

BOUNDS ON THE SELF-AVOIDING-WALK CONNECTIVE CONSTANT

by Gordon SLADE

This lecture reviews the current status of upper and lower bounds on the connective constant for self-avoiding walks on the hypercubic lattice \mathbf{Z}^d , for dimensions $d \geq 2$.

1 Introduction

An n -step *self-avoiding walk* on the d -dimensional hypercubic lattice \mathbf{Z}^d is an ordered set $\omega = (\omega(0), \omega(1), \dots, \omega(n))$, with each $\omega(i) \in \mathbf{Z}^d$, $|\omega(i+1) - \omega(i)| = 1$ for all i (Euclidean distance), and $\omega(i) \neq \omega(j)$ for $i \neq j$. Let c_n denote the number of n -step self-avoiding walks with $\omega(0) = 0$. It is clear that $c_{n+m} \leq c_n c_m$, and hence the sequence $\{\log c_n\}$ is subadditive. From this it follows that the limit $\mu \equiv \lim_{n \rightarrow \infty} c_n^{1/n}$ exists, and that $c_n \geq \mu^n$ for all n . This limit μ is known as the *connective constant*, and was first noted to exist in [14].

In fact it is believed that $c_n \sim A\mu^n n^{\gamma-1}$ as $n \rightarrow \infty$, with γ a *universal* critical exponent. “Universal” means dependent only on the spatial dimension and not on other details of the walk’s definition; for example γ is believed to be the same for self-avoiding walks on all two-dimensional lattices such as the square lattice or the triangular lattice. By contrast μ , being roughly a measure of the average number of possible next steps available for a long self-avoiding walk, is not a universal quantity. Because of this lack of universality, the connective constant has received less attention in the literature than the

critical exponents, but nevertheless the determination of the value of μ has been a question considered by many authors since the earliest mathematical work on self-avoiding walks.

The author's own interest in bounds on μ was aroused in the course of joint work with Takashi Hara [16, 15], in which a computer-assisted proof of existence of critical exponents for the self-avoiding walk in dimensions $d \geq 5$ required accurate numerical lower bounds on μ . We developed a new method for obtaining such bounds [15, Appendix A], based on loop-erasure and restoration, which was further extended in collaboration with Alan Sokal [18], and which is described below. It gives the current best lower bounds in dimensions $d \geq 3$. For $d = 2$ the best lower bound is due to Conway and Guttmann [3] and makes use of extensive walk enumerations; it also is described below. The best upper bounds on μ are due to Alm [1], and are described in the final section. These bounds also make use of enumeration data.

The precise value of μ is of course not known in any dimension $d \geq 2$ ($\mu = 1$ for the trivial case of $d = 1$). Early guesses that in two dimensions μ equals $1 + \sqrt{2} = 2.4142\dots$ or $e = 2.7182\dots$ have been ruled out by the rigorous bounds. There is one exception where μ is believed to be known exactly: for the 2-dimensional hexagonal (also called the honeycomb) lattice there is strong evidence [24], but as yet no proof, that $\mu = \sqrt{2 + \sqrt{2}}$.

The simplest bounds on μ are $d \leq \mu \leq 2d - 1$. This follows from the bounds $d^n \leq c_n \leq (2d)(2d-1)^{n-1}$, which themselves follow by counting walks which only take steps in positive coordinate directions (for the lower bound), and by counting walks having no steps which reverse their predecessor (the upper bound). Table 1 gives the current status of improvements to these simple bounds, for dimensions two through six. Table 1 also gives estimates of the precise value of μ , which have been obtained from series extrapolation methods: values of c_n are enumerated on a computer for n as large as is feasible, and then μ is estimated from this data. For $d = 2$ the current world record [2] is $c_{39} = 113\,101\,676\,587\,853\,932$, but larger values of n are likely in the near future. For $d = 3$ the record [11] is $c_{21} = 235\,710\,090\,502\,158$.

d	lower bound	estimate	upper bound
2	2.620 02 ^a	2.638 158 5 (10) ^d	2.695 76 ^b
3	4.572 140 ^c	4.683 907 (22) ^e	4.756 ^b
4	6.742 945 ^c	6.772 0 (5) ^f	6.832 ^b
5	8.828 529 ^c	8.838 6 (8) ^g	8.881 ^b
6	10.874 038 ^c	10.878 8 (9) ^g	10.903 ^b

Table 1: Rigorous lower and upper bounds on the connective constant μ , together with estimates of actual values, for dimensions 2,3,4,5,6. Estimated errors in the last digit(s) are shown in parentheses. References: a) [3], b) [1], c) [18], d) [12, 2], e) [7], f) [8], g) [9].

2 Lower bounds

Section 2.1 below describes the $d = 2$ Conway-Guttmann lower bound of Table 1, which is obtained using walk enumerations combined with a method due to Kesten [19]. This method works in all dimensions, but sufficient enumerations for good bounds have been done only for $d = 2$. Section 2.2 describes the Hara-Slade-Sokal lower bounds, which are based on loop-erasure and do not use enumeration data; this method gives good results in dimensions $d \geq 3$.

2.1 The irreducible-bridge method

Given a walk ω we denote the components of a site $\omega(i) \in \mathbf{Z}^d$ by $(\omega_1(i), \dots, \omega_d(i))$. An n -step *bridge* in \mathbf{Z}^d is an n -step self-avoiding walk ω with $\omega(0) = 0$, $\omega(1) = (1, 0, \dots, 0)$, and $1 \leq \omega_1(i) \leq \omega_1(n)$ for all $i = 1, \dots, n$. Let b_n denote the number of n -step bridges for $n \geq 1$, and set $b_0 = 1$. An n -step *irreducible bridge* is an n -step bridge which cannot be broken into an m -step and an $(n - m)$ -step subwalk (with $m \neq 0, n$) such that each subwalk is itself a bridge (or a translate of a bridge). Let i_n denote the number of n -step irreducible bridges. These counts satisfy the renewal equation

$$b_n = \delta_{n,0} + \sum_{k=1}^n i_k b_{n-k}. \quad (2.1)$$

We define for $z \geq 0$ the generating functions

$$B(z) = \sum_{n=0}^{\infty} b_n z^n \quad (2.2)$$

$$I(z) = \sum_{n=1}^{\infty} i_n z^n. \quad (2.3)$$

It is known that $B(z)$ and $I(z)$ both have radius of convergence equal to μ^{-1} , with $\lim_{z \nearrow \mu^{-1}} B(z) = \infty$ (see [22] for proofs and references to the original literature). Hence it follows from (2.1) that

$$B(z) = \frac{1}{1 - I(z)} \quad \text{for } z \leq \mu^{-1}, \quad (2.4)$$

with

$$I(\mu^{-1}) = \sum_{n=1}^{\infty} i_n \mu^{-n} = 1. \quad (2.5)$$

Suppose now that we have a sequence l_n of nonnegative lower bounds for i_n , *i.e.*, $0 \leq l_n \leq i_n$ for all $n \geq 1$, and define

$$L(z) = \sum_{n=1}^{\infty} l_n z^n. \quad (2.6)$$

Both L and I are increasing, and $L(z) \leq I(z)$. It follows that the root z^* of the equation $L(z^*) = 1$ obeys $z^* \geq \mu^{-1}$ and hence gives a lower bound for μ :

$$\mu \geq \frac{1}{z^*}. \quad (2.7)$$

This method is due to Kesten [19].

In two dimensions, Conway and Guttmann used (2.7) with $l_n = i_n$ for $n \leq 40$; l_n equal to a good lower bound on i_n for $41 \leq n \leq 124$; and $l_n = 0$ for $n \geq 125$. With this highly nontrivial enumeration done, the resulting bound $\mu \geq 2.62$ is within 0.7% of the best numerical estimate. Details of the method of enumeration can be found in [3].

2.2 The loop-erasure method

The loop-erasure method has several refinements, and here the focus will be on the simplest version. The description closely follows [18].

First some notation is needed. Let $\Omega(x, y)$ denote the set of all self-avoiding walks of any length (including zero if $x = y$) which begin at x and end at y . Let $\Omega_0(x, y)$ denote the corresponding set of simple random walks. We denote the *two-point function* or *Green function* for self-avoiding walks by

$$G(x, y; z) = \sum_{\omega \in \Omega(x, y)} z^{|\omega|}, \quad (2.8)$$

where $|\omega|$ denotes the length of ω and z is a nonnegative parameter. This series converges when $z < \mu^{-1}$, and is known to diverge when $z > \mu^{-1}$ [13]. The *susceptibility*

$$\chi(z) = \sum_{x \in \mathbf{Z}^d} G(0, x; z) = \sum_{n=0}^{\infty} c_n z^n \quad (2.9)$$

also has radius of convergence μ^{-1} . Given a set of sites $A \subset \mathbf{Z}^d$, the simple random walk Green function is given by

$$C^A(x, y; z) = \sum_{\omega \in \Omega_0(x, y): \omega \cap A = \emptyset} z^{|\omega|}. \quad (2.10)$$

If A is the empty set then it will be omitted as a superscript. The series converges for $z \leq 1/2d$ when $A = \emptyset$ and $d > 2$, and converges for $z \leq 1/2d$ in all dimensions $d > 0$ if A is nonempty. The simple random walk susceptibility is given by

$$\chi_0(z) = \sum_{x \in \mathbf{Z}^d} C(0, x; z) = \frac{1}{1 - 2dz}. \quad (2.11)$$

A relationship between the self-avoiding walk and simple random walk Green functions can be derived using a loop-erasure algorithm which has been studied extensively by Lawler [21]. Given a walk $\omega \in \Omega_0(x, y)$, the algorithm associates to ω a self-avoiding walk $\rho \in \Omega(x, y)$ by erasing loops chronologically, as follows. Let t_1 be the *last* time such that $\omega(t_1) = \omega(0) = x$, and then replace the loop $L_0 = (\omega(0), \omega(1), \dots, \omega(t_1))$ by the single site $\omega(0)$, producing a new walk $\rho^{(1)} \in \Omega(x, y)$. In other words we have erased the largest possible loop at the site x . (If $t_1 = 0$ then we have erased nothing.) The walk $\rho^{(1)}$ visits x exactly once, but it may visit the site $\rho^{(1)}(1)$ repeatedly.

Let t_2 denote the *last* time that $\rho^{(1)}(t_2) = \rho^{(1)}(1)$, and replace the loop $L_1 = (\rho^{(1)}(1), \dots, \rho^{(1)}(t_2))$ by the single site $\rho^{(1)}(1)$ as before. Note that the erased loop L_1 cannot pass through $\omega(0) = x$. This procedure gives rise to a walk $\rho^{(2)}$, which visits each of $\rho^{(2)}(0)$ and $\rho^{(2)}(1)$ exactly once. Repeating this procedure by removing loops successively yields a result which is devoid of loops, or in other words which is self-avoiding.

This defines a mapping from $\Omega_0(x, y)$ into the set $\mathcal{R}(x, y)$ whose elements are of the form $(\rho, L_0, L_1, \dots, L_n)$, where $\rho \in \Omega(x, y)$ is an n -step self-avoiding walk (for some n) and each $L_i \in \Omega_0(\rho(i), \rho(i))$ corresponds to an erased loop. We refer to ρ as the self-avoiding *backbone* of ω . In fact this mapping is a bijection between $\Omega_0(x, y)$ and the subset of $\mathcal{R}(x, y)$ for which the loop L_i attached at $\rho(i)$ does not intersect any of the previous backbone sites $\rho(0), \dots, \rho(i-1)$, for all $i = 1, \dots, |\rho|$.

Let $\rho[0, j]$ denote the set of sites $\{\rho(0), \dots, \rho(j-1)\}$, for $j = 1, \dots, |\omega|$, and let $\rho[0, 0)$ be the empty set. In view of the above bijection,

$$C(x, y; z) = \sum_{\rho \in \Omega(x, y)} z^{|\rho|} \prod_{j=0}^{|\rho|} C_0^{\rho[0, j]}(\rho(j), \rho(j); z). \quad (2.12)$$

An upper bound on (2.12) can be obtained by relaxing the avoidance constraints on the attached loops. We do this by replacing the restriction that the loop attached at $\rho(j)$ avoid all of $\rho[0, j]$ by the weaker restriction that it avoid only the smaller set

$$\rho[j-k, j] \equiv \{\rho(j-k), \dots, \rho(j-1)\}, \quad (2.13)$$

where k is a (small) fixed nonnegative integer. [For $k = 0$, $\rho[j, j] = \emptyset$; and for $k > j$ we omit the nonexistent points $\rho(i)$ with $i < 0$.] This gives the inequality

$$C(x, y; z) \leq \sum_{\rho \in \Omega(x, y)} z^{|\rho|} \prod_{j=0}^{|\rho|} C^{\rho[j-k, j]}(\rho(j), \rho(j); z). \quad (2.14)$$

For $j \geq k$, the set of sites $\rho[j-k, j]$ is the range of a $(k-1)$ -step self-avoiding walk starting at a nearest neighbour of $\rho(j)$, so a further upper bound follows by taking the maximum over all such sets. Taking into account translation invariance, this leads us to define

$$\Lambda(k; z) = \max_A C^A(0, 0; z), \quad (2.15)$$

where the maximum ranges over all k -element sets A which are the range of a $(k-1)$ -step self-avoiding walk starting at a nearest neighbour of the origin. Then we have

$$\begin{aligned} C(x, y; z) &\leq \sum_{\rho \in \Omega(x, y)} z^{|\rho|} \Lambda(0; z) \Lambda(1; z) \cdots \Lambda(k-1; z) \Lambda(k; z)^{|\rho|+1-k} \\ &\equiv \alpha_k(z) G(x, y; z \Lambda(k; z)) , \end{aligned} \quad (2.16)$$

where

$$\alpha_k(z) \equiv \left[\prod_{i=0}^{k-1} \Lambda(i; z) \right] \Lambda(k; z)^{1-k} . \quad (2.17)$$

Summing over $y \in \mathbf{Z}^d$, this gives the basic loop-erasure-and-restoration inequality

$$\frac{\chi_0(z)}{\alpha_k(z)} \leq \chi(z \Lambda(k; z)) . \quad (2.18)$$

Elementary facts about simple random walk imply that

$$\lim_{z \uparrow (2d)^{-1}} \frac{\chi_0(z)}{\alpha_k(z)} = \infty \quad (2.19)$$

for all $k \geq 0$ and all $d > 0$; this is simplest in dimensions $d > 2$ since the denominator on the left side remains bounded away from zero and infinity in the limit. From this, it is now easy to obtain a lower bound on μ . By (2.19) and (2.18), $\chi((2d)^{-1} \Lambda(k; (2d)^{-1})) = +\infty$. Since $\chi(x) < \infty$ for $x < 1/\mu$, we have

$$\frac{\Lambda(k; (2d)^{-1})}{2d} \geq \frac{1}{\mu} , \quad (2.20)$$

or in other words

$$\mu \geq \frac{2d}{\Lambda(k; (2d)^{-1})} \quad \text{for } k \geq 0, d > 0 . \quad (2.21)$$

The $k = 0$ version of this bound is not new: it is an immediate consequence of combined results of Fisher [4] and of Fröhlich, Simon and Spencer [6], and was also proved by Lawler [20] for $d > 4$ using loop erasure in a different way.

With $k = 1$, (2.21) gives the exact answer $\mu \geq 1$ in the trivial case $d = 1$. For $d = 2$ and $k = 1$, it gives the rather poor bound $\mu \geq 2$. For

$d = 3$ and $k = 1$, it already does better than all previously known bounds, yielding $\mu \geq 4.4758$. This improves the bound $\mu \geq 4.352$ obtained using the irreducible-bridge method with $l_n = i_n$ for $n \leq 11$ and $l_n = 0$ otherwise [10].

The evaluation of the lower bound (2.21) requires calculation of the denominator. This involves special difficulties for $d = 2$, so we restrict attention in the following to $d > 2$. In this case, for $k = 0$ the denominator of (2.21) is simply $C(0, 0; 1/2d)$, for which there is an integral representation

$$C(x, y; 1/2d) = \int_{[-\pi, \pi]^d} \frac{e^{ik \cdot (x-y)}}{1 - d^{-1} \sum_{j=1}^d \cos k_j} \frac{d^d k}{(2\pi)^d}. \quad (2.22)$$

This integral can be transformed into a 1-dimensional integral of modified Bessel functions, and then accurately evaluated numerically using the methods of [15, Appendix B]. Larger values of k (we used $k \leq 4$) can then be handled using the recursion (for $b \notin A$)

$$C^{A \cup \{b\}}(x, y; z) = C^A(x, y; z) - \frac{C^A(x, b; z)C^A(b, y; z)}{C^A(b, b; z)}. \quad (2.23)$$

The maximum in (2.15) is computed by evaluating the right side for all possible configurations of A , making the obvious use of symmetry. The optimization problem of predicting which set A gives the maximum for fixed $|A| = k$ appears to be difficult.

Improvements to the results described above were obtained by using the loop-erasure algorithm in conjunction with memory-2 walk rather than simple random walk. Memory-2 walk is obtained by putting the uniform measure on the set of n -step simple random walks having no immediate reversals, which means that $\omega(i+2) \neq \omega(i)$ for all i . The above analysis can be extended to memory-2 walks, with some changes, and leads to improved bounds. This involves evaluation of the memory-2 Green function, which can be reduced to the integrals (2.22). Some further improvements can be obtained by partially recovering losses suffered when the maximum over A is taken in deriving (2.16), yielding the $d \geq 3$ lower bounds of Table 1. Details can be found in [18].

For $d = 2$ the method produces the very weak bound $\mu \geq 2.3057$. The bounds improve as the dimension increases; in fact as $d \rightarrow \infty$ the best of the lower bounds has $1/d$ behaviour given by the right side of

$$\mu \geq 2d - 1 - \frac{1}{2d} - \frac{3}{(2d)^2} - \frac{18}{(2d)^3} - \frac{122}{(2d)^4} + O(d^{-5}). \quad (2.24)$$

This compares well with the expansion

$$\mu = 2d - 1 - \frac{1}{2d} - \frac{3}{(2d)^2} - \frac{16}{(2d)^3} - \frac{102}{(2d)^4} + O(d^{-5}) \quad (2.25)$$

(see [5, 23], and [17] for the error term).

3 Upper bounds

This section briefly describes Alm's method [1] for obtaining upper bounds on μ . The basic idea is to take the limiting value of the n -th root of a sequence of upper bounds on c_n . To formulate these bounds some notation is needed.

Given positive integers $r < s$, and a list of all possible r -step self-avoiding walks $\gamma^{(1)}, \dots, \gamma^{(c_r)}$, let $g_{i,j}(r, s)$ denote the number of s -step self-avoiding walks whose first r steps are given by $\gamma^{(i)}$ and whose last r steps are given by $\gamma^{(j)}$. Let $G(r, s)$ denote the $c_r \times c_r$ matrix whose elements are the $g_{i,j}(r, s)$. Because of the potential for trapping, there are values of i, j, r, s for which zero matrix entries arise. This can be overcome by taking s large compared to r , and by discarding any r -step walks which inherently give rise to trapping. This leads to a possibly smaller matrix with strictly positive entries; for simplicity the notation $G(r, s)$ will still be used to denote this diminished matrix. By the Perron-Frobenius theorem, the eigenvalue of $G(r, s)$ having largest magnitude is simple and positive. Denote this eigenvalue by $\lambda_1 = \lambda_1(r, s)$. Alm's method is then based on the fact that

$$\mu \leq [\lambda_1(r, s)]^{1/(s-r)}; \quad (3.1)$$

the proof of this inequality is discussed below.

To prove (3.1), first note that given two s -step self-avoiding walks, one beginning with $\gamma^{(i)}$ and ending with $\gamma^{(k)}$, and another beginning with $\gamma^{(k)}$ and ending with $\gamma^{(j)}$, these walks can be joined, with an overlap of r steps, to form an $[r + 2(s - r)]$ -step walk. All possible self-avoiding walks of this length can be formed in this way, so

$$g_{i,j}(r, r + 2(s - r)) \leq \sum_k g_{i,k}(r, s) g_{k,j}(r, s) = [G^2(r, s)]_{i,j}. \quad (3.2)$$

Repetition of this argument gives

$$g_{i,j}(r, r + m(s - r)) \leq [G^m(r, s)]_{i,j}. \quad (3.3)$$

For a positive matrix A with entries $a_{i,j}$, we will use the norm $\|A\| = \sum_{i,j} a_{i,j}$. Then $\|G(r, s)\| = c_s$. By (3.3),

$$c_{r+m(s-r)} = \|G(r, r + m(s-r))\| \leq \|G^m(r, s)\| \quad (3.4)$$

and hence

$$\begin{aligned} \mu &= \lim_{m \rightarrow \infty} \|G(r, r + m(s-r))\|^{1/[r+m(s-r)]} \\ &\leq \lim_{m \rightarrow \infty} \|G^m(r, s)\|^{1/[r+m(s-r)]} = [\lambda_1(r, s)]^{1/(s-r)}, \end{aligned} \quad (3.5)$$

where the fact that λ_1 is the largest eigenvalue was used in the last step. This proves (3.1).

Alm computes $\lambda_1(r, s)$ numerically, and observes that $[\lambda_1(r, s)]^{1/(s-r)}$ is decreasing (and hence gives improved bounds) as a function of r and s with $r < s$, and conjectures that this is always the case. The special case $r = 0$ of this conjecture says that $c_s^{1/s}$ is decreasing; this has not been proved. According to the conjecture the best bounds are obtained by taking r and s as large as possible, but this is balanced practically by the exponentially increasing size of the matrix $G(r, s)$ as r increases and the increase in the amount of enumeration data needed as s increases.

Symmetry can be used to reduce dramatically the size of the matrix G , and this is discussed in [1]. The $d = 2$ upper bound is obtained using $s = 24$ and $r = 8$; taking advantage of symmetry reduces the size of the matrix from $c_8 \times c_8 = 5916 \times 5916$ to 740×740 . Smaller matrices and less extensive enumerations are used in higher dimensions.

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