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Critical exponents for lattice animals with fixed cyclomatic index

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Abstract. We derive an inequality between the number of trees and the number of lattice animals with exactly c cycles, $a_n(c)$, for all positive c. If we assume that $a_n(c) \sim n^{-\theta_c}\lambda_c^n$, $n \to \infty$, c fixed, we use this to show that $\theta_c = \theta_0 - c$ where θ_0 is the corresponding exponent for trees.

1. Introduction

Lattice animals are connected subgraphs of a regular lattice. They have received considerable attention over the past ten years, partly because they are a useful model of excluded volume effects in branched polymer molecules in dilute solution (Lubensky and Isaacson 1979). One question of particular interest is the asymptotic behaviour of the number (a_n) of animals with n vertices (weakly) embeddable in a given lattice. Klarner (1967) used concatenation arguments to show that

$$0 < \lim_{n \to \infty} n^{-1} \log a_n = \sup_{n > 0} n^{-1} \log a_n \equiv \log \lambda < \infty. \tag{1.1}$$

By analogy with related problems one would expect that

$$a_n \sim n^{-\theta} \lambda^n \tag{1.2}$$

and (1.1) then implies that $\theta \geqslant 0$.

If we write $a_n(0)$ for the number of trees with n vertices, Klein (1981) has shown that

$$0 < \lim_{n \to \infty} n^{-1} \log a_n(0) = \sup_{n > 0} n^{-1} \log a_n(0) \equiv \log \lambda_0 < \infty. \tag{1.3}$$

Clearly $\lambda_0 \leqslant \lambda$ and this inequality is probably strict (Gaunt *et al* 1982). Again the expected asymptotic behaviour is

$$a_n(0) \sim n^{-\theta_0} \lambda_0^n. \tag{1.4}$$

Lubensky and Isaacson (1979) have argued that $\theta_0 = \theta$ and this is supported by several numerical studies (see, e.g., Duarte and Ruskin 1981, Gaunt *et al* 1982). Parisi and Sourlas (1981) have related the lattice animal exponent (θ) in d dimensions to the exponent characterising the Yang-Lee edge singularity in $d-2$ dimensions. This implies that $\theta = 1$ in two dimensions and $\theta = \frac{3}{2}$ in three dimensions.

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In order to relate trees to animals Lubensky and Isaacson (1979) introduced a cycle fugacity and argued that the corresponding critical exponent was independent of this fugacity. This led to the loose idea that cycles were unimportant in determining the critical behaviour of lattice animals. Whittington *et al* (1983) studied the number, $a_n(c)$, of lattice animals with n vertices and cyclomatic index c. These are referred to as c-animals. The cyclomatic index is the number of independent cycles; for instance a theta graph has $c=2$. They showed that

$$\lim_{n\to\infty} n^{-1}\log a_n(c) = \log\lambda_0 \tag{1.5}$$

for all c. Assuming that

$$a_n(c) \sim n^{-\theta_c}\lambda_0^n \tag{1.6}$$

they showed that

$$\theta_c \geqslant \theta_{c+1} \geqslant \theta_c - 1 \tag{1.7}$$

and presented numerical evidence that $\theta_1 = \theta_0 - 1$ and $\theta_2 = \theta_0 - 2$. This, together with (1.7), led them to conjecture that

$$\theta_c = \theta_0 - c. \tag{1.8}$$

More recent numerical studies by Wilkinson (1986) and Lam (1987) are all consistent with (1.8).

In this paper we prove (1.8) for the square lattice. We assume the *existence* of the exponent θ_0. Otherwise the arguments are rigorous.

The idea of the proof is to show that cycles can be introduced into a tree at a vertex of degree 4 and at certain vertices of degree 3, to give distinct animals with cycles. We show that there is a positive value of ε such that 'most' (in a sense which will be made precise) trees with n vertices have at least εn vertices at which this transformation can take place. By choosing c of these εn vertices and carrying out these transformations at c vertices, we obtain an inequality which is essentially

$$a_{n+c}(c) \geqslant An^c a_n(0) \tag{1.9}$$

for some positive constant A. This, together with the inequality

$$a_n(c) \leqslant 2dna_n(c-1) \tag{1.10}$$

derived by Whittington *et al* (1983), gives (1.8).

2. Proof of results

We restrict our attention to weak embeddings (i.e. subgraphs) in the square lattice. A tree (T) of n vertices has vertex set V and edge set E. The vertices have coordinates (x_i, y_i), $i = 1, 2, \ldots, n$, and we define the top vertex (bottom vertex) as the vertex having maximum (minimum) x coordinate and, in case of ambiguity, the vertex in this subset having maximum (minimum) y coordinate. Since the tree is connected, every vertex has degree 1, 2, 3 or 4 for $n>1$. A vertex is a member of set V_1 if it is of degree 4 and is a member of V_2, V_3, V_4 or V_5 if it is of degree 3 and is not connected to the neighbouring vertex in the south, west, north or east direction respectively (see figure 1). We consider a tree that has at least one vertex which is a member of V_1, V_2 or V_3. We number this vertex v_0 and suppose it has coordinates (x, y).

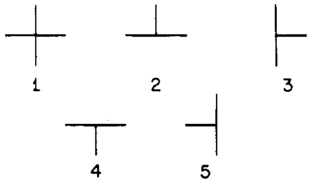

Figure 1. On the square lattice a vertex of degree greater than two must be of one of the five types shown.

Theorem 1. Every tree (with n vertices) containing a vertex $v_0 \in V_1$, V_2 or V_3 can be converted into a 1-animal (with $n+1$ vertices) containing a 4-cycle in which v_0 is the bottom vertex of the 4-cycle. The resulting 1-animal can have at most three trees rooted at a vertex in $V_1 \cup V_2 \cup V_3$ as precursors.

Proof. Let v_t be the top vertex of the tree, with coordinates (x_t, y_t). Since $v_0 \in V_1$, V_2 or V_3 then v_0 is connected to v_1 and v_2 with coordinates $(x+1, y)$ and $(x, y+1)$ respectively. We consider three subcases as follows.

(i) There is no vertex in the tree with coordinates $(x+1, y+1)$ (in this case $v_0 \in W_1$).

(ii) There is a vertex $v_3 \in V$ with coordinates $(x+1, y+1)$ and either $(v_1 - v_3) \in E$ or $(v_2 - v_3) \in E$ (then $v_0 \in W_2$).

(iii) $v_3 \in V$ but $(v_1 - v_3) \notin E$ and $(v_2 - v_3) \notin E$ (then $v_0 \in W_3$).

Note that since T is a tree it is not possible for both $(v_1 - v_3) \in E$ and $(v_2 - v_3) \in E$.

For the three cases we have three different constructions.

(i) Add v_3 at $(x+1, y+1)$ and the edges $(v_1 - v_3)$ and $(v_2 - v_3)$.

(ii) If $(v_1 - v_3) \in E$, add $(v_2 - v_3)$, and the vertex $v_{t'}$ with coordinates $(x_t + 1, y_t)$ and the edge $(v_t - v_{t'})$. If $(v_2 - v_3) \in E$, add $(v_1 - v_3)$, and the vertex $v_{t''}$ with coordinates $(x_t, y_t + 1)$ and the edge $(v_t - v_{t''})$.

(iii) The tree must contain at least one of two vertices having coordinates $(x+2, y+1)$ and $(x+1, y+2)$. We call these vertices v_4 and v_5, respectively. In addition, at least one of the edges $e_4 = (v_3 - v_4)$ and $e_5 = (v_3 - v_5)$ must be a member of E. v_3 is connected to v_0 through one and only one of e_4 and e_5. Delete the edge e_4 or e_5 on this connected path, add the edges $(v_1 - v_3)$ and $(v_2 - v_3)$ and the vertex $v_{t'} = (x_t + 1, y_t)$ and edge $(v_t - v_{t'})$ if e_4 is deleted, or the vertex $v_{t''} = (x_t, y_t + 1)$ and edge $(v_t - v_{t''})$ if e_5 is deleted.

The connected graph resulting from each of these constructions has $n+1$ vertices and $n+1$ edges so that it is a 1-animal.

Let $\mathscr{T}$ be the set of trees such that $T \in \mathscr{T}$ iff $V_1(T) \cup V_2(T) \cup V_3(T)$ is not empty. Let $\mathscr{T}_R$ be the set of rooted trees obtained by rooting each member (T) of $\mathscr{T}$ at each vertex $v_0 \in V_1(T) \cup V_2(T) \cup V_3(T)$. Let $\mathscr{T}_{R_k} \subset \mathscr{T}_R$ such that the tree $T \in \mathscr{T}_R$ is a member of $\mathscr{T}_{R_k}$ iff $v_0(T) \in W_k(T)$.

The transformation defined above maps a member of $\mathscr{T}_{R_k}$ uniquely into a 1-animal so that this transformation from $\mathscr{T}_{R_k}$ is 1-1 and onto the image set of $\mathscr{T}_{R_k}$. Hence, since k has three possible values, each 1-animal can have at most three precursors in the set of rooted trees.

Let $b_n(\varepsilon)$ be the number of trees with n vertices, more than εn of which are members of $V_1 \cup V_2 \cup V_3$. Let $a_n(c)$ be the number of c-animals with n vertices. From theorem

1 we have

$$a_{n+1}(1) \geq \binom{\varepsilon n}{1} b_n(\varepsilon)/3 \tag{2.1}$$

for any ε such that $\varepsilon n \geq 1$, since the tree can be rooted in at least

$$\binom{\varepsilon n}{1}$$

ways.

Suppose that we consider a tree with n vertices containing at least c vertices in $V_1 \cup V_2 \cup V_3$. We can choose c of these vertices and order them lexicographically (i.e. first in increasing order of x coordinate and, in case of ambiguity, in increasing order of y coordinate). By carrying out the above transformation successively at these ordered vertices we obtain c-animals having $n+c$ vertices. The resulting c-animal has at most 3^c precursors in the set of trees. If the tree has more than εn vertices in $V_1 \cup V_2 \cup V_3$ the c vertices can be chosen in at least

$$\binom{\varepsilon n}{c}$$

ways and

$$a_{n+c}(c) \geq \binom{\varepsilon n}{c} b_n(\varepsilon)/3^c \tag{2.2}$$

for $\varepsilon n \geq c$.

We now proceed to derive a lower bound on $b_n(\varepsilon)$ to establish that enough trees have sufficiently many vertices in $V_1 \cup V_2 \cup V_3$ that (2.2) implies (1.9). We accomplish this by proving a series of lemmas.

Lemma 1. If $t_n(\varepsilon, >)$ is the number of trees with n vertices containing more than εn vertices of degree greater than two then

$$b_n(\varepsilon/5) \geq t_n(\varepsilon, >)/2. \tag{2.3}$$

Proof. Suppose that $S_n(\varepsilon, >)$ is the set of trees with n vertices having more than εn vertices of degree greater than two. We construct subsets $S_{nm}(\varepsilon, >)$ such that a tree $T \in S_n(\varepsilon, >)$ is a member of $S_{nm}(\varepsilon, >)$ if m is the smallest number such that the number of vertices in $V_m(T)$ is at least as large as the number in $V_k(T)$, $k = 1, \ldots, 5$, $k \neq m$. Thus T can be a member of only one subset $S_{nm}(\varepsilon, >)$. $|S_{n2}(\varepsilon, >)| \geq |S_{n3}(\varepsilon, >)| \geq |S_{n4}(\varepsilon, >)| \geq |S_{n5}(\varepsilon, >)|$ where we write $|\cdot|$ for the cardinality of a set. Hence

$$\sum_{k=1}^{3} |S_{nk}(\varepsilon, >)| \geq |S_n(\varepsilon, >)|/2 = t_n(\varepsilon, >)/2. \tag{2.4}$$

Any $T \in S_{nm}(\varepsilon, >)$ is also a member of $S_n(\varepsilon, >)$ and hence has at least $n\varepsilon/5$ vertices in $V_m(T)$. Therefore the number of trees having at least $n\varepsilon/5$ vertices in $V_1 \cup V_2 \cup V_3$ is bounded below by $\Sigma_{k=1}^{3} |S_{nk}(\varepsilon, >)|$ and this, together with (2.4), implies (2.3).

Lemma 2 (Lipson and Whittington 1983). If $t_n(\varepsilon, \leq)$ is the number of trees with n vertices containing at most εn vertices of degree greater than 2 then there exists a positive constant $\lambda(\varepsilon)$ such that the limit

$$\lim_{n \to \infty} n^{-1} \log t_n(\varepsilon, \leq) \equiv \log \lambda(\varepsilon) < \infty \tag{2.5}$$

exists.

Lemma 3. $\lambda(\varepsilon)$ is a log concave function of ε in $[0, 1]$.

Proof. By an argument exactly analogous to that of Lipson and Whittington (1983) leading to their equation (2.21), it is easy to prove that

$$t_n(\varepsilon_1, \leqslant) t_n(\varepsilon_2, \leqslant) \leqslant t_{2n+q}((\varepsilon_1+\varepsilon_2)/2, \leqslant) \tag{2.6}$$

where q is the smallest integer greater than or equal to $4/(\varepsilon_1+\varepsilon_2)$. Taking logarithms, dividing by n and taking the limit $n\to\infty$ with ε_1 and ε_2 fixed we have

$$\log \lambda(\varepsilon_1) + \log \lambda(\varepsilon_2) \leqslant 2 \log \lambda((\varepsilon_1+\varepsilon_2)/2). \tag{2.7}$$

Since $\lambda(\varepsilon)$ is a non-decreasing function of ε bounded below (by the growth constant for self-avoiding walks) and above (by the growth constant for animals) then (2.7) implies that $\lambda(\varepsilon)$ is a log concave function of ε in $[0, 1]$ (Hardy *et al* 1934).

Lemma 4. $\log \lambda(\varepsilon)$ is a continuous function of ε in $[0, 1]$.

Proof. Since $\log \lambda(\varepsilon)$ is a non-decreasing concave function of ε in $[0, 1]$ it is continuous in $(0, 1]$ (Hardy *et al* 1934). Hence we need only establish continuity at $\varepsilon = 0$. To do this we construct an upper bound on $t_n(\varepsilon, \leqslant)$, as follows. We write n_k for the number of vertices of degree k in a tree. Let $u_n(\varepsilon)$ be the number of trees with n vertices having at most εn vertices of degree not equal to 2. Then

$$t_n(\varepsilon, \leqslant) \leqslant u_n(4\varepsilon) \tag{2.8}$$

since

$$m = n_1 + n_3 + n_4 = 2 + 2n_3 + 3n_4 \leqslant 4\varepsilon n \tag{2.9}$$

provided that $2/n \leqslant \varepsilon \leqslant \frac{1}{4}$. We can bound $u_n(4\varepsilon)$ by

$$u_n(4\varepsilon) \leqslant \sum_{m \leqslant 4\varepsilon n} T(m) \binom{n-2}{m-2} \mathrm{e}^{n(\kappa + g\sqrt{\varepsilon})} \tag{2.10}$$

where $T(m)$ is the number of (unlabelled) trees, in a graph theoretic sense, and g is some fixed positive number. The second term in (2.10) is the number of ways of distributing the $n_2 = n - m$ vertices of degree 2 among the $m-1$ branches of each tree, and the final term is an upper bound on the number of ways of embedding the branches independently in the lattice, derived from the results of Hammersley and Welsh (1962). κ is the connective constant of the lattice, given by

$$\kappa = \lim_{n\to\infty} n^{-1} \log c_n \tag{2.11}$$

where c_n is the number of n-step self-avoiding walks on the lattice. Clearly $\lambda(0) = \mathrm{e}^{\kappa}$. Since there exist positive constants B and β (Otter 1948) such that

$$T(m) \leqslant B\beta^m \tag{2.12}$$

we have, from (2.10)

$$u_n(4\varepsilon) \leqslant 4\varepsilon n B \beta^{4\varepsilon n} \binom{n-2}{4\varepsilon n - 2} \mathrm{e}^{n(\kappa + g\sqrt{\varepsilon})} \tag{2.13}$$

provided that $\varepsilon \leqslant \frac{1}{8} + 1/(4n)$. Then from (2.8) and (2.13)

$$\begin{aligned} \log \lambda(\varepsilon) &= \lim_{n\to\infty} n^{-1} \log t_n(\varepsilon, \leqslant) \\ &\leqslant 4\varepsilon \log \beta - 4\varepsilon \log 4\varepsilon - (1-4\varepsilon)\log(1-4\varepsilon) + \kappa + g\sqrt{\varepsilon} \end{aligned} \tag{2.14}$$

and

$$\lim_{\varepsilon \to 0} \log \lambda(\varepsilon) = \kappa = \log \lambda(0) \tag{2.15}$$

establishing continuity at $\varepsilon = 0$.

Lemma 5. There exists $\varepsilon_0 > 0$ such that for all $\varepsilon < \varepsilon_0$,

$$\lim_{n \to \infty} (t_n(\varepsilon, >)/a_n(0)) = 1. \tag{2.16}$$

Proof. Since $\lambda(\varepsilon)$ is continuous in $[0, 1]$ and $\lambda(0) < \lambda(1)$ (Gaunt *et al* 1982) there exists $\varepsilon_0 > 0$ such that for all $\varepsilon < \varepsilon_0$, $\lambda(\varepsilon) < \lambda(1)$. We can write

$$t_n(\varepsilon, >)/a_n(0) = 1 - t_n(\varepsilon, \leqslant)/a_n(0) \tag{2.17}$$

$$= 1 - [\lambda(\varepsilon)/\lambda(1)]^n \, e^{O(n)} \tag{2.18}$$

and letting $n \to \infty$ proves the lemma.

Lemma 6. There exists an $A>0$ and an integer N such that for all $n > N$

$$b_n(\varepsilon) \geqslant A a_n(0) \tag{2.19}$$

for any $\varepsilon \leqslant \varepsilon_0/5$.

Proof. (2.19) follows immediately from (2.3) and (2.18).

Theorem 2. If $\lim_{n\to\infty}[\log(a_n(0)/\lambda_0^n)/\log n] = -\theta_0$ exists then

$$\lim_{n \to \infty} [\log(a_n(c)/\lambda_0^n)/\log n] = -\theta_c$$

exists for all c and

$$\theta_c = \theta_0 - c. \tag{2.20}$$

Proof. It follows from (2.2) and (2.19) that

$$a_{n+c}(c) \geqslant A \binom{\varepsilon n}{c} a_n(0)/3^c \tag{2.21}$$

and from (1.10) that

$$a_n(c) \leqslant (2dn)^c a_n(0). \tag{2.22}$$

Dividing by λ_0^n, taking logarithms and dividing by $\log n$ in (2.21) and (2.22) and then letting $n \to \infty$ with c fixed proves the theorem and in particular gives (2.20).

3. Discussion

The proof given in the previous section is specifically for the square lattice. However, it can be generalised to work for the d-dimensional hypercubic lattice with relatively minor modifications. For lemmas 2–6 the proofs for arbitrary d are almost identical to those for $d = 2$ and the only serious differences arise in theorem 1 and lemma 1. In theorem 1 the sets of vertices corresponding to V_1, V_2 and V_3 will be sets of vertices

(v_0) with degree $3, 4, \ldots, 2d$ which have incident on them the two edges $(x_1, x_2, \ldots, x_d)-(x_1+1, x_2, \ldots, x_d)$ and $(x_1, x_2, \ldots, x_d)-(x_1, x_2+1, \ldots, x_d)$ where $(x_1, x_2, \ldots, x_d)$ are the coordinates of v_0. In lemma 1 the inequality corresponding to (2.3) is

$$b_n(\varepsilon/k) \geq (1/l)t_n(\varepsilon, >) \tag{3.1}$$

where

$$k = \sum_{j=3}^{2d} \binom{2d}{j} = 2^{2d} - 2d^2 - d - 1 \tag{3.2}$$

and

$$l = \max_{j\geq 3} \binom{2d}{j}\binom{2d-2}{j-2}^{-1} = d(2d-1)/3. \tag{3.3}$$

The proof follows the same lines as that given in § 2.

To summarise we have shown that if the critical exponent (θ_0) for trees exists then the corresponding exponent (θ_c) for c-animals exists and is given by $\theta_c = \theta_0 - c$. Apart from its relevance to the effect of cyclomatic index on the statistics of lattice animals this result is also relevant to recent work by Dickman and Schieve (1984, 1986) on the collapse transition of lattice animals.

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