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Bounds on connective constants for self-avoiding walks

A J Guttmann

Department of Mathematics, Statistics and Computer Science, The University of Newcastle, NSW 2308, Australia

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Abstract. New lower bounds on the connective constant of the square and simple cubic lattice self-avoiding walks are obtained, by enumerating a particular subset of self-avoiding walks and using a result of Kesten. We find $\mu(\text{sq}) > 2.5680$ and $\mu(\text{SC}) > 4.352$.

1. Introduction

The improvement of numerical bounds on the connective constant of self-avoiding random walks (SAWS) on lattices has taken place in a sequence of steps of about ten years' duration. The earliest substantive effort recorded in the literature appears to be the work of Wakefield (1951), who obtained upper and lower bounds for SAWS on the square and tetrahedral lattices.

In 1959 Fisher and Sykes obtained very good estimates for upper and lower bounds on a range of two- and three-dimensional lattices. Indeed, their lower bounds, obtained without the aid of a computer, are still the best extant for many lattices. The important theoretical work of Kesten (1963) subsequently allowed Beyer and Wells (1972) to improve on Fisher and Sykes' lower bound in the case of the square lattice, though as we shall show, their derivation appears to be flawed. In 1976 Wall and White computerised the method of finding upper bounds introduced by Wakefield, and confirmed some of Fisher and Sykes's results on the square lattice, though the hand calculations of Fisher and Sykes went further! Wall and White also confirmed and extended Wakefield's (1951) upper bound on the connective constant of the tetrahedral lattice.

More recently, Ahlberg and Janson (1982) have introduced a new method for obtaining upper bounds which, while it does not improve on Fisher and Sykes' results for the square lattice, does give the best current upper bound for the triangular, honeycomb, simple cubic (SC), body-centred cubit (BCC) and face-centred cubic (FCC) lattices.

In this paper we present new and improved lower bounds for the connective constant of the square and simple cubic lattices, using a method based on a result of Kesten (1963).

In § 2 we review the methods that have been used to obtain bounds, and in § 3 we develop and apply enumerations necessary to utilise Kesten's method.

2. Methods of establishing bounds

A SAW of n steps on a regular, infinite, lattice is a non-cyclic continuous path connecting $n+1$ vertices of the lattice. Let c_n denote the numbers of n-step SAWs per lattice site, so that c_1 is just the coordination number of the lattice. Hammersley and Morton (1954) have proved that $\lim_{n\to\infty}(1/n)\ln c_n = \inf_{n>0}(1/n)\ln c_n$ exists and is greater than zero. This limit is called the connective constant, is usually denoted μ, and represents the average number of choices that can be made at each step by an infinitely long walk. The stronger result that $\lim_{n\to\infty} c_{n+2}/c_n = \mu^2$ was proved by Kesten (1963) for the hypercubic lattice. The best available result for the rate of approach to the limit is that of Hammersley and Welsh (1962) who proved that $c_n = \mu^n \exp(\mathrm{O}(\sqrt{n}))$. It is widely believed, and supported by an overwhelming weight of numerical evidence and heuristic argument, that $c_n = \mu^n \exp(\mathrm{O}(\log n))$, but this result has resisted all attempts at its proof. For a fuller discussion see Whittington (1982).

The method first used by Wakefield (1951) and subsequently by Fisher and Sykes (1959) and Wall and White (1976) to obtain upper bounds proceeds by determining the number of restricted n-step random walks $b_n^{(r)}$, which are random walks that are only permitted cycles of at least r steps. Thus by inspection $b_n^{(r)} \geq c_n$ for all $r<\infty$, while $\lim_{r\to\infty} b_n^{(r)}/c_n = \inf_{r>0} b_n^{(r)}/c_n = 1$. The determination of the analogous connective constant ν_r for the random walks $b_n^{(r)}$ is then a Markovian problem which can be solved for low values of r. As shown by Fisher and Sykes, $\nu_r \geq \mu$, and upper bounds are thereby obtained by calculating ν_r for $r=2,3,4,\ldots$. Unfortunately, the difficulty of evaluating ν_r increases rapidly with increasing values of r, and it is this limitation which prevents bounds being arbitrarily sharpened. By employing a clever numerical procedure, Fisher and Sykes were able to obtain ν_r for $r=2(2)12$ for the square lattice. Their result $\mu \leq \nu_{12} = 2.712$ disproved a conjecture of Lehman and Weiss (1958) that $\mu = \mathrm{e} = 2.718\,28\ldots$. Subsequently Beyer and Wells (1972) expressed doubts as to the reliability of the numerical technique employed by Fisher and Sykes, but since then Wall and White (1976) confirmed all Fisher and Sykes's results up to ν_{10}, at which point they stopped. There appears no reason to doubt the correctness of the result for ν_{12} therefore.

In order to obtain lower bounds, Fisher and Sykes considered a sequence of proper subsets of SAWs. For fixed n the sequence has increasing cardinality. For the square lattice the sequence was generated by first restricting steps in the x direction to being only in the positive x direction, and then effectively allowing an increasing number of steps in the negative x direction, restricted to ensure that the SAW property was not violated. Then, having proved a lemma that the analogous connective constant $\lambda_r \leq \mu$, where r is the size of the 'backward' portion of the walk, evaluation of λ_r for increasing values of r provided a sequence of lower bounds. In this way the bound $2.577 \leq \mu$ was obtained for the square lattice, disproving a conjecture of Temperley (1956) that $\mu = \sqrt{2}+1$. Beyer and Wells (1972) point out that this lower bound is not correct due to minor numerical errors. After correction, the best bound obtained was $\mu \geq 2.542$.

A more systematic approach to lower bounds was given by Kesten (1963), on which both this work and that of Beyer and Wells (1972) is based. In order to discuss this method, it is necessary to introduce three proper subsets of the set of SAWs. For ease of visualisation we restrict the discussion to the square lattice, though the argument applies directly to the general d-dimensional hypercubic lattice. Consider a cartesian coordinate system at the origin of the walk, with axes parallel to the lattice axes, and calibrated in units of a lattice spacing. Then we define terminally attached walks (TAWS) as SAWS whose first step is along the positive x axis, and which subsequently never have x coordinate less than 1. That is, after the first step, the walk is confined to lie on the right of the y axis. We denote the cardinality of n-step TAWS by t_n, and clearly $t_n < c_n$ for $n > 0$. The next class of walks we consider are called bridges. Let $x_{\max}$ denote the (not necessarily unique) maximal x coordinate of an n-step TAW. If the x coordinate of the $(n+1)$th vertex (i.e. the last vertex) is equal to $x_{\max}$, then this TAW is a bridge. Denoting the cardinality of n-step bridges by b_n, it is clear that $b_n \leqslant t_n$. Finally, we define the class of irreducible bridges as those bridges which cannot be decomposed into two concatenated bridges, and denote the class of irreducible bridges by s_n.

Kesten proved the important lemma

$$b_n = \sum_{k=1}^{n} s_k b_{n-k}, \qquad n \geqslant 1. \tag{2.1}$$

If one defines the bridge and irreducible bridge generating functions, $B(x)$ and $S(x)$ respectively, by $B(x) = \Sigma_{n \geqslant 0} b_n x^n$ and $S(x) = \Sigma_{n \geqslant 1} s_n x^n$, it follows from the above lemma that $B(x) = 1/[1 - S(x)]$. Now since the TAWS, bridges and irreducible bridges all have the same connective constant as the SAWS on the same lattice, Kesten observed that if μ_N is the (unique) positive solution of the equation

$$\sum_{n=1}^{N} s_n \mu_N^{-n} = 1. \tag{2.2}$$

then $\mu_N \leqslant \mu$.

Thus enumeration of irreducible bridges allows a monotonic non-decreasing sequence of lower bounds on μ to be obtained, by solving the sequence of polynomial equations given by (2.2) with increasing N, and is the approach used in this paper.

The earlier calculation of Beyer and Wells (1972) also made use of Kesten's result, but in a less direct manner. From (2.1) Kesten showed that $1/\mu$ is a singular point of the bridge generating function $B(x)$, so that the equation $1/B(x) = (\Sigma_{n \geqslant 0} b_n x^n)^{-1} = 0$ has $x_c = 1/\mu$ as a root. Beyer and Wells point out that the equation $1/\tilde{B}(x) = (\Sigma_{n \geqslant 0} \tilde{b}_n x^n)^{-1} = 0$, with $0 \leqslant \tilde{b}_n \leqslant b_n$, has as its root $\tilde{x}_c \geqslant x_c = 1/\mu$, so that $1/\tilde{x}_c$ provides a lower bound to μ. They then express the function $\tilde{B}(x)$ as the ratio of two polynomials, so that $1/\tilde{B}(x) = 0$ corresponds to a zero of the denominator polynomial. In order to evaluate the polynomial coefficients, certain subclasses of TAWS are enumerated. Their denominator polynomial is of the form $1 - \Sigma_{n \geqslant 0} a_n c^n$, where all the a_n's that have been evaluated (up to a_{20}) are non-negative. A necessary and sufficient condition for the validity of their approach is that $a_n \geqslant 0$ for all $n > 0$, and this question is not addressed. Apart from this objection in principle, errors in their enumeration have also been detected, so that, for example, their function $\phi^2(x)$ deviates from its definition at $O(x^6)$. One is therefore forced to conclude that their work does not provide a reliable bound.

The method proposed by Ahlberg and Janson requires the retention of detailed configurational information, so that the set of n-step walks must be classified into a number of disjoint subsets, and they demonstrate this approach in the case of the square lattice. If this detailed configurational information is *not* available, they prove that an upper bound is given by $\min(\mu_a, \mu_b)$ where $\mu_a = (c_n/c_1)^{1/n-1}$ and μ_b is the positive root of

$$qx^{n-1} = [c_n - (q-2)c_{n-1}]x + (q-2)[(q-1)c_{n-1} - c_n], \qquad n > 2, \quad (3.1)$$

where $q = c_1$ is the coordination number of the lattice. This result allows them to obtain the best available upper bounds for all common lattices except the square lattice, for which the result of Fisher and Sykes is still the best.

In § 3 we describe the method whereby we have obtained the best current lower bounds for the square and simple cubic lattice connective constants.

3. Derivation of lower bounds

In order to use Kesten's result (2.2), it is clear that enumeration of irreducible bridges is required. The topological constraint imposed by the definition of irreducibility is difficult to incorporate into an enumeration program. However, by using Kesten's lemma (2.1), one need only enumerate all bridges, and then determine the number of irreducible bridges from (2.1).

A Fortran program was written that generated all TAWS, making use of obvious symmetries, and then tested to see which TAWS were bridges. The exponential complexity of the problem means that the time required to enumerate TAWS at each order rapidly limits the viability of the computation, while the non-Markovian nature of the problem, which requires that all TAWS of length n be stored in order to generate

Table 1. Coefficients of the bridge and irreducible bridge generating functions for the square and simple cubic lattices.

	Square lattice		Simple cubic	
n	b_n	s_n	b_n	s_n
0	1		1	
1	1	1	1	1
2	3	2	5	4
3	7	2	21	12
4	17	2	89	36
5	41	2	381	112
6	101	4	1 673	392
7	251	10	7 401	1 428
8	631	26	32 989	5 380
9	1 591	56	147 077	19 972
10	4 029	118	657 485	74 992
11	10 235	256	2 939 725	279 976
12	26 083	586		
13	66 653	1 386		
14	170 689	3 262		
15	437 947	7 690		
16	1 125 515	18 206		
17	2 896 883	43 520		
18	7 466 063	104 892		
19	19 265 059	254 040		
20	49 763 899	617 440		
21	128 670 737	1 505 906		
22	332 909 215	3 687 276		

TAWS of length $n+1$, means that storage capacity also becomes a limiting factor. By judicious data structuring we were able to evaluate bridges of length 22 steps on the square lattice and 11 steps on the simple cubic lattice. Application of (2.1) then gave the cardinality of irreducible bridges to the same order. These results are shown in table 1 below. Using equation (2.2), we then solved the polynomial equation $\sum_{n=1}^{N} s_n \bar{\mu}_N^{-n} = 1$ with $N = 22$ and 11 for the square and simple cubic lattices respectively. This gave $\mu_{22}(\mathrm{sq}) = 2.5680$ and $\mu_{11}(\mathrm{SC}) = 4.352$. These lower bounds may be compared with the current series estimates of $\mu(\mathrm{sq}) = 2.6381$ and $\mu(\mathrm{SC}) = 4.6835$, so that the square lattice estimate is 2.7% below the series estimate, while the simple cubic result is some 7.6% below the series estimate.

Very recently Nienhuis (1982) has presented very convincing physical arguments (though not rigorous mathematical ones) that, for the honeycomb lattice, the exact value of μ is $(2+\sqrt{2})^{1/2} = 1.847\,759\ldots$. Unfortunately there is no obvious way to generalise Nienhuis's technique so that it applies to the square or triangular lattices.

In table 2 we summarise the best available upper and lower bounds, and the single exact result for the two-dimensional lattices, and the best unbiased series estimates (where available). It is important to quote unbiased series estimates, as Nienhuis (1982) also gives strong arguments to suggest that the exponent characterising the growth in the cardinality of the walks is not $\frac{1}{3}$, as has been assumed by all biased series estimates, but is slightly higher, at $\frac{11}{32} = 0.343\,75$.

Table 2. Upper and lower bounds on the connective constant of the SAW problem on a range of common lattices. Exact and conjectured results and unbiased series estimates are also tabulated.

Lattice	Lower bound	Best series estimate	Exact or conjectured estimate	Upper bound
Honeycomb	1.7872[a]	1.8481[h]	1.847 759[c]	1.895[d]
Square	2.5680[b]	2.6381[g]	—	2.712[a]
Kagomé	2.4453[a]	2.555[a]	—	2.6968[a]
Triangular	3.8404[a]	4.1517[f]	—	4.354[d]
Tetrahedral	2.5325[a]	2.878[i]	—	2.9175[e]
Simple-cubic	4.352[b]	4.684[f]	—	4.781[d]
Body-centred cubic	5.187[a]	6.529[f]	—	6.695[d]
Face-centred cubic	7.644[a]	10.037[f]	—	10.361[d]
Hydrogen-peroxide	1 69[j]	1.956[k]	—	1.979[j]
Hyper-kagomé	2.335[j]	—	—	—
Hyper-triangular	3.38[j]	4.6181[k]	—	4.76[j]

[a] Fisher and Sykes (1959)
[b] This work
[c] Nienhuis (1982)
[d] Ahlberg and Janson (1982)
[e] Wall and White (1976)
[f] Guttman *et al* (1968)
[g] Sykes *et al* (1972)
[h] Guttmann and Sykes (1973)
[i] Essam and Sykes (1963)
[j] J Wilker and S G Whittington (unpublished)
[k] Leu (1969)

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