Upper bounds for the connectivity constant

By

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Abstract. A new method to calculate rigorous upper bounds for the connectivity constant is described. For the square lattice, a computer calculation yields the bound 2.7272. Slight improvements of the bounds of the connectivity constant for other lattices and the time constant for first-passage percolation are also obtained.

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1. Introduction

We are studying self-avoiding paths on a lattice. We will only consider lattices such that all vertices are equivalent (every vertex can be mapped on any other vertex by some symmetry operation) and that all edges from a vertex to its neighbours are equivalent. Later on we will specialize to the square lattice where the vertices are the points with integer coordinates in the plane and the neighbours of a vertex are the four vertices at unit distance.

A self-avoiding path of length n is a sequence of $n+1$ mutually distinct vertices such that any two successive vertices in the sequence are neighbours. The number of such paths having a prescribed first vertex is denoted by f_n. Thus f_1 is the number of neighbours of a vertex. Hammersley [1] proved that, for large n, $f_n^{1/n}$ converges to a limit, the connectivity constant. This was strengthened by Kesten [2] who proved that f_{n+2}/f_n converges. Other aspects of self-avoiding path theory and many references are given by Domb [3].

Section 2 presents a new method to obtain a rigourous upper bound of the connectivity constant, given a count of all self-avoiding paths of a certain length, partitioned according to the first few steps.

Section 3 describes briefly such a counting on a computer.

Section 4 gives the numerical results.

2. A bound for the connectivity constant

The following notations will be used: λ is the connectivity constant. Γ_n is the set of self-avoiding paths of length n having a prescribed first vertex. Thus f_n is the cardinality of Γ_n. If $\gamma \in \Gamma_k$, where $k \leq n$, f_n^γ is the number of self-avoiding paths of length n that begin with γ. Thus

$$f_n = \sum_{\gamma \in \Gamma_k} f_n^\gamma, \quad k \leq n .$$

Let $m,n \geq k$. Any path of length $m+n-k$ may be decomposed in a head consisting of the n first steps and a tail consisting of the last m steps, with k steps overlapping. We sort all paths in Γ_{m+n-k} according to the overlapping part and obtain the inequality

$$f_{m+n-k} \leq \sum_{\Gamma_k} f_n^\gamma f_m^{\gamma^*} \qquad \text{(where } \gamma^* \text{ is } \gamma \text{ reversed).}$$

For $k=0$ this reduces to the submultiplicativity $f_{m+n} \leq f_m f_n$, which implies that $\lambda = \lim f_n^{1/n}$ exists and $\lambda \leq f_n^{1/n}$ [1]. For $k=1$, Γ_1 consists of f_1 paths and, by symmetry, $f_n^\gamma = f_n/f_1$. Hence the inequality is $f_{m+n-1} \leq f_n \cdot f_m / f_1$ which yields the known bound $\lambda \leq (f_n/f_1)^{\frac{1}{n-1}}$ [4]. We will derive still better bounds using higher k. We assume that the values of f_n^γ are known for one choice of k and n. We do not know the values of f_m^γ (for large m) but, if δ is the last step of γ, $f_m^\gamma \leq f_{m-k+1}^\delta = f_{m-k+1}/f_1$.

Choose a positive number A. If $f_n^\gamma \leq A$, $f_n^\gamma f_m^{\gamma^*} \leq A f_m^{\gamma^*}$, and if $f_n^\gamma > A$, $f_n^\gamma f_m^{\gamma^*} = A f_m^{\gamma^*} + (f_n^\gamma - A) f_m^{\gamma^*} \leq A f_m^{\gamma^*} + (f_n^\gamma - A) f_{m-k+1}/f_1$. Hence, if $(f_n^\gamma - A)_+$ denotes $\max(f_n^\gamma - A, 0)$,

$$f_{m+n-k} \leq \sum_{\Gamma_k} (A f_m^{\gamma^*} + (f_n^\gamma - A)_+ f_{m-k+1}/f_1) = A f_m + \frac{1}{f_1} \sum_{\Gamma_k} (f_n^\gamma - A)_+ f_{m-k+1} .$$

Replacing m by $m+k-1$, this may be written as

$$f_{m+n-1} \le A f_{m+k-1} + B f_m, \quad m \ge 1, \text{ where } B = \frac{1}{f_1} \sum_{\Gamma_k} (f_n^{\gamma} - A)_+ .$$

This difference inequality implies that λ is less than the unique positive root of $x^{n-1} = A x^{k-1} + B$. To obtain a slightly more convenient form of this, let $f_{n,k}^i$, $i = 1,2,\ldots,f_k/f_1$, be the numbers f_n^{γ} for all $\gamma \in \Gamma_k$ starting in a particular direction, arranged in decreasing order. By symmetry, each of these numbers is repeated f_1 times in the full sequence $\{f_n^{\gamma}\}_{\gamma \in \Gamma_k}$. Furthermore, choose A as $f_{n,k}^j$ for some j, $1 \le j \le f_k/f_1$. Then

$$B = \sum_{i=1}^{f_k/f_1} (f_{n,k}^i - A)_+ = \sum_{i=1}^{j} (f_{n,k}^i - f_{n,k}^j) .$$

We have proved the following theorem:

<u>Theorem</u>. <u>Let</u> $f_{n,k}^i$ <u>be as above. If</u> $k < n$ <u>and</u> $j \le f_k/f_1$, <u>then the connective constant is less than or equal to the unique positive root of</u>

$$x^{n-1} = f_{n,k}^j x^{k-1} + \sum_{i=1}^{j} (f_{n,k}^i - f_{n,k}^j) .$$

<u>Remarks</u>. 1. It is not difficult to show that, given n and k, the best choice of j is approximately λ^{k-1}. (Thus j is close to its upper bound f_k/f_1.)

2. A reasonable guess is that the best choice of k slowly increases with increasing n. This is supported by the results in Section 4.

If only the total number f_n of self-avoiding paths is known, but we also know f_{n-1}, crude estimates yield the following bound. If $f_n/f_{n-1} > f_1 - 2$, it is better than $(f_n/f_1)^{\frac{1}{n-1}}$.

<u>Corollary</u>. <u>If</u> $n > 2$, <u>then the connective constant is less than the positive root of</u>

$$f_1 x^{n-1} = (f_n - (f_1 - 2) f_{n-1}) x + (f_1 - 2)((f_1 - 1) f_{n-1} - f_n) .$$

Proof. Choose $k=2$ and $j = f_2/f_1 = f_1 - 1$. Thus $\lambda^{n-1} \leq f^j_{n,2}(\lambda-j) + \sum_{i=1}^{j} f^j_{n,2}$. Now $\sum_{i=1}^{j} f^i_{n,2} = f_n/f_1$, and every $f^i_{n,2}$ equals some f^γ_n, $\gamma \in \Gamma_2$. Let $\delta \in \Gamma_1$ be the second step of γ. Then $f^i_{n,2} = f^\gamma_n \leq f^\delta_{n-1} = f_{n-1}/f_1$. Thus

$$f^j_{n,2} = f_n/f_1 - \sum_{1}^{j-1} f^i_{n,2} \geq \frac{f_n - (j-1)f_{n-1}}{f_1}.$$

Hence, since $\lambda \leq j$,

$$\lambda^{n-1} \leq \frac{f_n - (j-1)f_{n-1}}{f_1}(\lambda - j) + \frac{f_n}{f_1} = \frac{f_n - (j-1)f_{n-1}}{f_1}\lambda + \frac{j(j-1)f_{n-1} - (j-1)f_n}{f_1}.$$

3. Computational algorithms for the square lattice

We will describe how an electronic computer can be used to count the number of self-avoiding paths which belong to Γ_n .

Each path may be represented by a Boolean lattice. If a vertex is on a path it contains 1 and otherwise 0 . Thus all possible paths may be represented by a three-dimensional matrix P(I,X,Y) , where I is an index of the path and (X,Y) is a vertex. The memory of a computer is a Boolean lattice. Most economically each vertex corresponds to a bit (instead of a word or a byte). A path of the length m is constructed from one of the length $m-1$ by addition of one vertex at the head. All possible paths of length $m-1$ and directions must be tried in each iteration. Obviously, one has to remember which vertex of a path is the head. The heads are represented by a matrix H(I, J(X,Y)) where J a one to one integer valued function of (X,Y) . Also the form

$$P(I,X,Y) = P(I, J(X,Y))$$

is used in our programme. This reduces the number of index operations and the storage. The index I is orders of magnitudes too large to permit P and H to be contained in the primary storage. Therefore secondary storage (discs) are used to buffer in and out sub-matrices.

Symmetry may be used to reduce the number of paths to be counted. Only paths which start along the x-axis and first turn off into the positive Y direction are needed. This subset we denote by Γ_n^{-} and the number of paths by g_n . We have $f_n = 8g_n - 4$.

One choice for the function J is

$$J_n(X,Y) = nX + (n-1)Y + n^2 - 4n + 2 .$$

The maximum of the J function, $2(n-1)^2$, is the number of bits required to represent any path and $\frac{2(n-1)^2}{w}$ words have to be reserved for the second index of P and H .

For $n > 17$ storage and computing times required are too large within our present resources. The calculations can be extended thanks to the fact that continuations can be performed at the start instead of at the end. We may connect paths of length k to paths of length $n-k$ at the origin and thus avoid intermediate iterations and any storage beyond the length $n-k$. The number of paths is obtained from

$$f_n = \frac{3}{4} f_{n-k} f_k - 4\,C_{n-k,k}$$

where $C_{n-k,k}$ is the number of pairs of intersecting paths, one belonging to Γ_{n-k} and starting along the positive x-axis and the other belonging to Γ_k and starting in one of the three other directions. The latter set of paths is denoted by $\Gamma_k^{\sim}$. When only the set Γ'_{n-k} is stored, one may use

$$C_{n-k,k} = \sum_{\substack{\delta \in \Gamma'_{n-k} \\ \gamma \in \Gamma_k^{\sim}}} \varepsilon_{\gamma\delta} + \sum_{\substack{\delta \in \Gamma'_{n-k} \\ \gamma \in \Gamma_k^{\sim} \\ \delta \neq \overline{\delta}}} \varepsilon_{\overline{\gamma}\delta}$$

where $\varepsilon_{\gamma\delta}$ is 1 if γ and δ have at least one crossing and otherwise it is 0. $\overline{\gamma}$ is the path γ reflected in the x-axis. The terms f_n^{γ} are obtained by means of the partial sums for γ isomorphic to a given one.

We programmed the cases $k = 2,3,4$. A developed version which permits k close to $n/2$ would be better especially for f_n. To perform this in an efficient way we need to store also the paths of $\Gamma_k^{\sim}$ and to have an AND-operation which turns on only bits which are in both of the matched paths. Also one needs a fast test if not all words representing this intersection are zero. Vector processors may turn out to be efficient [5]. Very large integers need to be represented in our calculations. 60-bit computers would avoid the early difficulties we have had.

4. Numerical results

Table 1 contains the number of self-avoiding paths on the square lattice for $n \leq 21$. This is only a part of the table of [6] which covers $n \leq 24$. Table 2 contains (for $12 \leq n \leq 21$) the best upper bounds of the connectivity constant given by Section 2 with $k \leq 4$. (Only these k were tried. It is conceivable that higher k gives even better bounds.) The optimal choices of k and j are 3 and 8 (or 9), respectively, for $12 \leq n \leq 16$ and 4 and 20 (or 21) respectively, for $17 \leq n \leq 21$. For comparison, Table 2 also contains the estimates $(f_n/4)^{\frac{1}{n-1}}$.

The best upper bound of the connectivity constant is thus 2.7272 , obtained for $n=21$, $k=4$. Table 3 lists the numbers $f^i_{n,k}$ for this case. However, the better bound 2.7248 is reported by Wall and White [7]. A lower bound is 2.581 obtained by Beyes and Wells [8]. There are suggestive indications that the true value is 2.639 [9].

For other lattices, our theorem seems to yield a similar improvement. However, we have only computed $f^i_{n,k}$ for small n and we have not obtained any new bounds. The corollary and published values of f_n [6], [10] yield the upper bounds: triangular 4.354 $(n=17)$, honeycomb 1.895 $(n=34)$, simple cubic 4.781 $(n=19)$, body-centered cubic 6.695 $(n=15)$, face-centered cubic 10.361 $(n=12)$.

Another result of our calculations is that the lower bound of the time constant for first-passage percolation with exponential passage time distribution is increased to 0.29853 (by the method of [11], with $n=17$) .

Table 1: The number of selfavoiding paths for a square lattice

n	f_n
1	4
2	12
3	36
4	100
5	284
6	780
7	2172
8	5916
9	16268
10	44100
11	120292
12	324932
13	881500
14	2374444
15	6416596
16	17245332
17	46466676
18	124658732
19	335116620
20	897697164
21	2408806028

Table 2: Upper bounds to the connectivity constant for the square lattice

n	the theorem	$(f_n/4)^{\frac{1}{n-1}}$
12	2.7635	2.7947
13	2.7586	2.7878
14	2.7529	2.7805
15	2.7487	2.7748
16	2.7442	2.7689
17	2.7405	2.7642
18	2.7364	2.7593
19	2.7333	2.7553
20	2.7299	2.7512
21	2.7272	2.7478

Table 3: $f^i_{21,4}$ for the square lattice. (By symmetry, all but one occur in pairs.)

27541881	25911043	24697573
27158763	25911043	23992012
27158763	25911043	23992012
26795760	25693180	21553753
26795760	25693180	21553753
25924031	25302172	18509645
25924031	25302172	18509645
25911043	24697573	15880838
		15880838

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