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Limiting ring closure probability on the square lattice

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Abstract. A Monte Carlo technique is described for estimating the number of tadpoles of a given size, which are weakly embeddable in a given lattice. Data are reported for the square lattice for tadpoles with up to twenty edges in the head and up to fifty edges in the tail. These data are combined with good self-avoiding walk extrapolants to yield estimates of the limiting probability (p_k) of forming a head with k edges, and it is suggested that

$$p_k \sim k^{-\alpha}$$

where $\alpha \simeq 2{\cdot}13$.

1. Introduction

A tadpole is a connected graph which is homeomorphic to the graph shown in figure 1. The graph has all vertices of degree two except one vertex of degree three and one vertex of degree one. The 'head size' of the tadpole is the number of edges in the circuit and the 'tail size' is the number of edges in the simple chain from the vertex of degree one to the vertex of degree three. We shall be concerned with the number ($T_{h,t}$) of tadpoles with head size h and tail size t which are weakly embeddable in a lattice. It appears that the method which we shall describe can be applied, with only minor modifications, to any lattice but we shall be concerned with its application to the square lattice and we shall only report results obtained for this lattice.

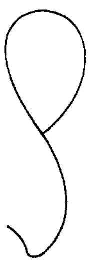

Figure 1. A tadpole is a connected graph with one vertex of degree one, one vertex of degree three and all other vertices of degree two.

The numbers of tadpoles weakly embeddable in a lattice are important in the high temperature susceptibility expansion of the Ising model (Stanley 1971). The number (and generating function) of self-avoiding walks on a lattice can be expressed as a recurrence relation involving the number (and generating function) of tadpoles on the lattice (Sykes 1961, Ree Chay 1971) and this number is therefore important in models of the excluded volume effect in polymers. In connection with these problems the numbers of tadpoles with a fairly small total number of edges have been enumerated exactly (on the square lattice for $h+t \leqslant 24$). Wall *et al* (1955) obtained Monte Carlo estimates of numbers of tadpoles in connection with their work on self-avoiding walks but since their estimation procedures were primarily directed to self-avoiding walks, tadpoles appeared only as a by-product of this work.

Two lattice parameters which are of particular interest in connection with excluded volume problems are the initial and limiting ring closure probabilities on the lattice. Let c_k be the number of k step self-avoiding walks and u_k be the number of otherwise self-avoiding k step walks which return to the origin at the kth step. The initial ring closure probability p_k^0 is defined as

$$p_k^0 = u_k/(q-1)c_{k-1} \tag{1}$$

where q is the coordination number of the lattice. The limiting ring closure probability p_k is defined as

$$p_k = \lim_{t\to\infty} 2T_{k,t}/(q-1)c_{k+t-1} \tag{2}$$

where the factor of two appears since the head of a tadpole can be walked in two directions (notice that a tadpole as defined here is an undirected graph).

Wall *et al* (1955) suggested that

$$p_k^0 \sim k^{-\alpha^0} \tag{3}$$

and that

$$p_k \sim k^{-\alpha} \tag{4}$$

and, from Monte Carlo calculations and heuristic arguments, proposed that $\alpha = \alpha^0 = 2$ in two and three dimensions. Since then, Edwards (1965) (using selfconsistent field arguments) suggested that $\alpha^0 = 9/5$ in three dimensions and Martin *et al* (1967) (from exact enumeration studies) suggested that $\alpha^0 = 23/12$ in three dimensions and 11/6 in two dimensions. To the authors' knowledge, the only estimate of α which has appeared in the literature is that of Wall *et al.* Unfortunately, exact enumeration does not seem to be well suited to estimating α since both large heads and long tails appear to be necessary.

2. Sampling scheme

The general idea of the sampling scheme is to generate a random sample of self-avoiding polygons (heads) of h edges and to estimate how many tails of length t can be grown from each head. If the number of self-avoiding polygons is known, either from enumeration or Monte Carlo work, this is sufficient to estimate the number of tadpoles $T_{h,t}$.

The first problem is to generate a random sample of polygons. We have used a variant of the method described by Whittington and Valleau (1969) in which sampling is carried out over a realization of a Markov chain (with uniform unique limit distribution) defined on the set of polygons. A polygon is represented by a sequence of vectors and a new polygon can be generated by a permutation of a pair of vectors such that the new graph has all vertices distinct (ie is a (self-avoiding) polygon). The transitions we have used are: (*a*) permutation of an adjacent pair of vectors and (*b*) permutation of a pair of vectors separated by a third vector. If a polygon j can be reached from a polygon i by such a transition we say that j is adjacent to i, and write $j \in S(i)$ where $S(i)$ is the adjacency set of polygon i, and has n_i members. Define

$$\begin{aligned} q_{ij} &= 1 \qquad \text{if } j \in S(i) \\ &= 0 \qquad \text{otherwise} \end{aligned} \tag{5}$$

and

$$p_{ij} = q_{ij}/n_i \qquad j \neq i. \tag{6}$$

If we define

$$p_{ii} = 1 - \sum_{j \neq i} p_{ij} \tag{7}$$

then $||p_{ij}||$ is the transition probability matrix of a Markov chain defined on the polygons. Clearly the Markov chain is reducible since two polygons are consequents only if their vector sets are permutations of one another. This reducibility provides a convenient stratification and we sample on each class independently though this requires knowledge of the number of polygons in each class. For each class the limit distribution is not uniform but we wish to construct a sampling Markov chain whose limit distribution is uniform. We have chosen to use the above Markov chain but to accept each state j in a realization of the process as a member of the sample, with probability $1/n_j$. If, after state j is reached, a random number, uniformly distributed in (0, 1), is less than $(1/n_j)$, state j is accepted as a member of the sample. Otherwise state j is rejected and the next state in the realization of the process is considered. Since $\{n_i\}$ is the limit distribution of $\|p_{ij}\|$ this ensures that the states are sampled with equal probability and the procedure has the advantage that the correlation between successive states in the sample is smaller than would be the case if each state was accepted and suitably weighted. A difficulty with the method is that, with the transitions used here, some states are not consequents of the simple rectangular polygons and are never included in the sample. This problem should not be serious since the numbers of polygons concerned are small and the probability of successfully growing a tail from these heads should not differ drastically from the average probability for polygons in that class.

3. Results and discussion

We have estimated the numbers of tadpoles, weakly embeddable in the square lattice, with head sizes ranging from four to twenty and with tail sizes up to thirty or, in some cases, up to fifty. These numbers have been tabulated by Trueman (1972) and are not reproduced here. We are primarily interested in the probability that a walk, self-avoiding at $(n-1)$ steps, will form a tadpole with head size h at the nth step, that is, in the ratio

$$p_{h,n-h} = 2T_{h,n-h}/3c_{n-1}.$$

To obtain these ratios we require the numbers of self-avoiding walks c_n. Exact values of c_n are available (Sykes *et al* 1972) up to $n = 24$ and we have estimated c_n for $n > 24$ by the extrapolation formula where $\gamma = 1/3$,

$$c_n = (\beta_1 + \beta_2/n)n^{\gamma}\mu^n$$

$\mu = 2{\cdot}639$ and β_1 and β_2 are obtained by least squares fitting to the exact data. Because of the alternation on the square lattice, it is convenient to use different extrapolators depending upon whether n is even or odd. For n even, we found $\beta_1 = 1{\cdot}215$ and $\beta_2 = 0{\cdot}351$ and for n odd, $\beta_1 = 1{\cdot}212$ and $\beta_2 = 0{\cdot}427$. We would expect β_1 to be the same in each case and indeed they are very similar. To check these extrapolators we have obtained Monte Carlo estimates of c_n for $n > 24$ and the agreement between the Monte Carlo values and the extrapolated values is excellent. Using these extrapolated values of c_n together with Monte Carlo estimates of $T_{h,t}$ we have estimated $p_{h,t}$. Some of the results are shown in figure 2. It is clear that, for each value of h, $p_{h,t}$ tends to a limiting ring closure probability

$$p_h = \lim_{t\to\infty} p_{h,t}$$

for each h. The uncertainties in p_h are very small compared to the differences between p_h for different values of h. A log–log plot of the dependence of p_h on h is shown in

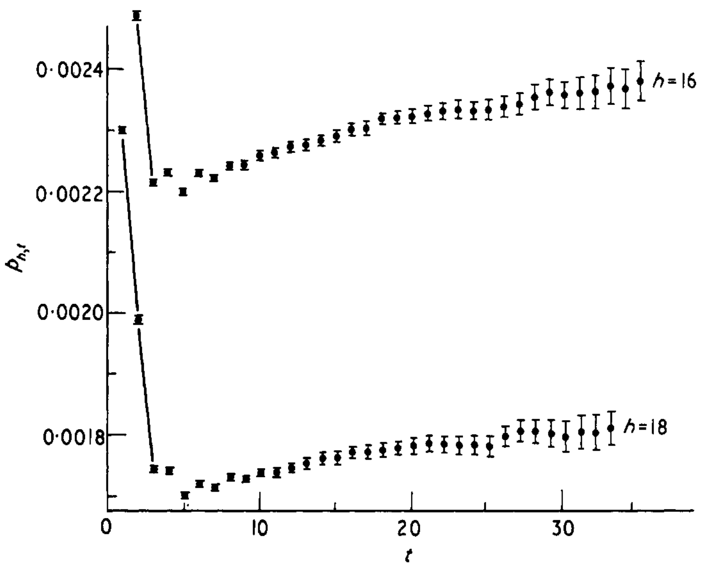

Figure 2. Dependence of $p_{h,t}$ on t for $h = 16$ and $h = 18$.

figure 3. Except for the $h = 4$ point, the log–log dependence is linear and the gradient is $-2{\cdot}13 \pm 0{\cdot}01$. This result is interesting in view of Wall's suggestion that

$$p_h \sim h^{-\alpha}$$

with $\alpha = 2$. Our results support his suggested functional form but with $\alpha = 2{\cdot}13$. Since the probability of initial ring closure is now thought to behave as

$$p_h^0 \sim h^{-11/6}$$

in two dimensions, it appears that the initial ring closure probability decreases less rapidly with increasing h than does the limiting ring closure probability. For the initial ring closure probability the exponent depends on dimensionality but seems to be lattice independent. We are currently investigating the lattice and dimensionality dependence of the exponent for the limiting ring closure probability.

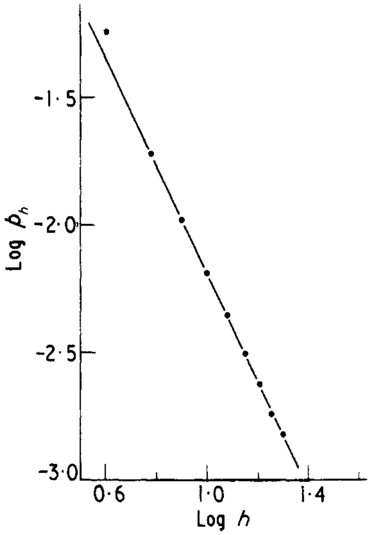

Figure 3. Dependence of limiting ring closure probability (p_h) on head size (h).

Acknowledgments

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