Lattice Animals: Rigorous Results and Wild Guesses

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1. Introduction

We consider the d-dimensional hypercubic lattice with vertices being the integer points in $\mathbb{R}^d$. Two points are connected by an edge if they are unit distance apart. We write $(x_1, x_2, \ldots, x_d)$ for the coordinates of a vertex v and $e = (v_1, v_2)$ for the edge joining the vertices v_1 and v_2 whose coordinates must differ by unity in exactly one coordinate.

A *bond animal* is a connected subgraph of the lattice and a *site animal* is a connected section graph of the lattice. The distinction is that for each pair of vertices v_1 and v_2 in a site animal, which differ by unity in exactly one coordinate, the edge $e = (v_1, v_2)$ must be in the site animal. That is, for site animals, edges are induced by the vertices. We shall be interested in the number of bond or site animals, with n vertices, where two animals are identical if one can be translated into the other. We write A_n for the number of site animals with n vertices and a_n for the number of bond animals with n vertices. For instance, for the square lattice (i.e. $d = 2$), $a_1 = 1$, $a_2 = 2$, $a_3 = 6$, $a_4 = 23$, $a_5 = 95$, $\ldots$ and $A_1 = 1$, $A_2 = 2$, $A_3 = 6$, $A_4 = 19$, $A_5 = 63$, $\ldots$.

In each case an interesting subset is the corresponding set of animals without cycles which we call *bond trees* and *site trees*. We write t_n and T_n for the numbers of bond trees and site trees with n vertices. Again in $d = 2$, $t_1 = 1$, $t_2 = 2$, $t_3 = 6$, $t_4 = 22$, $t_5 = 87$, $\ldots$ and $T_1 = 1$, $T_2 = 2$, $T_3 = 6$, $T_4 = 18$, $T_5 = 55$, $\ldots$.

These animals and trees have been considered as models of branched polymers with excluded volume in much the same way that self-avoiding walks have been used as models of linear polymers with excluded volume, and the techniques used to handle the animal problem are closely related to techniques in the theory of self-avoiding walks (Hammersley 1957; Kesten 1963). Lattice animals are also closely related to percolation clusters although the associated weights are different in the two problems (Broadbent and Hammersley 1957; Kesten 1982).

A good deal of the literature on site animals uses the language of polyominoes. A *cell* of the square lattice is the boundary and interior of a unit square having its vertices at lattice vertices and a *polyomino* is a connected set of cells which are joined at their edges (Golomb 1954; Klarner 1967). Because the square lattice is self-dual the number of polyominoes with n cells is precisely the number of site animals with n vertices. (Where polyominoes are regarded as distinct when one cannot be translated into another, they are sometimes called *fixed* polyominoes.)

The primary interest is in the asymptotic behaviour of a_n, A_n, t_n and T_n. There are many papers which develop methods for obtaining bounds on $A_n^{1/n}$ and we shall review some of these. Concatenation arguments easily establish the existence of the limit $\lim_{n\to\infty}(1/n)\log A_n$ once an upper bound on $A_n^{1/n}$ is available and we shall indicate the corresponding arguments to establish the existence of the limits, the growth constants,

$$\begin{aligned}\Lambda_0 &= \lim_{n\to\infty} T_n^{1/n}\\ \lambda_0 &= \lim_{n\to\infty} t_n^{1/n}\\ \Lambda &= \lim_{n\to\infty} A_n^{1/n}\\ \lambda &= \lim_{n\to\infty} a_n^{1/n}.\end{aligned} \tag{1.1}$$

In fact the only difficulty is to show that $a_n^{1/n}$ is bounded above. The inequalities $\Lambda_0 \le \Lambda$ and $\lambda_0 \le \lambda$ are immediate and we show that

$$\Lambda_0 < \Lambda < \lambda_0 < \lambda. \tag{1.2}$$

Roughly speaking, Sections 2–4 describe what is now known rigorously. Section 5 looks at the rates of approach to the limits in (1.1). There, very little is known but there are some informed guesses based on field theoretic arguments and numerical results. It seems that all four limits are approached at roughly the same rate, that this rate is characterized by a critical exponent and that the exponent is independent of the dimension of the problem for $d \ge 8$, but depends on d (but not on the particular lattice in $\mathbb{R}^d$) for $d < 8$. In Section 6 we consider animals on a lattice subset and, in particular, animals in wedge and slab geometries. Section 7 contains a collection of unsolved problems.

Like many other combinatorial problems these are closely connected to problems in physics, are easy to state and understand, but are remarkably difficult to solve.

2. Existence of Limits

We first prove that $a_n^{1/n}$ is bounded above, using a method which is an extension of an idea due to Klarner (1967).

We define the top (bottom) vertex of a set S_0 of vertices as follows. First construct the subset $S_1 \subset S_0$ such that the coordinate x_1 of every vertex in S_1 has the maximum (minimum) value over all vertices in S_0. We then recursively construct $S_k \subset S_{k-1}$ such that the coordinate x_k of every vertex in S_k has the maximum (minimum) value over all vertices in S_{k-1}. Let j be the smallest integer such that S_j contains precisely one vertex, and call this vertex t (respectively b), the top (respectively bottom) vertex of S_0.

We now construct a unique ordering of the vertices and edges of a bond animal. A vertex can have up to $2d$ edges emanating from it and we assign an order $l_1, l_2, \ldots, l_{2d}$. We specify the added constraint that the edge in the $-\hat{x}_1$ direction comes before the edges in the $\pm\hat{x}_2$ directions in this ordering. We number the bottom vertex v_1. The k edges incident on the bottom vertex are numbered $1, 2, \ldots, k$ according to their order in the list $\{l_i\}$, and the vertices connected to the bottom vertex through these edges are numbered $2, \ldots, k+1$. We now continue this numbering at vertex v_2, labelling any edges incident on v_2 and vertices connected to v_2, which have not previously been labelled, and so on through v_3, v_4, $\ldots$.

We next code the animal, proceeding through the vertices in order, using the following procedure. The vertex v_k, $k > 1$, is connected by an edge to at least one vertex v_j with $j < k$. Let j be the smallest such value and let r be the order of the edge (v_k, v_j) emanating from v_k in the ordering $\{l_i\}$ described above. Then number the ith edge (in the ordering $\{l_i\}$) emanating from v_k with the number $s_i = (i - r) \bmod (2d)$ for each $i = 1, \ldots, 2d$, $i \neq r$. Place the number zero in the $\{(2d-1)(k-1) + s_i\}$th location of a vector of length $(2d-1)n$ if the ith edge is not in the animal or if it is incident on v_m for some $m < k$. Otherwise place the number 1 in the $\{(2d-1)(k-1) + s_i\}$th location of the vector. In the special case $k = 1$, assume the edge $(v_1 - \hat{x}_2, v_1)$ is in the animal and then proceed as for v_k. In this way there is a vector of length $(2d-1)n$ associated with each animal. The total number of ones in this vector is equal to the total number of bonds in the animal. If an animal has b bonds these can be chosen in at most $\binom{(2d-1)n}{b}$ ways and the number of animals satisfies

$$\begin{aligned} a_n &\leq \sum_{b=n-1}^{dn} \binom{(2d-1)n}{b} \\ &\leq (d-1)n \binom{(2d-1)n}{\lfloor (d-1/2)n \rfloor} \end{aligned} \tag{2.1}$$

($\lfloor x \rfloor$ denotes the greatest integer less than or equal to x) and it follows that

$$a_n^{1/n} \leq 2^{2d-1} \tag{2.2}$$

for all n.

Each animal with n vertices can be concatenated with each animal with m vertices by translating so that the coordinates $(x_1(b), x_2(b), \dots)$ of the bottom vertex of one animal and the coordinates $(x_1(t), x_2(t), \dots)$ of the top vertex of the second animal are such that

$$\begin{aligned} x_1(b) &= x_1(t) + 1 \\ x_j(b) &= x_j(t) \quad \forall j \neq 1. \end{aligned} \tag{2.3}$$

Adding an edge to join these two adjacent vertices results in an animal with $m + n$ vertices and every pair of m and n animals gives a distinct $(n + m)$-animal so that

$$a_n a_m \leq a_{n+m}. \tag{2.4}$$

From (2.2) and (2.4) it follows that

$$\sup_{n>0} n^{-1} \log a_n = \lim_{n\to\infty} n^{-1} \log a_n = \log \lambda \leq (2d-1) \log 2, \tag{2.5}$$

where λ is called the *growth constant* of bond animals. Similar concatenation arguments establish the existence of the limits in (1.1) since T_n, t_n and A_n are all less than or equal to a_n and so $T_n^{1/n}$ etc. are all bounded above.

3. Upper and Lower Bounds on the Growth Constants

In this section we give a brief account of several methods for finding upper and lower bounds on the growth constants. Perhaps the most obvious approach for obtaining a lower bound is to use (2.5) directly since (2.5) implies that

$$a_n^{1/n} \leq \lambda \quad \forall n, \tag{3.1}$$

and with corresponding inequalities for Λ_0, Λ and λ_0. The numbers of bond and site animals and bond and site trees are known exactly for small n (see e.g. Gaunt et al. 1976, Gaunt and Ruskin 1978, Redelmeier 1981, Gaunt et al. 1982). For instance, using Redelmeier's result that $A_{24} = 5239988770268$ on the square lattice, we have $\Lambda \geq 3.388$. By noticing that the concatenation can be carried out in each of d directions (3.1) can be improved to

$$(dn)^{1/n} \leq \lambda \tag{3.2}$$

and, for site animals on the square lattice, we have $\Lambda \geq 3.487$. Similar calculations yield $\Lambda_0 \geq 3.1533$, $\lambda_0 \geq 4.1507$ and $\lambda \geq 4.3486$.

An alternative but closely related method has been discussed by Rands and Welsh (1981). This is related to an idea of Moser described in Klarner and Rivest (1973). We call an animal α *composite* if there exist two animals

α_1 and α_2 which yield α under the concatenation described in Section 2. If no such pair of animals exists we call α a *prime animal with respect to bond decomposition.* If we write p_n for the number of these prime animals with n vertices then

$$a_n = p_n + \sum_{i=1}^{n-1} p_{n-i} a_i, \quad n \geq 1. \tag{3.3}$$

If we construct generating functions

$$A(x) = \sum_{n=0}^{\infty} a_n x^n \tag{3.4}$$

and

$$P(x) = \sum_{n=1}^{\infty} p_n x^n \tag{3.5}$$

then

$$A(x) = 1 + P(x)A(x) \tag{3.6}$$

and $A(x)$ is singular when $P(x) = 1$.

If a_n is known exactly for $n \leq N$ then p_n can be determined for $n \leq N$ from (3.3). If we write $P_N(x)$ for the polynomial with degree N whose coefficients are equal to the coefficients of $P(x)$ up to x^N then Rogers (1979) shows that the unique positive zero $(1/\lambda_N)$ of $P_N(x) - 1 = 0$ is such that $\lambda_N \leq \lambda$ and converges to λ as $N \to \infty$. Using this method Rands and Welsh show that, for the square lattice, $\Lambda \geq 3.57$.

A substantial improvement results from a comparatively minor change in the concatenation operation. Instead of joining the top vertex of one animal to the bottom vertex of a second animal by adding a bond, they construct an animal by superimposing the top vertex of one and the bottom vertex of another. This gives another definition of primality (prime with respect to site decomposition) and the previous argument goes through with only minor changes. The resulting bound is improved to $\Lambda \geq 3.7355$.

The configurational data which are now known exactly allow these bounds to be improved and corresponding bounds to be determined for the other growth constants. For the square lattice, Redelmeier's results for site animals give $\Lambda \geq 3.791$. The second concatenation approach can be used for bond animals and for bond trees on the square lattice and, using the available counts (Gaunt and Ruskin 1978; Gaunt et al. 1982), we obtain the bounds $\lambda \geq 4.544$ and $\lambda_0 \geq 4.462$. This second concatenation does not work for site trees (since two site trees concatenated in this way do not necessarily yield a tree) but, using the results of Gaunt et al. (1976), the first concatenation gives $\Lambda_0 \geq 3.300$.

The first concatenation argument can be extended in the following way. With the definition of top and bottom vertex given in Section 2, an animal is composite if there exists an edge in the x_1-direction which when removed decomposes the animal into two animals whose top and bottom vertices were incident on this edge. If no such edge exists we call the animal *prime with respect to* x_1.

We now extend our definitions of top and bottom vertices to *i-top* and *i-bottom* vertices in the following way. We first construct the set of vertices such that coordinate x_i has maximum (minimum) value, and the subset of this such that x_{i+1} has maximum (minimum) value, and so on, cyclically, to x_{i-1}. This gives a unique i-top (i-bottom) vertex.

If an animal is prime with respect to x_1 we can look for a further decomposition removing an edge in the x_2-direction to give two animals whose 2-top and 2-bottom vertices were incident on this edge. If no such edge is present the animal is *prime with respect to* x_2, and so on. This implies that the p_n of (3.3) can be written in terms of the numbers $p_n(2)$ of animals prime with respect to x_2 as

$$p_n = p_n(2) + \sum_{i=1}^{n-1} p_{n-i}(2) p_i \tag{3.7}$$

and, in terms of their generating functions,

$$P(x) = \big(1 + P(x)\big) P_2(x) \tag{3.8}$$

where

$$P_2(x) = \sum_{n=1}^{\infty} p_n(2) x^n. \tag{3.9}$$

Hence

$$A(x) = \frac{\big(1 - P_2(x)\big)}{\big(1 - 2P_2(x)\big)} \tag{3.10}$$

and A has a singular point at the positive root of $P_2(x) = 1/2$.

This approach gives an improved bound for site trees on the square lattice, $\Lambda_0 \geq 3.381$, but does not improve the bounds for Λ, λ_0, or λ. We note that this approach does not generalize to the site decomposition process.

All of these methods for deriving lower bounds rely on counting animals exactly for small n. The bounds are capable of improvement by determining further terms in the series but the computational effort required is considerable.

We also mention, without much detail, several other approaches to computing lower bounds. We focus on site animals on the square lattice but the methods could be extended to other cases. If a site animal is such that the bonds in each row (column) of the lattice are contiguous we call the animal *row (column) convex.* An animal is *convex* if it is both row and column convex. Clearly these are subsets of the site animals and counting these subsets yields lower bounds on Λ, though these problems are also interesting in their own right. Row convex animals have been counted by Klarner (1965) and convex animals by Klarner and Rivest (1974) and by Delest and Viennot (1984). On a different tack, Read (1962) has used a transfer matrix method to count site animals confined between two parallel lines. Although each of these approaches has attractive features we believe that the renewal sequence method of Rands and Welsh shows most promise for calculating good lower bounds.

In his original paper on site animals Eden (1961) shows that $\Lambda \leq 27/4$ in $d = 2$. (Our argument in Section 2 that $\lambda \leq 2^{2d-1}$ is based on his approach.) Klarner and Rivest (1973) have reformulated Eden's approach in a way which allows successive improvement and we sketch their argument here. Each site animal is associated with a unique spanning tree and these trees can be regarded as a sequence of 'twigs', chosen from a fixed finite set. The number of site animals is bounded above by the number of ways of concatenating the twigs. Based on this argument, there is a particular set of twigs which gives the Eden bound $\Lambda \leq 27/4$. We note that this argument and the same set of twigs also works for bond trees and gives $\lambda_0 \leq 27/4$ in $d = 2$. Furthermore, this same set of twigs can be used to obtain the upper bound $\lambda \leq 8$ in $d = 2$ derived by us in Section 2. Klarner and Rivest describe a procedure for choosing sets of twigs which lead to successive improvements of the bound on Λ. Their best bound obtained in this way is $\Lambda \leq 4.649551$.

4. Applications of a Pattern Theorem

To motivate this section we begin by describing some work by Kesten (1963) on the number of self-avoiding walks on a lattice. Kesten defined a pattern to be any finite self-avoiding walk, i.e. any finite sequence of edges such that no vertex of the lattice is visited more than once. He proved that if there exists a self-avoiding walk on which the pattern appears three times then the pattern appears at least once on all except exponentially few sufficiently long self-avoiding walks. Kesten used this theorem to establish that, if c_n is the number of n-step self-avoiding walks, the limit $\lim_{n\to\infty} c_{n+2}/c_n$ exists. The theorem has proved useful in a variety of other areas, e.g. in studying walks confined to a subset of a lattice (Hammersley and Whittington 1985).

Recently Madras (1988) has proved a corresponding pattern theorem for lattice animals and related structures which we state as follows.

We focus on the case of bond animals though the theorem applies to certain subsets of these as well. Let L be the simple hypercubic lattice in $\mathbb{R}^d$ and let $P = (P_1, P_2)$ be a *proper pattern* if P_1 and P_2 are disjoint subsets of L such that for any n there exists an animal with $m > n$ vertices weakly embeddable in L which contains all of P_1 and none of P_2. The number $a_n(\overline{P})$ of animals with n vertices in which P does not occur is such that

$$\limsup_{n\to\infty} n^{-1} \log a_n(\overline{P}) < \log \lambda. \tag{4.1}$$

The theorem is valid if bond animals are replaced by site animals or by bond trees; i.e.

$$\limsup_{n\to\infty} n^{-1} \log A_n(\overline{P}) < \log \Lambda \tag{4.2}$$

and

$$\limsup_{n\to\infty} n^{-1} \log t_n(\overline{P}) < \log \lambda_0. \tag{4.3}$$

It is easy to prove that $\Lambda_0 \leq \Lambda \leq \lambda_0 \leq \lambda$ and Rands and Welsh (1981) conjectured that $\Lambda < \lambda_0$ while Gaunt et al. (1982) conjectured that $\Lambda_0 < \Lambda$ and $\lambda_0 < \lambda$. Each of these strict inequalities can be established by an application of Madras' pattern theorem. If we consider P_1 to be the elementary square and P_2 to be the empty set, $P = (P_1, P_2)$ occurs in both site animals and in bond animals but not in site trees or bond trees and this immediately gives

$$\Lambda_0 < \Lambda \tag{4.4}$$

and

$$\lambda_0 < \lambda. \tag{4.5}$$

Following Klarner (1967) we construct a spanning tree for each site animal. The vertices of the spanning tree are those of the animal and are numbered according to the vertex numbering scheme described in Section 2. We complete the spanning tree by adding edges as follows. We join the first and second vertices. We then consider each vertex in turn and add an edge to join this vertex to the vertex with smallest number which is adjacent to it in the lattice. These spanning trees are a subset of the bond trees and correspond 1-1 with the site animals. It is clear that the pattern in which P_1 is $\sqsupset$ and P_2 is the complement of P_1 in $\square$ can appear in a bond tree but not in the spanning tree (as defined above) of a site animal. Hence

$$\Lambda < \lambda_0. \tag{4.6}$$

Madras et al. (1988) gave an alternative proof that $\lambda_0 < \lambda$ and this argument can be strengthened to show that

$$\lambda - \lambda_0 \geq (0.00003758)\lambda_0 \geq 0.0001677. \tag{4.7}$$

5. The Subdominant Asymptotic Behaviour

The results described up to now tell us nothing about the rates of approach to the limits in (1.1). Physicists (e.g. Lubensky and Isaacson 1979) expect that

$$a_n \sim Cn^{-\theta}\lambda^n \tag{5.1}$$

which implies that the limit

$$\lim_{n\to\infty}\left(\frac{\log[a_n/\lambda^n]}{\log n}\right) = -\theta \tag{5.2}$$

exists. Proving that this limit exists would be a major advance. Similarly, it is believed that

$$t_n \sim C_0 n^{-\theta_0}\lambda_0^n \tag{5.3}$$

and there are arguments (and some numerical results) suggesting that $\theta = \theta_0$ (Lubensky and Isaacson 1979; Duarte and Ruskin 1981; Gaunt et al. 1982). The value of θ is believed to be lattice independent and to depend only on the dimension. (Notice that λ is lattice dependent.) In addition, θ is believed to be independent of d for $d \geq d_c = 8$, where d_c is called the *upper critical dimension.* For self-avoiding walks, the existence of an upper critical dimension has now been established (Slade 1987). There is an intriguing proposal (Parisi and Sourlas 1981) that θ is connected to the Yang-Lee edge singularity exponent in $d-2$ dimensions and, since this exponent is known exactly for $d=0$ and 1, this suggests that $\theta(d=2)=1$ and $\theta(d=3)=3/2$. These values are certainly consistent with the available numerical evidence.

An attempt has been made to connect the results on trees with those on animals by asking for the number of animals with fixed cyclomatic index. If $a_n(c)$ is the number of bond animals with n vertices and c elementary cycles then $a_n(0) \equiv t_n$ and

$$a_n = \sum_{c\geq 0} a_n(c). \tag{5.4}$$

It is fairly easy to prove that

$$\lim_{n\to\infty} n^{-1}\log a_n(c) \equiv \log\lambda_c \tag{5.5}$$

exists and that

$$\lambda_c = \lambda_0 \quad \forall c. \tag{5.6}$$

By analogy with (5.1) one expects that

$$a_n(c) \sim C_c n^{-\theta_c}\lambda_0^n \tag{5.7}$$

and it has been shown (Soteros and Whittington 1988) that if θ_0 exists then θ_c exists (in an analogous way to (5.2)) and that

$$\theta_c = \theta_0 - c. \tag{5.8}$$

While there are heuristic arguments (Whittington, Torrie, and Gaunt 1983) that this is consistent with $\theta = \theta_0$, much remains to be done in this area.

6. Lattice Animals on Lattice Subsets

In this section we consider the number of lattice animals with n vertices, confined to lie in a subset of the square lattice. This is closely related to some work on self-avoiding walks in restricted geometries (Hammersley and Whittington 1985) and to similar problems in percolation theory (Grimmett 1983) and the Ising problem (Chayes and Chayes 1986).

We shall consider two particular cases: animals in wedges and animals in slits. We define an *f-wedge* of the square lattice to be the subset of the square lattice $\{(x, y) : x \geq 0, 0 \leq y \leq f(x)\}$ where $f(x)$ is a non-negative function of x. We now ask for the number $a_n(f)$ of animals with n vertices with one vertex at the origin and with all other vertices in the f-wedge. It is easy (following a line of argument due to Hammersley and Whittington (1985)) to show that, provided that $\lim_{x\to\infty} f(x) = \infty$,

$$\lim_{n\to\infty} n^{-1} \log a_n(f) = \log \lambda \tag{6.1}$$

independent of f. A situation of some physical interest is when

$$f(x) = \alpha x. \tag{6.2}$$

If one assumes that

$$a_n(\alpha x) \sim n^{-\theta(\alpha)} \lambda^n \tag{6.3}$$

the question is: how does θ depend on α? Of course, this is all modulo the existence of the exponent θ. There are some numerical results due to De'Bell and Lookman (1985) but nothing else. In the case of self-avoiding walks there are some definite predictions from conformal invariance arguments and these are in good agreement with the numerical results of Guttmann and Torrie (1984) and Cardy and Redner (1984). (The conformal invariance argument does not work for animals since there is no Hamiltonian formulation of the animal problem.)

The corresponding slit problem asks for the number $a_n(L)$ of animals with n vertices such that no vertex has y coordinate less than zero or greater than L and at least one vertex has y coordinate zero. Two animals are considered identical if one can be translated into the other in the x-direction. By concatenation in the x-direction it is easy to show that

$$\lim_{n\to\infty} n^{-1} \log a_n(L) = \sup_{n>0} n^{-1} \log a_n(L) = \log \lambda(L) \tag{6.4}$$

and interest focuses on the L-dependence of $\lambda(L)$.

Madras' pattern theorem readily establishes that

$$\lambda(L+1) > \lambda(L) \tag{6.5}$$

and, following Hammersley and Whittington (1985), it is easy to prove that

$$\lim_{L\to\infty} \lambda(L) = \lambda. \tag{6.6}$$

Can one say anything further about the L dependence? It is presumably the case that $\log \lambda(L)$ is a concave function of L, and a reasonable guess (supported by a scaling argument) would be that

$$\log \lambda - \log \lambda(L) \sim L^{-\phi} \tag{6.7}$$

but this seems to be difficult to prove.

7. Unsolved Problems

In this final section we list some of the unsolved problems which we have mentioned earlier.

(i) Calculate any of the growth constants for any non-trivial lattice.
(ii) Show that $a_n = \lambda^n e^{O(\log n)}$.
(iii) Prove that the $\log n$ term in (ii) has the same coefficient for trees and for animals, and for the site and bond cases.
(iv) Provide some rigorous results on the sub-dominant term for animals in a wedge of angle α.
(v) Investigate the L dependence of $\lambda(L)$ for animals in a slit geometry.

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