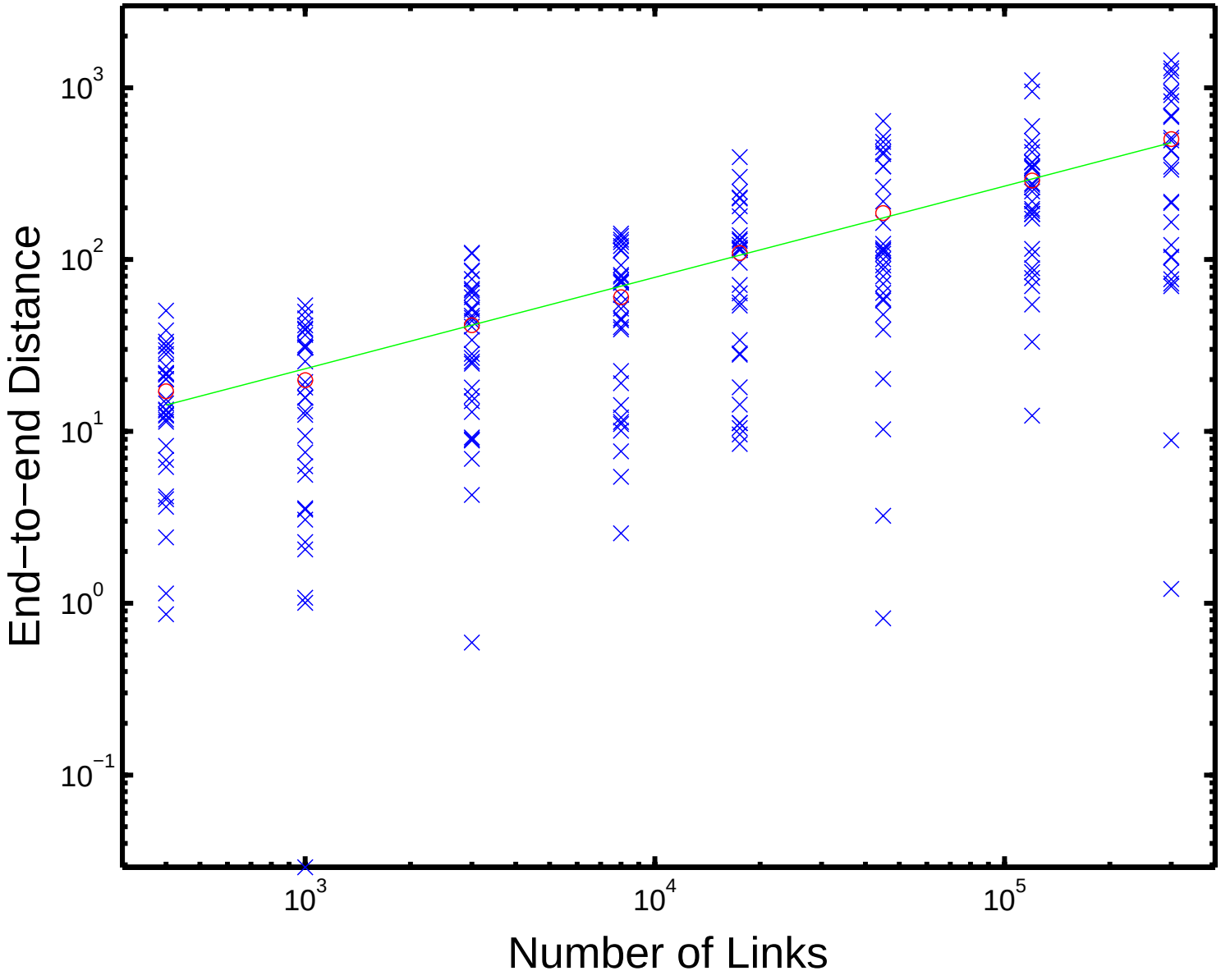
$$(1, 0) + \sum_{k=1}^{n-1} (\cos(\theta_k), \sin(\theta_k)).$$

The end-to-end length of the polymer, r, is then given by

$$r = \left| (1, 0) + \sum_{k=1}^{n-1} (\cos(\theta_k), \sin(\theta_k)) \right|.$$

The average value of this quantity for a given polymer determines many of its physical and chemical properties.

We carry out the above simulation for various values of n ranging


End−to−end Distance
Number of Links
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{3}
10^{4}
10^{5}

from 400 to 300,000. For a fixed n, the results obtained for r vary drastically from run to run (as shown by the blue crosses in the figure), assuming of course one uses a different sequence of random numbers each time.

To make better sense of the data, the simulation is repeated 30 times for each given n, and the average end-to-end length, $\bar{r}$ is computed. The result as shown by the red circles clearly follows a more distinctive trend.

On theoretical grounds, it is clear that the polymer here executes a random-walk with a step size of 1 starting at the origin. Thus from statistics one expects that $\bar{r}$ is proportional to $\sqrt{n}$, and so we can write

$$\bar{r} = \alpha n^p,$$

where α and p are unknown parameters. Of course we expect that p should be $1/2$. These parameters can be extracted from the simulation data.

To see how to do that, we take the logarithm of the above relation

to give

$$\log \bar{r} = \log \alpha + p \log n.$$

This is a linear equation with $\log n$ as the independent variable, and with $\log \bar{r}$ as the dependent variable. Thus the parameters $\log \alpha$ and p can be determined by treating the above equation as a linear least-squares problem. We find that p is indeed about 0.5, plus or minus a few percent error.

In a given polymer, there is generally a sizable variation in the number of monomer units. Monte Carlo is a powerful method for studying various properties of polymers. More meaningful modeling must take into account of many other physical and chemical factors. For example, a polymer executes more like a self-avoiding random walk than a pure random walk, since there are repulsive forces between a link and its nearest neighbors. The angle between adjacent links is far from uniformly random since there are usually some preferred orientations. Moreover we also need to work with a three-dimensional model.