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Figure eights on the square lattice: enumeration and Monte Carlo estimation

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Abstract. This paper concerns the numbers of figure eights weakly embeddable in a lattice, important in the theories of self-avoiding walks and the Ising problem. Two Monte Carlo techniques for estimating such numbers are outlined and have been applied to the case of the square lattice. Enumerations have also been carried out for this lattice, and extrapolation formulae have been sought on the basis of these results. It appears that, as one goes to large graphs having a given number of edges, the numbers of figure eights will become comparable to those of self-avoiding polygons, and may be larger. Some rigorous, but rather weak, bounds are established for the numbers of such figure eights.

1. Introduction

In this paper we investigate the number of figure eights†† of given size which are weakly embeddable in the two dimensional square lattice. A figure eight is a connected graph homeomorphic to the graph shown in figure 1, having one articulation point

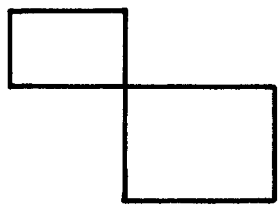

Figure 1. The two self-avoiding circuits of a figure eight meet each other only at a single vertex.

and a cyclomatic index of 2. We represent by $(m, n)_8$ the number of figure eights with m edges in one circuit and n in the other. Since each vertex is of even degree, the number of figure eights is of importance in the calculation of the partition function of the Ising model (Domb 1960, Green and Hurst 1965). In addition, the number of self-avoiding walks on a lattice is related to the numbers of certain simpler classes of graphs, including figure eights, by Sykes' 'counting theorem' (Sykes 1961). Although figure eights have been enumerated in connection with these problems, very few data have been published (Domb 1960) and no attempt appears to have been made to establish how the number of figure eights depends on the number of edges in the graph.

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†† For a discussion of the relevant graph theory terminology see Sykes *et al.* (1966).

We have developed two Monte Carlo techniques for estimating the numbers of figure eights, and we report some results obtained in this way, together with some exact enumeration data. We derive some rigorous bounds on $(m, n)_8$, and attempt to find formulae describing our results. In particular, we discuss the relationship of the total number of figure eights of m edges to the number of polygons of m edges.

2. Monte Carlo calculations

The Monte Carlo method which we have used for most of this work depends on the fact that a figure eight can be considered as two self-avoiding polygons joined at a vertex in such a way that no other intersection between the two polygons occurs. We generate a random sample of polygons of n edges and, for each polygon in the sample, we count the number of ways in which each polygon of m edges can be added to each vertex to generate a figure eight. If the number of n-gons is known, this allows us to estimate the number of figure eights $(m, n)_8$. The method is evidently most convenient when m is much less than n; we have used it only for $n \leqslant 20$ and $m = 4$ and 6. One could go to larger values of m, however, by considering samples from the population of m-gons, rather than counting all the possible ways of adding an m-gon.

The random sample of polygons was generated by a Monte Carlo technique described previously (Whittington and Valleau 1969). The idea is to sample along a realization of a suitable Markov chain defined on a set of polygons which are consequents of one another. Since each polygon is to have the same weight, this sampling Markov chain must have a uniform limit distribution and therefore a doubly stochastic transition probability matrix; in practice, the Markov chain was chosen to be symmetric. It is important to notice that for the transition probabilities used (Whittington and Valleau 1969), the Markov chain defined on the whole population of polygons is reducible; it is thus necessary to know the number of polygons in each closed subset. In the case $n = 20$, Monte Carlo estimates (Whittington and Valleau 1969) of the proportions in the subsets were combined with Sykes' enumeration (Sykes 1969, private communication) of the total number $(20)_p$ of such polygons. For $n = 18$, we enumerated the polygons in each subset†; these numbers combine to give a total number of 18-step polygons agreeing with the result of Rushbrooke and Eve (1959) and of Hiley and Sykes (1961).

An alternative Monte Carlo approach, which we tried out in a few cases, involved applying to figure eights a capture–recapture estimation scheme, similar to that described previously for polygons (Whittington and Valleau 1969). A random sample of figure eights is generated, again by sampling along a realization of a suitable Markov chain with a uniform unique distribution, and the number of times that a figure eight recurs in the realization is noted. The data can then by analysed (using for example the method of DeLury (1958)) to estimate the total number of figure eights. This method is more convenient than the other when $m \simeq n$, and also has the advantage that the total number of polygons of n edges need not be known. It has the disadvantage that, at least with the transition probabilities which we have used (Whittington and Valleau 1969), the number of closed subsets which must be sampled increases rapidly with the size of the figure eight.

† The separate subsets are characterized by the number of vertical steps in the polygon. Their numbers would be important in the study of lattices which were rectangular rather than square, so we report them here ($n = 18$).

Vertical steps	2	4	6	8
Number of polygons	1	85	1476	6072

3. Results

The exact enumerations were done by hand, all enumerations being carried out at least twice by independent enumeration schemes; the results are given in table 1. The results accompanied by an error bound were obtained by the first Monte Carlo method described above; the error given is one standard deviation. Estimates of $(4, 16)_8$ and $(6, 16)_8$ were obtained in both ways and (table 1) agree to better than $\frac{1}{2}\%$. Several results were checked by the capture–recapture method and in all cases agreed within the standard deviation; we have not reported these results here.

Table 1. Numbers, $(m, n)_8$, of figure eights having m edges in one loop and n edges in the other and which are weakly embeddable in the square lattice. Standard deviations are given for the Monte Carle estimates; the rest have been enumerated

$n \backslash m$	4	6	8	10
4	2			
6	8	8		
8	32	64	124	
10	144	288	1096	2388
12	708	1408	5304	22888
14	3696	7248	27096	—
16	20296	39056	—	—
	20287 (2%)	39172 (2%)		
18	$1{\cdot}158 \times 10^5$ (1%)	$2{\cdot}188 \times 10^5$ (1%)	—	—
20	$6{\cdot}69 \times 10^5$ (1%)	$1{\cdot}241 \times 10^6$ (1%)	—	—

4. Discussion

A figure eight can be considered as two polygons joined at a vertex and satisfying certain non-intersection criteria. As an upper bound on the number of figure eights, we consider the number of graphs formed by joining two polygons at a vertex in the absence of these constraints. Each m-gon can then be joined to each n-gon at each vertex of each polygon, i.e. in mn ways. If we write $(m)_\mathrm{p}$ for the number of m-gons, then evidently

$$(m, n)_8 \leqslant mn(m)_\mathrm{p}(n)_\mathrm{p}.$$

In the appendix we prove a slightly stronger upper bound, and also give a lower bound, obtaining:

$$2(m)_\mathrm{p}(n)_\mathrm{p} \leqslant (m, n)_8 \leqslant \tfrac{1}{4}mn(m)_\mathrm{p}(n)_\mathrm{p}.$$

These bounds are too weak to be of much practical importance, except in checking the asymptotic validity of extrapolation formulae.

The forms of these bounds suggest that one might look at extrapolation formulae of the type

$$(m, n)_8 \propto (mn)^{\xi}(m)_\mathrm{p}(n)_\mathrm{p}$$

or

$$(m, n)_8 \propto (mn)^{\xi'}\mu^{m+n}$$

where the second form comes from the first using the good polygon extrapolation formula (Fisher and Sykes 1959, Rushbrooke and Eve 1959, Hiley and Sykes 1961)

$$(m)_\mathrm{p} \propto m^{\beta-1}\mu^m.$$

A comparison with the second form has been made in figure 2, using the accepted value of μ, $2{\cdot}6390$ (Hiley and Sykes 1961); the values of $(m, n)_8$ for the cases $m = n$

have been multiplied by 2 when drawing figure 2, in order to compensate for the additional symmetry present. Except for the graphs $(4, n)_8$, one finds a rough agreement with this form; the slope of the line drawn through the points is roughly 2·0,

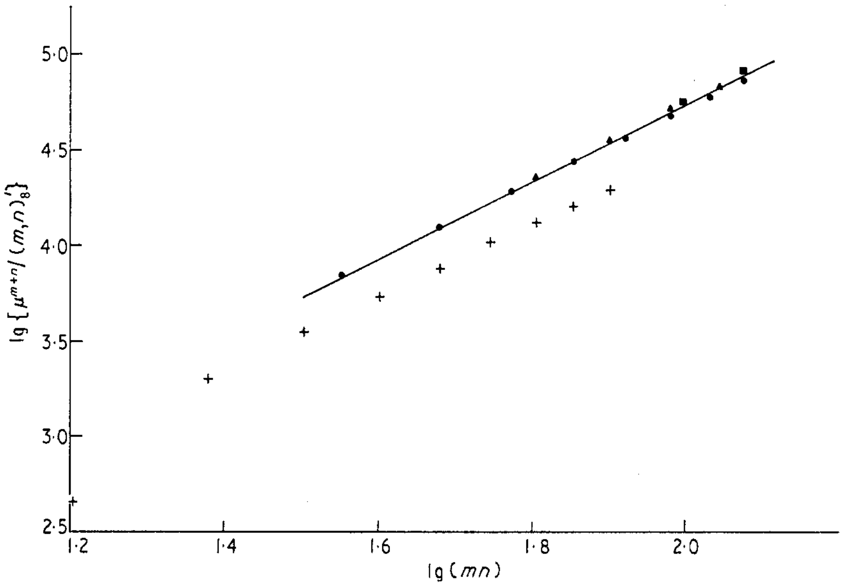

Figure 2. Graph of lg $\{\mu^{m+n}/(m, n)_8\}$ against lg (mn) (except that the values of $(m, n)_8$ have been doubled for the cases $m = n$ to allow for the extra symmetry): + $m = 4, n = 4, 6, \ldots 20$; ● $m = 6, n = 6, 8, \ldots 20$; ▲ $m = 8, n = 8, 10, 12, 14$; ■ $m = 10, n = 10, 12$.

which would correspond to

$$(m, n)_8 \propto (mn)^{1/2}(m)_p(n)_p.$$

The agreement with this form is not entirely satisfactory, however. A closer look at the data suggests that the lines $(6, n)_8$, $(8, n)_8$ and $(10, n)_8$ have in fact slightly different slopes, increasing in that order, while the slopes of $(4, n)_8$ and $(6, n)_8$ seem to be slowly decreasing as n increases.

Table 2. The total numbers of polgons, $(m)_p$, and of figure eights, $(m)_8$, having m edges which are weakly embeddable in the square lattice; r_m is the ratio $(m)_p/(m)_8$

m	$(m)_p$	$(m)_8$	r_m
8	7	2	3·5000
10	28	8	3·5000
12	124	40	3·1000
14	588	208	2·8269
16	2938	1120	2·6232
18	15268	6200	2·4626
20	81826	35236	2·3222
22	449572	$2·048 \times 10^5$ (0·6%)	2·195 (0·6%)

If we define the total number of figure eights $(m)_8$, then the ratios $r_m = (m)_p/(m)_8$ appear (table 2) to obey fairly well the simple relationship

$$r_m = \alpha + \beta/m;$$

a graph is shown in figure 3. A least-squares analysis based on the exact data of $m = 10(2)20$ yields

$$\alpha = 1{\cdot}158 \pm 0{\cdot}010$$

$$\beta = 23{\cdot}39 \pm 0{\cdot}13$$

the standard error of the estimate is small: 0·0056. However, for large m there is a downward trend from this straight line†, emphasized when the $m = 22$ result is

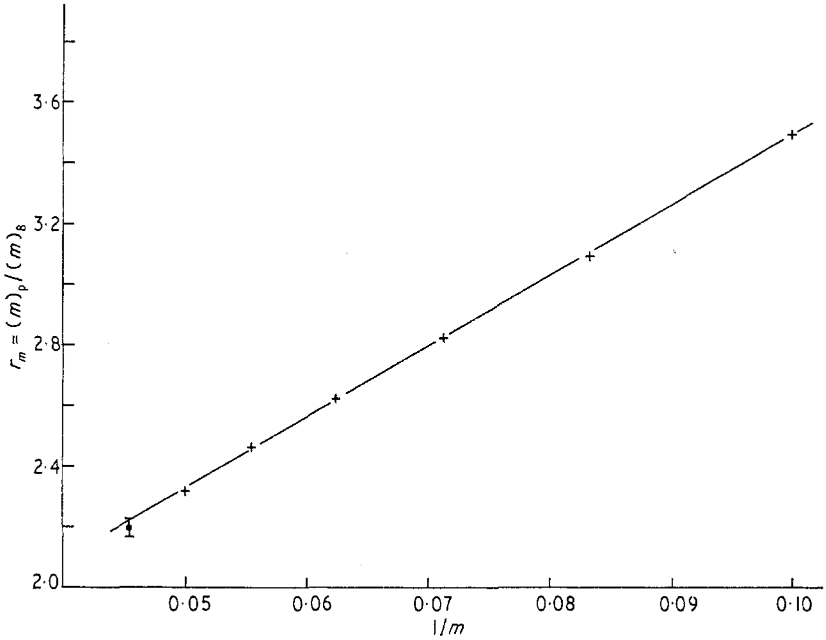

Figure 3. Graph of $r_m = (m)_p/(m)_8$ as a function of $1/m$. The line is that obtained from the least-squares analysis mentioned in the text, using $m = 10(2)20$. The error bar for $m = 22$ corresponds to the 95% confidence limit (two standard deviations) of the Monte Carlo estimate for $(4, 18)_8$.

included (figure 3). This can be taken into account by adding a third parameter and fitting the data to

$$r_m = a + b/\sqrt{m} + c/m$$

when a least-squares analysis gives $a = 0{\cdot}818$, $b = 2{\cdot}45$, $c = 19{\cdot}00$. The data therefore suggest that for large m the ratio r_m tends to a constant‡ in the region of unity, so that the numbers of polygons and of figure eights are similar. This means that they must make similar contributions to the higher terms in the series expansions of the Ising partition function: the polygon numbers no longer dominate the behaviour, as they do for the lower terms.

† Since submitting this paper we have learned that M. F. Sykes has enumerated many figure eights, including nearly all those reported here. Our enumeration results are identical to his, and our Monte Carlo estimates are within a standard deviation. Use of his results would allow a point for $m = 24$ to be added to the r_m curve: this point confirms the 'downward' trend indicated by our data. We wish to thank Dr. Sykes for permission to mention his results.

‡ The present data do not allow one to exclude the possibility that r_m may eventually approach zero, as suggested by a referee. In that case the figure eight contributions would eventually swamp those of the polygons in the higher terms of the Ising partition functions.

Acknowledgments

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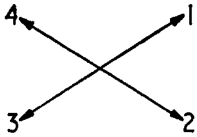
Appendix

In order to establish an upper limit on the number of figure eights $(m, n)_8$, consider joining two polygons $\mathscr{M}$ and $\mathscr{N}$ of m and n steps. A vertex like $\urcorner$, pointing north-east, on $\mathscr{M}$, can only join on $\mathscr{N}$, a vertex $\llcorner$, pointing south-west. Let us relabel these directions



and call M_1 the number of vertices on $\mathscr{M}$ pointing in direction 1, etc. The number of ways of joining $\mathscr{M}$ and $\mathscr{N}$, J, is governed by

$$J \leqslant M_1N_3 + M_2N_4 + M_3N_1 + M_4N_2 = 2(M_1N_1 + M_2N_2) \tag{A1}$$

where the second form follows from the fact that $M_1 = M_3$, $M_2 = M_4$ and similarly for N_1, N_3 and N_2, N_4. Now necessarily

$$\sum_1^4 M_i \leqslant m, \qquad \sum_1^4 N_i \leqslant n$$

so that

$$M_1 + M_2 \leqslant \tfrac{1}{2}m, \qquad N_1 + N_2 \leqslant \tfrac{1}{2}n. \tag{A2}$$

If we define μ, ν by

$$M_1 - M_2 = \tfrac{1}{2}\mu, \qquad N_1 - N_2 = \tfrac{1}{2}\nu \tag{A3}$$

then it follows from (1) and (2) that:

$$J \leqslant \tfrac{1}{4}mn + \tfrac{1}{4}\mu\nu. \tag{A4}$$

To consider $(m, n)_8$ we have eventually to average over all the $\mathscr{M}$ and $\mathscr{N}$, however, and in this average the final term of (4) will disappear. This is because for any pair $\mathscr{M}, \mathscr{N}$ we shall also encounter a pair $\mathscr{M}\mathscr{N}'$, for example, in which $\mathscr{N}'$ is simply $\mathscr{N}$ rotated through $\pi/2$, so that $N_1' = N_2$, $N_2' = N_1$. This has the effect of reversing the sign of ν (3), $\nu' = -\nu$, so that the result corresponding to (4) becomes $J \leqslant \frac{1}{4}mn - \frac{1}{4}\mu\nu$. Averaging over all the polygons, therefore, the $\mu\nu$ terms disappear, and one obtains

$$\langle J \rangle \leqslant \tfrac{1}{4}mn$$

which gives the upper limit on $(m, n)_8$ quoted in the paper.

To establish a lower limit on $(m, n)_8$ we define an 'upper right-hand corner' of any polygon $\mathscr{M}$: this vertex is in the top-most row of vertices of the polygon, and it is the most rightward of the vertices in that row. Evidently it exists, and so does a lower left-hand corner on $\mathscr{N}$, and they can certainly be joined to form a permissible figure eight. The argument can be repeated for an upper left-hand corner on $\mathscr{M}$ and a lower right-hand corner on $\mathscr{N}$, so that

$$J \geqslant 2$$

leading to the lower bound on $(m, n)_8$ quoted in the paper. One might expect to push this argument a little further, but in the case $m = n$, one then runs the risk of counting the same figure eight twice (as one can see for the case $(4, 4)_8$, for which the result is in fact $(4, 4)_8 = 2(4)_p(4)_p$). Where $m \neq n$ one can at least consider the other two 'corners', however, and obtain

$$(m, n)_8 \geqslant 4(m)_p(n)_p, \qquad m \neq n.$$

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