Enumeration Bounds via an Isoperimetric-Type Inequality

N Madras
Department of Mathematics and Statistics, York University, 4700 Keele Street, Toronto, Ontario, Canada M3J 1P3
E-mail: madras@mathstat.yorku.ca

Abstract. In 1949, Loomis and Whitney published a geometrically intuitive inequality that bounds the cardinality of a $d$-dimensional set in terms of the cardinalities of its projections onto the coordinate hyperplanes. We show how this inequality can be used to prove two results in the asymptotic enumeration of lattice animals: a bound on the critical exponent for the number of lattice animals in arbitrary dimension, and a bound on the growth constant for the number of “almost unknotted” embeddings of graphs in the cubic lattice.

1. Introduction
In this paper, I shall describe three apparently unrelated rigorous mathematical results: an old inequality of Loomis and Whitney (1949); a bound on the critical exponent for the number of lattice animals (Madras 1995); and the evaluation of the growth constant for a certain class of knotted graph embeddings in the cubic lattice (work in preparation by the author with D.W. Sumners and S.G. Whittington). The connection among them is that the proofs of the second and third results use the first result in fundamental and somewhat unexpected ways.

The three results will be described in the three remaining sections of the paper.

2. The Loomis-Whitney inequality
Let $S$ be a subset of $d$-dimensional Euclidean space $\mathbb{R}^d$. In the applications of the present paper, we will be thinking of $S$ as a finite set, and more specifically as a finite subset of the $d$-dimensional hypercubic lattice $\mathbb{Z}^d$.

For each $k = 1, \ldots, d$, we define $\text{Proj}_k(S)$ to be the projection of $S$ onto the coordinate hyperplane parallel to the $x_k$-axis, i.e.

$$\text{Proj}_k(S) = \{(x_1, \ldots, x_{k-1}, x_{k+1}, \ldots, x_d) : (x_1, \ldots, x_{k-1}, u, x_{k+1}, \ldots, x_d) \in S \text{ for some } u \in \mathbb{R}\}.$$

Thus $\text{Proj}_k(S)$ is a subset of $\mathbb{R}^{d-1}$. Also, we shall use the notation $|\cdot|$ to denote cardinality.

The Loomis-Whitney inequality is the following result.

**Theorem 1** (Loomis and Whitney (1949)). Let $S$ be a subset of $\mathbb{R}^d$. Then

$$|S|^{d-1} \leq \prod_{k=1}^{d} |\text{Proj}_k(S)|.$$
Loomis and Whitney also show that this holds if $S$ is an open set and we interpret $| \cdot |$ as Lebesgue measure (in $d$ or $d - 1$ dimensions, as appropriate).

Some remarks on this result are in order. First, the inequality is obvious for $d = 2$, since in that case $S$ is a subset of the Cartesian product $\text{Proj}_1(S) \times \text{Proj}_2(S)$. Indeed, the elegant proof of Loomis and Whitney uses this as a starting point, and proceeds by induction on $d$. Also, notice that equality holds if $S$ is a (hyper)rectangle.

Finally, we note the following consequence of the Arithmetic-Geometric Mean Inequality and Theorem 1:

**Corollary 2.** Let $S$ be a subset of $\mathbb{R}^d$. Then

$$|S|^{(d-1)/d} \leq \frac{1}{d} \sum_{k=1}^{d} |\text{Proj}_k(S)|.$$  

This corollary has a natural interpretation. The right-hand side is the average size of a projection of $S$ onto a coordinate hyperplane. This should be a lower bound for any reasonable definition of the “surface measure” of the set $S$. Thus we conclude that the surface measure of a $d$-dimensional object of volume $V$ should be at least $V^{(d-1)/d}$. This assertion, with an optimal multiplicative constant, is the prototypical isoperimetric inequality. Such inequalities have a broad range of applications throughout mathematics.

### 3. Critical Exponent for Lattice Animals

In this section we shall work on the hypercubic lattice $\mathbb{Z}^d$, where $d \geq 2$. We say that a site $(x_1, \ldots, x_d)$ of this lattice is lexicographically smaller than another site $(y_1, \ldots, y_d)$ if $x_I < y_I$, where $I$ is the smallest value of $i$ for which $x_i \neq y_i$.

A lattice animal is a finite connected subgraph of $\mathbb{Z}^d$ (some authors refer to these as bond animals). For each positive integer $N$, we define $A_N$ to be the set of all lattice animals in $\mathbb{Z}^d$ having exactly $N$ sites and whose lexicographically smallest site is the origin. Also, we define

$$a_N := |A_N|,$$

which is the number of bond animals in $\mathbb{Z}^d$ with $N$ sites, modulo translation.

Klarner (1967) proved rigorously that there is a finite number $\lambda$ such that

$$\lim_{N \to \infty} a_N^{1/N} = \lambda = \sup_{N \geq 1} a_N^{1/N}. \quad (3.1)$$

To prove that this limit exists, one uses the following concatenation argument. Fix positive integers $N$ and $M$. Consider any pair of animals $\alpha$ in $A_N$ and $\beta$ in $A_M$, and let $y[\alpha]$ be the lexicographically largest site of $\alpha$. Now translate $\beta$ by the vector $y[\alpha] + (1, 0, \ldots, 0)$; then its lexicographically smallest site is adjacent to the lexicographically largest site of $\alpha$, and the two animals lie on opposite sides of the hyperplane $x_1 = y[\alpha]_1 + 0.5$ (see Figure 1). We can join these two animals by adding the single bond from $y[\alpha]$ to $y[\alpha] + (1, 0, \ldots, 0)$, and the result is a lattice animal $\Psi$ in $A_N \times A_M$. No animal $\Psi$ in $A_N \times A_M$ can be produced in this way from more than one pair of initial animals $(\alpha, \beta)$ in $A_N \times A_M$, since there is a unique hyperplane of the form “$x_1 = \text{constant}$” that has $N$ sites of $\Psi$ on its left and $M$ sites on its right. This observation implies the supermultiplicative inequality

$$a_N a_M \leq a_{N+M} \quad (N, M \geq 1) \quad (3.2)$$

which in turn implies Equation (3.1) by a standard lemma (e.g., Lemma 1.2.2 in Madras and Slade 1993).

Note that the finiteness of $\lambda$ must be established by an independent argument.

The true asymptotic behaviour of $a_N$ is believed to be

$$a_N \sim C\lambda^N N^{-\theta} \quad \text{as } N \to \infty, \quad (3.3)$$

where $C$ and $\theta$ are positive constants.
where $C$ is a lattice-dependent constant and $\theta$ is a critical exponent—that is, $\theta$ depends only on the spatial dimension of the lattice. It is believed that $\theta$ equals 1 for $d = 2$, equals 1.5 for $d = 3$, and gradually increases with $d$ up to the value of 2.5 which holds for all dimensions greater than 8. These values are well understood from physical arguments, but little has been proven from the viewpoint of rigorous mathematics. Hara and Slade (1992) used the lace expansion to prove this scaling behaviour in high dimensions, but in general dimensions we cannot yet prove rigorously that $\theta$ exists. Some bounds have been proven rigorously:

(a) “$\theta \geq 0$”: The mathematically rigorous bound is actually $a_N \leq \lambda^N$ for all $N$, which follows immediately from the second equality in (3.1).

(b) “$\theta \leq 5/2$”: This inequality holds at the level of the generating function in any dimension, i.e.

$$\sum_{N=1}^{\infty} N^2 a_N z^N \geq \text{const.} \sum_{N=1}^{\infty} \lambda^N N^{-1/2} z^N \quad \text{as } z \rightarrow \lambda^{-1}$$

(due to Bovier, Fröhlich, and Glaus 1984, Tasaki and Hara 1987, Hara and Slade 1990).

(c) “$\theta \geq (d - 1)/d$”: The actual assertion is that there exists a constant $K$ such that

$$a_N \leq K \lambda^N N^{-(d-1)/d} \quad \text{for every } N \geq 1$$

(due to Madras 1995). A similar result holds for other families of lattice objects (including bond trees and site animals on other lattices; see Madras 1995).

The rest of this section will explain the main ideas behind the inequality (3.4) above.
Figure 2. Proof of inequality (3.4): For the animals $\alpha$ and $\beta$ of Figure 1, we show four different choices of $z$ and the four different $\Psi$’s that result. Notice that in the lower right case, we chose $u$ to be $z + (1, 1)$, but we could also have chosen $u$ to be $z + (1, 0)$, which would give a slightly different $\Psi$.

The key to the proof of (3.4) is a variation on the traditional concatenation argument that we used to establish the supermultiplicative inequality (3.2), which we now explain.

Consider a pair of animals $\alpha$ in $A_N$ and $\beta$ in $A_M$, as we did in the paragraph leading to (3.2). Pick a site $z = (z_1, z_2, \ldots, z_d)$ of $\alpha$, and consider all translations of the animal $\beta$ by vectors $(t, z_2, \ldots, z_d)$ where $t$ is an integer. Since $\beta$ contains the origin, we know that the translated $\beta$ intersects $\alpha$ when $t = z_1$ (in fact, they intersect at $z$). Let $t[z]$ be the largest integer for which the translated $\beta$ intersects $\alpha$, and let $u$ be a site at which they intersect. Now, translate $\beta$ by $(t[z] + 1, z_2, \ldots, z_d)$ and call the resulting animal $\beta^*$. Observe that $\alpha$ and $\beta^*$ are disjoint, that $u$ is a site of $\alpha$, and that $u + (1, 0, \ldots, 0)$ is a site of $\beta^*$. Let $\Psi$ be the union of $\alpha$, $\beta^*$, and the bond from $u$ to $u + (1, 0, \ldots, 0)$. Then $\Psi$ is in $A_{N+M}$. See Figure 2.

The above procedure describes how to obtain an animal $\Psi$ in $A_{N+M}$ from a given triple $(\alpha, \beta, \tilde{z})$, where $\alpha \in A_N$, $\beta \in A_M$, and $\tilde{z} = (z_2, \ldots, z_d) \in \Proj_1(\alpha)$. If it were always possible to reconstruct the triple uniquely from a given $\Psi$, then we would obtain the inequality

$$a_N a_M N^{(d-1)/d} \leq a_{N+M}.$$

The factor $N^{(d-1)/d}$ comes from averaging $\Proj_1(\alpha)$ over all rotations of $\alpha$, and applying Corollary 2 of the Loomis-Whitney inequality. Unfortunately, this reconstruction is not possible in general; that is, a given animal $\Psi$ could arise from several different triples $(\alpha, \beta, \tilde{z})$ for a given $N$ and $M$. See Figure 3 for an example.

Fortunately, the reconstruction is possible in the special case that $N = M$. This is due to a simple graph-theoretical result: A connected graph with $2N$ sites has at most one bond whose deletion produces two components with exactly $N$ vertices in each. Therefore it is true that

$$a_N^2 N^{(d-1)/d} \leq a_{2N}$$

for every $N \geq 1$. (3.5)

Now it just remains to do a bit of analysis. The inequality (3.5) implies that

$$\left( N^{(d-1)/d} a_N \right)^2 \leq (2N)^{(d-1)/d} a_{2N}$$

(3.6)
Figure 3. The animal $\Psi$ in (a) could arise from two different triples $(\alpha, \beta, \tilde{z})$ when $N = 9$ and $M = 4$, as illustrated in (b) and (c).

for every $N \geq 1$. Next, define

$$Q_n := n^{(d-1)/d} a_n \quad \text{for } n = 1, 2, \ldots$$

Then the inequality (3.6) says that

$$Q_N^2 \leq Q_{2N},$$

which we can rewrite as

$$Q_N^{1/N} \leq Q_{2N}^{1/2N}.$$  

Similarly, we have $Q_{2N}^{1/2N} \leq Q_{4N}^{1/4N}$, and so on. Therefore

$$Q_N^{1/N} \leq Q_{2N}^{1/2N} \leq Q_{4N}^{1/4N} \leq Q_{8N}^{1/8N} \leq \ldots; \quad (3.7)$$

thus we have found an increasing subsequence of the sequence $\{Q_n^{1/n}\}$. We know that

$$\lim_{n \to \infty} Q_n^{1/n} = \lim_{n \to \infty} a_n^{1/n} = \lambda$$

from Equation (3.1). Therefore $\lambda$ is an upper bound of the increasing subsequence in (3.7). In particular, we deduce that the first term of the subsequence is less than $\lambda$:

$$Q_N^{1/N} \leq \lambda.$$ 

Since $Q_N = N^{(d-1)/d} a_N$, we can rewrite the above inequality as

$$a_N \leq N^{-(d-1)/d} \lambda N,$$

which is the desired result that $\theta \geq (d-1)/d$. See Madras (1995) for more details.

4. Almost Unknotted Embeddings in the Cubic Lattice

In this section, we will use the notation $\approx_{\Exp}$ to relate two sequences which have the same leading exponential order in $n$; thus,

$$f_n \approx_{\Exp} g_n \quad \text{if and only if} \quad \lim_{n \to \infty} \left( \frac{f_n}{g_n} \right)^{1/n} = 1.$$  

Similarly, we define the notation $\geq_{\Exp}$ by

$$f_n \geq_{\Exp} g_n \quad \text{if and only if} \quad \liminf_{n \to \infty} \left( \frac{f_n}{g_n} \right)^{1/n} \geq 1,$$
Figure 4. Two “theta graphs”, (a) $\theta_{3,N}$ and (b) $\theta_{4,N}$, with $N = 5$.

and analogously for $\omega$.

For background, we begin by considering the $d$-dimensional hypercubic lattice $\mathbb{Z}^d$. For a positive integer $N$, an $N$-step self-avoiding walk is a sequence of $N + 1$ distinct lattice sites $(w[0], w[1], \ldots, w[N])$ such that $w[i]$ and $w[i + 1]$ are nearest neighbours for each $i = 0, \ldots, N - 1$. An $N$-step self-avoiding polygon is a set of $N$ distinct nearest-neighbour bonds in the lattice whose union is a simple closed curve (that is, a cycle with no self-intersections). Let $c_N$ (respectively, $p_N$) denote the number of $N$-step self-avoiding walks (respectively, polygons) in $\mathbb{Z}^d$ up to translation. It is well known that there exists a constant $\mu$ (depending on the lattice) such that

$$c_N \exp \approx \mu^N$$

and

$$p_N \exp \approx \mu^N$$

(Hammersley and Morton 1954, Hammersley 1961, Kesten 1963).

For the rest of this section, we shall consider properties related to knotting, so we restrict our discussion to the three-dimensional cubic lattice $\mathbb{Z}^3$. We shall use $\mu$ to denote the constant for self-avoiding walks in $\mathbb{Z}^3$.

Knots in long polymers are a problem of considerable theoretical and practical importance (Flapan 2000, Sauvage and Dietrich-Buchecker 1999, Sumners 1990). Let $p_N[0]$ denote the number of $N$-step self-avoiding polygons in $\mathbb{Z}^3$ (up to translation) that are unknotted. It has been proven rigorously that there is a constant $\mu_0$ such that

$$p_N[0] \exp \approx \mu_0^N$$

and that $\mu_0$ is strictly less than $\mu$ (Sumners and Whittington 1988, Pippenger 1989; see Section 8.4 of Madras and Slade 1993 for a brief discussion). This tells us that nontrivial knots are very common in long polymer loops.

We can view a self-avoiding polygon as an embedding of a loop in $\mathbb{Z}^3$. What about embeddings of other graphs? For simplicity, consider two “theta graphs”, $\theta_{3,N}$ and $\theta_{4,N}$, defined as follows. The graph $\theta_{k,N}$ consists of $kN$-step paths which all have the same initial site and the same final site but are otherwise disjoint (see Figure 4). Let $e(\theta_{k,N})$ denote the number of embeddings of $\theta_{k,N}$ in $\mathbb{Z}^3$. Thus, $e(\theta_{k,N})$ counts a special set of lattice animals, with $kN$ bonds and two vertices of degree $k$, that can be expressed as the union of $kN$-step self-avoiding walks that are mutually avoiding except at their endpoints. Corollary 2 of Soteros (1992) tells us that

$$e(\theta_{k,N}) \exp \approx \mu^{kN}$$

for $k = 3$ or 4.

Next, we define $e_0(\theta_{k,N})$ to be the number of embeddings of $\theta_{k,N}$ in $\mathbb{Z}^3$ such that no cycle is knotted. An embedding of a graph is said to be almost unknotted if the embedding is knotted, and if the deletion of any single bond will produce an unknotted embedding. Define $e_{AU}(\theta_{k,N})$ to be the number of almost
unknotted embeddings of $e(\theta_{k,N})$ in $\mathbb{Z}^3$. Clearly, if an embedding of $\theta_{3,N}$ or $\theta_{4,N}$ is almost unknotted, then no cycle can be knotted; hence
\[ e_{AU}(\theta_{k,N}) \leq e_0(\theta_{k,N}) \quad \text{for every } N. \tag{4.1} \]
The following result is intuitively plausible, but not as easy to prove as one might first guess.

**Theorem 3** (Madras, Sumners and Whittington, in preparation). For $k = 3, 4$, we have
\[ e_{AU}(\theta_{k,N}) \exp(\mu_0^N). \]

A construction due to Sumners and Whittington exhibits a large class of almost unknotted embeddings, and this leads to a bound in one direction, namely
\[ e_{AU}(\theta_{k,N}) \geq \mu_0^N \]
for $k = 3, 4$. The challenge that we shall take up here is how to prove the reverse inequality. In view of inequality (4.1), it will suffice to prove that
\[ e_0(\theta_{k,N}) \leq \mu_0^N . \tag{4.2} \]

First we observe that it is easy to prove the inequality (4.2) for $k = 4$. To do this, observe that we can express any embedding of $\theta_{4,N}$ as the union of two $2N$-step self-avoiding polygons whose intersection is a set of precisely two vertices. Moreover, if every cycle of the embedding is unknotted, then these two self-avoiding polygons must be unknotted. Therefore
\[ e_0(\theta_{4,N}) \leq (p_{2N}[0])^2 \exp(\mu_0^{2N})^2; \]
which proves the inequality (4.2) for $k = 4$.

This simple method does not work for $k = 3$. We can decompose $\theta_{3,N}$ into a $2N$-step self-avoiding polygon and an $N$-step self-avoiding walk, but since the walk is not a loop we cannot really talk about it being unknotted. In particular, this only leads to the bound $e_0(\theta_{3,N}) \leq \mu_0^{2N} \mu_0^N$, which is inadequate. Alternatively, we can express $\theta_{3,N}$ as the union of three overlapping $2N$-step unknotted self-avoiding polygons. It turns out that the Loomis-Whitney inequality is exactly what makes this alternative approach work.

We now prove inequality (4.2) for $k = 3$. Fix $N$, and let $M = e_N$. Consider a list $\omega^1, \ldots, \omega^M$ of all $N$-step self-avoiding walks in $\mathbb{Z}^3$ that start at the origin. Now define the set $S$ to be the set of all ordered triples $(i, j, k)$ in $\{1, \ldots, M\}^3$ with the property that $\omega^i \cup \omega^j \cup \omega^k$ is an embedding of $\theta_{3,N}$ with no knotted cycle. Then
\[ |S| = e_0(\theta_{3,N}) \times 3! \times 2 \tag{4.3} \]
(the factor $3!$ comes from the number of permutations of $(i, j, k)$, and the factor 2 arises because each embedding of $\theta_{3,N}$ has two vertices which could serve as the origin).

Now consider the projections of the set $S$. For example, $\text{Proj}_{1}(S)$ is the set of all ordered pairs $(j, k)$ in $\{1, \ldots, M\}^2$ for which there exists an $i$ having the property that $\omega^i \cup \omega^j \cup \omega^k$ is an embedding of $\theta_{3,N}$ with no knotted cycle. In particular, if $(j, k)$ is in $\text{Proj}_{1}(S)$, then $\omega^j \cup \omega^j \cup \omega^k$ must form an unknotted cycle (i.e., an unknotted self-avoiding polygon). Any unknotted $2N$-step self-avoiding polygon corresponds to $4N$ such pairs $(j, k)$ [this is because there are $2N$ choices for the origin, and because $(k, j)$ determines the same polygon as $(j, k)$]. Therefore
\[ |\text{Proj}_{1}(S)| \leq 4N p_{2N}[0] \exp(\mu_0^{2N}) \tag{4.4} \]
and similarly for the other two projections. Finally, we use the Loomis-Whitney inequality:

\[
12^2 e_0(\theta_{3,N})^2 = |S|^{3-1} \leq \prod_{t=1}^3 |\text{Proj}_t(S)| \leq \text{Exp} \leq (\mu_0 N)^3
\]

[by (4.3)] [Loomis-Whitney] [by (4.4)].

This shows that the inequality (4.2) holds for \( k = 3 \).

This method can be generalized beyond theta graphs to prove that \( \mu_0 \) is the growth constant for any (topological) graph that has an almost unknotted embedding in \( \mathbb{Z}^3 \) and no cut edge (Madras, Sumners and Whittington, in preparation).

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