MONTE CARLO STUDIES OF LINEAR SELF-AVOIDING WALK POLYMERS IN VARIOUS DIMENSIONS

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Abstract

Self-avoiding walks are a more realistic model than random walks. This paper explores the properties of such walks in different dimensions by employing Monte Carlo computer simulations. The ability to construct such models and to develop a computer simulation are important skills for engineering and science students to acquire.

Introduction

In a previous publication in this journal, Zajac and Bishop [1] used a Monte Carlo (MC) growth method to simulate three dimensional self-avoiding linear N "bead" polymers. They computed a variety of properties such as the mean-square radius of gyration, $\langle S^2 \rangle$, its components along the principal orthogonal axes [2], λ_1, λ_2, and λ_3, the mean-square end-to-end distance, $\langle R^2 \rangle$, and the mean asphericity, $\langle A \rangle$. They found excellent agreement with theoretical values. In this work, their MC growth method for a three dimensional simple cubic lattice is extended to examine self-avoiding walk linear polymers on a square lattice in two dimensions and a hypercubic lattice in four and five dimensions. A wide variety of properties are computed and compared to theoretical predictions in order to examine the influence of spatial dimension on the system properties.

Method

The self-avoiding walk growth algorithm utilizes portions of the ideal linear polymer growth algorithm described in Barillas, Borgeson and Bishop [3], with major modifications to account for the self-avoidance condition. The first polymer bead is placed at the origin of a lattice. The second bead is randomly placed in any of the four possible lattice site locations in the two dimensional simulation and any of the eight possible locations in the four dimensional study or the ten possible locations in five dimensions.

Then a new random number is used to select the possible location where the third bead could be placed. However, before allowing that bead to be put at the new location, a test is made to ensure that another bead is not already occupying that lattice site. This procedure grows a non-intersecting chain and is continued until N beads have been successfully placed. Each bead is placed one unit apart from the previously placed bead. If at any time in the process the chain intersects itself, it is erased and a new chain is started. After each polymer is completely constructed, a number of properties are calculated for that configuration, as was done in Barillas, Borgeson and Bishop [3]. The process is continued until M independent samples have been created.

Figure 1 presents a typical configuration of a 25-bead self-avoiding walk, two dimensional chain. The underlying square lattice structure is readily apparent.

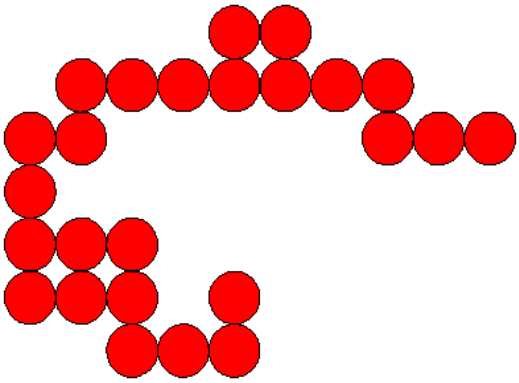

Figure 1: A configuration of a 25 bead self-avoiding walk, two dimensional chain.

Results

It becomes increasingly difficult to grow chains using this direct static sampling MC method [4]. Indeed, the probability of obtaining a chain with N beads decreases exponentially:

$$\text{Prob} = C\, e^{-\lambda N} . \qquad (1)$$

Here, C is a normalization coefficient and λ is the attrition constant. Table I presents the results of fitting Eq. 1 in the different current simulations, as well as, previous findings for three dimensions. The agreement between the MC λ values and the theoretical predictions is very good. The two dimensional value of the attrition constant is larger than the three dimensional value which in turn is larger than the four dimensional value which again is larger than the five dimensional value because growth in lower dimensions is quite hindered compared to higher dimensions; e.g. there is a larger chance of overlapping in lower dimensions.

Table I: The attrition constant, λ, in different dimensions.

Dimension	λ	Theory
2	0.400	0.416[b]
3	0.242[a]	0.248[b]
4	0.164	0.167[b]
5	0.123	0.123[b]

(a) reference[1] (b) reference [4]

All the data for the MC runs are contained in Tables II A, B and C. The components of $\langle S^2 \rangle$, along the principal orthogonal axes [2], are the eigenvalues of a real, symmetric square matrix and were obtained by the Jacobi method [5]. Since the polymer generation process provides M independent samples, the mean and standard deviation of the mean of general properties can be computed from the usual simple equations [6], but more care is needed in computing the errors of ratios [1]. In these tables the number in parenthesis denotes one standard deviation in the last displayed digit; for example $\langle \lambda_1 \rangle$ = 8.21(1) means that $\langle \lambda_1 \rangle = 8.21 \pm 0.01$.

The $\langle R^2 \rangle$ and $\langle S^2 \rangle$ data in these tables were fit by a weighted nonlinear least-squares program [6] to determine the exponent, 2ν, in their scaling laws [7]:

$$\langle R^2 \rangle = C_1 (N-1)^{2\nu} , \qquad (2a)$$

and

$$\langle S^2 \rangle = C_2 (N-1)^{2\nu} . \qquad (2b)$$

The coefficients, C_1 and C_2, are model dependent amplitudes but the exponent, 2ν, is universal. Table III contains the fit results, as well as, the known theoretical values. As the dimension increases the self-avoiding walk polymers behave more and more like a random walk ideal chain, which has an exponent value of 1.00. The self-avoidance condition causes the chains to be expanded and therefore the exponent will be larger at lower dimensions. The small chains examined here are not expected to yield the same values for properties

which have been predicted for very long chains.

Table IIA: Two Dimensional Properties as a function of N.

Property	20	25	30
M	121,875	16,587	2,222
$\langle\lambda_1\rangle$	8.21(1)	11.47(4)	15.17(14)
$\langle S^2\rangle$	9.51(1)	13.29(4)	17.53(13)
$\langle R^2\rangle$	66.74(12)	93.86(47)	123.78(169)
$\langle A\rangle$	0.502(1)	0.498(2)	0.508(5)
$\langle\lambda_1\rangle/\langle S^2\rangle$	0.864(1)	0.863(1)	0.866(2)
$\langle S^2\rangle/\langle R^2\rangle$	0.142(1)	0.142(15)	0.142(19)

Table IIB: Four Dimensional Properties as a function of N.

Property	20	25	30	35
M	598,520	263,714	115,879	50,766
$\langle\lambda_1\rangle$	3.49(1)	4.49(1)	5.49(1)	6.53(1)
$\langle S^2\rangle$	4.72(1)	6.07(1)	7.43(1)	8.83(1)
$\langle R^2\rangle$	28.42(2)	36.69(4)	45.02(8)	53.54(15)
$\langle A\rangle$	0.422(1)	0.421(1)	0.419(1)	0.419(1)
$\langle\lambda_1\rangle/\langle S^2\rangle$	0.740(1)	0.740(1)	0.739(1)	0.739(1)
$\langle S^2\rangle/\langle R^2\rangle$	0.166(1)	0.165(1)	0.165(1)	0.165(1)

Table IIC: Five Dimensional Properties as a function of N.

Property	20	25	30	35
M	1,178,090	637,943	345,029	186,678
$\langle\lambda_1\rangle$	3.04(1)	3.86(1)	4.68(1)	5.51(1)
$\langle S^2\rangle$	4.27(1)	5.42(1)	6.58(1)	7.76(1)
$\langle R^2\rangle$	25.21(1)	32.19(2)	39.20(4)	46.31(6)
$\langle A\rangle$	0.412(1)	0.410(1)	0.409(1)	0.408(1)
$\langle\lambda_1\rangle/\langle S^2\rangle$	0.713(1)	0.712(1)	0.711(1)	0.711(1)
$\langle S^2\rangle/\langle R^2\rangle$	0.169(1)	0.168(1)	0.168(1)	0.167(1)

Table III: Exponents in different dimensions.

Dimension	2ν $\langle R^2\rangle$	2ν $\langle S^2\rangle$	Theory
2	1.46(2)	1.44(1)	1.500[b]
3	1.19(1)[a]	1.18(1)[a]	1.176[b]
4	1.09(1)	1.08(1)	
5	1.04(1)	1.03(1)	

(a) reference[1] (b) reference [7]

The computer results displayed in Tables IIA, B and C are for finite N whereas the theoretical values are for infinite N. The data have been extrapolated in 1/N to 0 (e.g. N $\rightarrow\infty$) via the method reported in Barillas, Borgeson and Bishop [3]. The final extrapolated values are presented in Table IV along with known results. Nearly all of the simulation results reported in Table IV are within two standard deviations of the mean, or in the 95% confidence interval, compared to literature values. However, some of the earlier studies used only one value of N and thus, did not extrapolate to determine the long chain limit.

One can clearly see that the polymers are becoming less stretched out and are behaving more and more like random walk chains as the dimension is increased; e.g. $\langle S^2\rangle/\langle R^2\rangle$ is approaching the known value for random walks in all dimensions, 0.167 [7].

Table IV Comparison of Simulation and Literature Results.

Dimension	$\langle A\rangle$ MC	$\langle A\rangle$	$\langle\lambda_1\rangle/\langle S^2\rangle$ MC	$\langle\lambda_1\rangle/\langle S^2\rangle$	$\langle S^2\rangle/\langle R^2\rangle$ MC	$\langle S^2\rangle/\langle R^2\rangle$
2	0.495(9)	0.503(4)[b]	0.865(5)	0.870(15)[e]	0.142(75)	0.1403[g]
3	0.425(9)[a]	0.429(2) [c]	0.775(6)[a]	0.785[f]	0.156(5)[a]	0.1603(h)
4	0.414(2)	0.434(12)[d]	0.737(2)	0.749(38)[e]	0.163(3)	
5	0.403(2)	0.437(8) [d]	0.708(2)	0.726(21)[e]	0.165(2)	

(a) reference [1] (b) reference [8] (c) reference [9] (d) reference [10] (e) reference [11] (f) reference [12]] (g) reference [13] (h) reference [14]

Conclusion

We have investigated two, four and five dimensional self-avoiding linear polymers on square and hypercubic lattices, respectively, using a Monte Carlo growth method. Many different properties have been calculated. There is fine agreement with theoretical results and other simulations. The self-avoiding conditions are mitigated as the dimension is increased. Modeling projects such as the one described here provide a clear demonstration of some aspects of polymers and thus strongly enhance student understanding and intuition.

Appendix: The Manhattan College Undergraduate Research Program

Manhattan College has a long tradition of involving undergraduates in research and was one of the original members of the Oberlin 50. This is a group of undergraduate institutions whose students have produced many PhDs in engineering and science. At Manhattan College, students can elect to take an independent study course for three credits during the academic year. In addition, the College provides grant support to the students for ten weeks of work during the summer. I have personally recruited the students from my junior level course in Systems Programming. Previously published articles in this journal by Manhattan College student co-authors are a very effective recruitment tool. The students have also presented their results at a variety of undergraduate research conferences including the Hudson River Undergraduate Mathematics Conference and the Spuyten Duyvil Undergraduate Mathematics Conference.

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