The lace expansion and the enumeration of self-avoiding walks

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Abstract

The lace expansion is a recursion relation for the number of self-avoiding walks.

We discuss an algorithmic improvement for direct enumeration, called the two-step method. We describe the lace expansion, and explain its recent application to enumerate self-avoiding walks on $\mathbb{Z}^d$ up to $n = 30$ for $d = 3$, and up to $n = 24$ steps for *all* $d \geq 4$, and to extend $1/d$ expansions.

Joint work with Nathan Clisby (Melbourne) and Richard Liang (Berkeley).

Preprint soon at `http://www.math.ubc.ca/~slade`.

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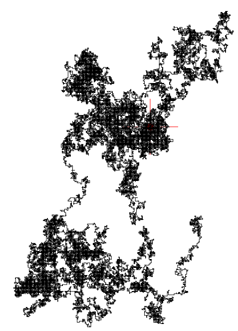
Simple random walk

Start at $0 \in \mathbb{Z}^d$. Choose one of the $2d$ neighbours at random and step to it. Continue with independent steps to a neighbour of current position.



Let $\omega(n)$ be the position after n steps. Let $s_n(x)$ be the number of n-step SRWs with $\omega(n) = x$.
Let s_n be the number of n-step SRWs.

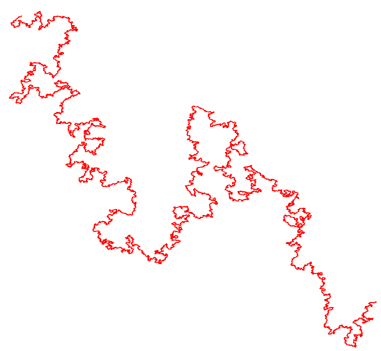
Recursion relation: $s_n(x) = \sum_{y \in \mathbb{Z}^d} s_1(y) s_{n-1}(x-y)$, which can easily be solved.
Sum over x: $s_n = 2d s_{n-1}$ which has solution $s_n = (2d)^n$.

Mean-square displacement: $E|\omega(n)|^2 = n$.

Self-avoiding walk

Let $\mathcal{S}_n(x)$ be the set of $\omega : \{0, 1, \ldots, n\} \to \mathbb{Z}^d$ with:
$\omega(0) = 0$, $\omega(n) = x$, $|\omega(i+1) - \omega(i)| = 1$, and $\omega(i) \neq \omega(j)$ for all $i \neq j$.
Let $\mathcal{S}_n = \cup_{x \in \mathbb{Z}^d} \mathcal{S}_n(x)$

Declare all walks in $\mathcal{S}_n$ to be equally likely: each has probability c_n^{-1} where $c_n = |\mathcal{S}_n|$.



Interested in c_n and $E|\omega(n)|^2 = c_n^{-1} \sum_{\omega \in \mathcal{S}_n} |\omega(n)|^2 = c_n^{-1} \sum_{x \in \mathbb{Z}^d} |x|^2 c_n(x)$.

Previously known values of c_n

$d = 2$ (Jensen 2004): $c_{71} = 4\,190\,893\,020\,903\,935\,054\,619\,120\,005\,916$

$d = 3$ (MacDonald et al 2000): $c_{26} = 549\,493\,796\,867\,100\,942$

$d = 4$ (Chen–Lin 2003): $c_{19} = 8\,639\,846\,411\,760\,440$

$d = 5$ (Chen–Lin 2003): $c_{15} = 192\,003\,889\,675\,210$

$d = 6$ (Chen–Lin 2003): $c_{14} = 373\,292\,253\,262\,692$

Critical exponents

Connective constant $\mu = \lim_{n\to\infty} c_n^{1/n}$ exists because $c_{n+m} \le c_n c_m$.
Easy: $d \le \mu \le 2d-1$.

Conjectured asymptotic behaviour:

$$c_n \sim A\mu^n n^{\gamma-1}, \quad E|\omega(n)|^2 \sim Dn^{2\nu}$$

with universal critical exponents γ and ν (and $\log$ corrections for $d=4$).

For $d=2$: $\gamma = \frac{43}{32}$ and $\nu = \frac{3}{4}$ will follow if scaling limit is $\mathrm{SLE}_{8/3}$ (Lawler–Schramm–Werner).
For $d=3$: no rigorous results.
For $d=4$: $\gamma=1$ and $\nu=\frac{1}{2}$ with $(\log n)^{1/4}$ corrections for hierarchical lattice (Brydges–Imbrie 2003).
For $d \ge 5$: $\gamma = 1$ and $\nu = \frac{1}{2}$ (Hara–Slade 1992).

How bad is it for $d = 2,3,4$? Best bound is $\mu^n \le c_n \le \mu^n e^{Cn^{2/(d+2)}\log n}$.
Not proved that $cn \le E|\omega(n)|^2 \le Cn^{2-\epsilon}$.

The two-step method

This is an exponentially improved method for direct enumeration of SAWs.

A *2-step walk* Ω is a SAW which takes steps $\pm e_i \pm e_j$.
The *weight* $W(\Omega)$ is the number of $2n$-step SAWs whose restriction to every second vertex is Ω.

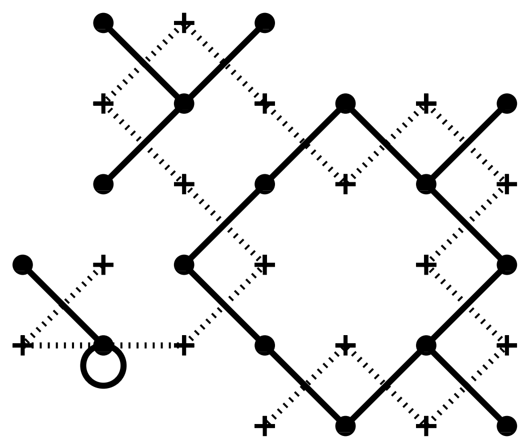
Then c_{2n} is the sum of $W(\Omega)$ over all Ω that take n steps.

In practice we find for $d = 3$ that the number of two-step walks taking n steps grows like $\approx (4.0)^{2n}$, yielding an exponential improvement over $\mu^{2n} \approx (4.68)^{2n}$.

The weight $W(\Omega)$ can be calculated in time $O(n)$:

The two-step method: Allocation graph

$W(\Omega)$ is computed using the *allocation graph* $\mathcal{G}_\Omega$: $W(\Omega) = I_\Omega 2^{|\mathcal{C}_\Omega|} \prod_{T \in \mathcal{T}_\Omega} N_T$



where $|\mathcal{C}_\Omega|$ is the number of unicyclic components, $\mathcal{T}_\Omega$ is the set of tree components, N_T is the number of vertices of a tree T, and

$$I_\Omega = \begin{cases} 1 & \text{if no component has two or more loops and/or cycles} \\ 0 & \text{otherwise.} \end{cases}$$

Proof. Count the number of *admissible* orientations of the allocation graph.

The lace expansion

Invented by Brydges–Spencer (1985) to analyse weakly SAW for $d > 4$.

Subsequently extended by several people to analyse:

lattice trees and lattice animals for $d > 8$,

percolation for $d > 6$,

oriented percolation, contact process, Ising model for $d > 4$,

SAW for $d \geq 5$.

Reference: G. Slade, The Lace Expansion and its Applications, Springer LNM 1879, (2006).

The lace expansion: Recursion relation

Identifies a function $\pi_m(x)$ such that for $n \geq 1$,

$$c_n(x) = \sum_{y \in \mathbb{Z}^d} c_1(y) c_{n-1}(x-y) + \sum_{m=2}^{n} \sum_{y \in \mathbb{Z}^d} \pi_m(y) c_{n-m}(x-y).$$

Let $\pi_m = \sum_{y \in \mathbb{Z}^d} \pi_m(y)$ and sum over $x \in \mathbb{Z}^d$ to get:

$$c_n = 2d c_{n-1} + \sum_{m=2}^{n} \pi_m c_{n-m}.$$

Knowledge of $(\pi_m)_{2 \leq m \leq n}$ is equivalent to knowledge of $(c_m)_{0 \leq m \leq n}$.

The lace expansion: smaller enumeration task

We enumerate π_m by counting *lace graphs*, which are self-avoiding returns and their generalisations.

In practice, we find that the ratio of SAWs to lace graphs is approximately

$$d = 2, n = 30 : \quad 36$$

$$d = 3, n = 30 : \quad 525$$

$$d = 4, n = 24 : \quad 1700$$

$$d = 5, n = 24 : \quad 6200$$

$$d = 6, n = 24 : \quad 20000$$

Determination of $(\pi_m)_{m \le M}$ in dimensions $d \le \frac{M}{2}$ gives $(\pi_m)_{m \le M}$ in *all* dimensions d. Thus $(\pi_m)_{m \le 24}$ in dimensions $d \le 12$ gives $(c_n)_{n \le 24}$ in *all* dimensions d.

The lace expansion: graphs

Given $\omega \in \mathcal{W}_m(x)$ = set of m-step simple random walks that start at the origin and end at x, let

$$U_{st}(\omega) = \begin{cases} -1 & \text{if } \omega(s) = \omega(t) \\ 0 & \text{if } \omega(s) \neq \omega(t). \end{cases}$$

For $0 \leq a < b$, let

$$K[a,b] = K_\omega[a,b] = \prod_{a \leq s < t \leq b} (1 + U_{st}).$$

Then

$$c_n(x) = \sum_{\omega \in \mathcal{W}_n(x)} K_\omega[0,n].$$

A *graph* is a set of pairs st with $s < t$. Let $\mathcal{B}_{[a,b]}$ denote the set of all graphs on $[a,b]$.

The lace expansion: connected graphs

Then

$$K[0,n] = \prod_{0\le s<t\le n} (1+U_{st}) = \sum_{\Gamma\in\mathcal{B}_{[0,n]}} \prod_{st\in\Gamma} U_{st}.$$

We say Γ is *connected* on $[a,b]$ if, as intervals of real numbers, $\cup_{st\in\Gamma}(s,t) = (a,b)$. The set of all connected graphs on $[a,b]$ is denoted $\mathcal{G}_{[a,b]}$. Let

$$J[0,n] = \sum_{\Gamma\in\mathcal{G}_{[0,n]}} \prod_{st\in\Gamma} U_{st}.$$

Then

$$K[0,n] = K[1,n] + \sum_{m=2}^{n} J[0,m]K[m,n].$$

Insert in

$$c_n(x) = \sum_{\omega\in\mathcal{W}_n(x)} K_\omega[0,n].$$

First term gives

$$\sum_{\omega\in\mathcal{W}_n(x)} K_\omega[1,n] = \sum_{y\in\mathbb{Z}^d} c_1(y)c_{n-1}(x-y).$$

The lace expansion: factorisation

Second term is

$$\sum_{m=2}^{n} \sum_{\omega \in \mathcal{W}_n(x)} J_\omega[0,m] K_\omega[m,n] = \sum_y \sum_{m=2}^{n} \sum_{\omega_1 \in \mathcal{W}_m(y)} J_{\omega_1}[0,m] \sum_{\omega_2 \in \mathcal{W}_{n-m}(x-y)} K_{\omega_2}[0,n-m].$$

This is

$$\sum_y \sum_{m=2}^{n} \pi_m(y) c_{n-m}(x-y)$$

with

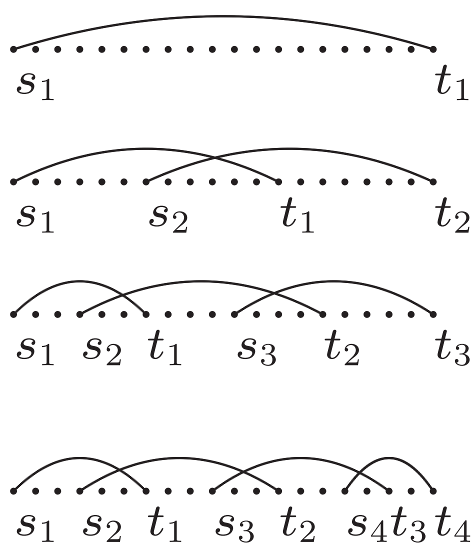
$$\pi_m(y) = \sum_{\omega \in \mathcal{W}_m(y)} J_\omega[0,m].$$

Altogether,

$$c_n(x) = \sum_y c_1(y) c_{n-1}(x-y) + \sum_y \sum_{m=2}^{n} \pi_m(y) c_{n-m}(x-y).$$

The lace expansion: laces

Given $\Gamma \in \mathcal{G}_{[0,n]}$, choose a 'minimal' connected $L \subset \Gamma$,
and let $\mathcal{C}(L)$ denote the edges which are *compatible* with L in the sense that L remains the minimal choice for $\Gamma = L \cup \{st\}$.
Examples of *laces* L with $N = 1, 2, 3, 4$ edges:



The lace expansion: resummation

Then

$$J[0,m] = \sum_{L \in \mathcal{L}_{[0,m]}} \prod_{st \in L} U_{st} \sum_{\Gamma \in \mathcal{G}_{[0,m]}(L)} \prod_{s't' \in \Gamma \setminus L} U_{s't'}$$

$$= \sum_{L \in \mathcal{L}_{[0,m]}} \prod_{st \in L} U_{st} \prod_{s't' \in \mathcal{C}(L)} (1 + U_{s't'})$$

$$= \sum_{N=1}^{\infty} (-1)^N \sum_{L \in \mathcal{L}^{(N)}_{[0,m]}} \prod_{st \in L} [-U_{st}] \prod_{s't' \in \mathcal{C}(L)} (1 + U_{s't'}),$$

so

$$\pi_m(x) = \sum_{N=1}^{\infty} (-1)^N \pi_m^{(N)}(x)$$

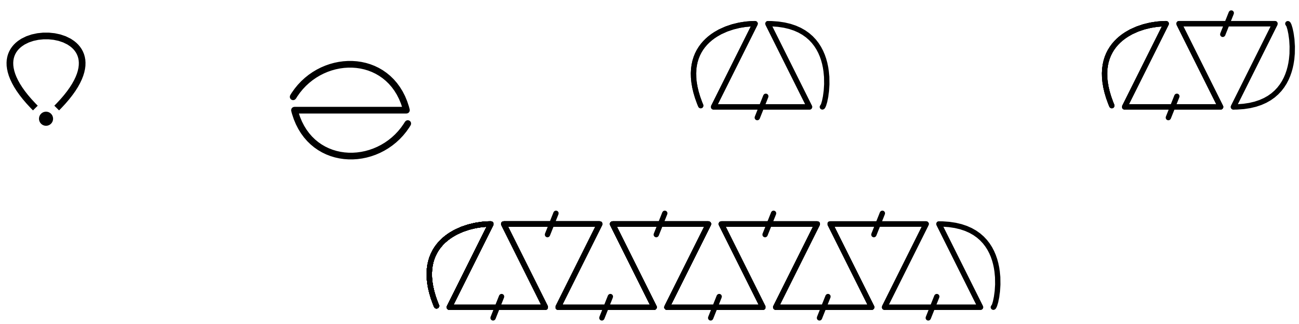
where

$$\pi_m^{(N)}(x) = \sum_{\omega \in \mathcal{W}_m(x)} \sum_{L \in \mathcal{L}^{(N)}_{[0,m]}} \prod_{st \in L} [-U_{st}(\omega)] \prod_{s't' \in \mathcal{C}(L)} (1 + U_{s't'}(\omega)).$$

The lace expansion: lace graphs

$$\pi_m^{(N)}(x) = \sum_{\omega \in \mathcal{W}_m(x)} \sum_{L \in \mathcal{L}_{[0,m]}^{(N)}} \prod_{st \in L} [-U_{st}(\omega)] \prod_{s't' \in \mathcal{C}(L)} (1 + U_{s't'}(\omega)).$$

The lace graphs are the walks that give nonzero products in the above sum, and this is what we enumerate.



Lace graphs for $N = 1, 2, 3, 4, 11$.

Values of $\pi_{m,\delta}$:

m	$\delta = 2$	$\delta = 3$	$\delta = 4$	$\delta = 5$	$\delta = 6$
4	-1	0	0	0	0
5	3	0	0	0	0
6	-8	-4	0	0	0
7	19	15	0	0	0
8	-50	-86	-27	0	0
9	121	300	106	0	0
10	- 305	-1 511	-1 340	- 248	0
11	736	5 297	5 333	966	0
12	-1 853	-25 566	-52 252	-25 020	-2 830
13	4 531	91 234	211 403	100 988	10 755
14	-11 444	- 435 330	-1 907 566	-1 850 364	- 515 509
15	28 294	1 586 306	7 854 601	7 635 822	2 029 500
16	-71 803	-7 568 792	-68 777 498	- 123 248 980	-64 816 437
17	179 006	28 105 857	288 074 727	517 006 517	260 695 401
18	- 455 588	- 134 512 520	-2 498 227 824	-7 899 351 270	-7 074 329 136
19	1 142 357	507 675 751	10 626 960 167	33 569 520 427	28 860 719 280
20	-2 914 236	-2 438 375 322	-92 047 793 514	- 500 752 577 733	- 724 291 034 691
21	7 341 457	9 330 924 963	396 919 882 288	2 150 581 793 271	2 984 307 507 943
22	-18 768 621	-44 965 008 206	-3 445 692 397 195	-31 789 616 257 271	-72 005 867 458 629
23	47 466 002	174 103 216 625	15 035 569 992 917	137 713 940 393 321	298 797 296 949 195
24	- 121 579 349	- 841 380 441 626	- 130 974 140 581 412	-2 032 548 406 479 564	-7 072 798 632 884 530
25	308 478 355	3 290 830 791 268			
26	- 791 455 148	-15 941 476 401 251			
27	2 013 666 265	62 897 919 980 935			
28	-5 174 044 897	- 305 298 415 550 796			
29	13 195 280 922	1 213 812 491 872 081			
30	-33 949 508 883	-5 901 490 794 431 276			

Results of enumerations

For $d = 3$:

$c_{26} = 549\,493\,796\,867\,100\,942$

$c_{30} = 270\,569\,905\,525\,454\,674\,614$

$c_{30}/c_{26} = 492.3\ldots$

For $d = 4$:

$c_{19} = 8\,639\,846\,411\,760\,440$

$c_{24} = 124\,852\,857\,467\,211\,187\,784$

$c_{24}/c_{19} = 14450.8\ldots$

For $d = 5$:

$c_{15} = 192\,003\,889\,675\,210$

$c_{24} = 63\,742\,525\,570\,299\,581\,210\,090$

$c_{24}/c_{15} = 3.3 \times 10^8$

For $d = 6$:

$c_{14} = 373\,292\,253\,262\,692$

$c_{24} = 8\,689\,265\,092\,167\,904\,101\,731\,532$

$c_{24}/c_{14} = 2.3 \times 10^{10}$

Results of enumerations: CPU time

Self-avoiding polygons $\pi_m^{(1)}$:
$d = 3$, $m = 30$ took 450 CPU hours;
$d = 3$, $m = 32$ took 5000 CPU hours;
$d = 4$, $m = 26$ took 180 CPU hours;
$d \geq 2$, $m = 24$ took a total of 980 CPU hours.

Lace graph enumerations π_m:
$d = 3$, $m = 30$ took 14400 CPU hours;
$d \geq 2$, $m = 24$ took 3400 CPU hours.

Self-avoiding walks c_n:
$d = 3$, $n = 30$ took 15000 hours;
$d \geq 2$, $n = 24$ took 4400 hours.

$1/d$ expansions

Recall the recursion relation

$$c_n = 2dc_{n-1} + \sum_{m=2}^{n} \pi_m c_{n-m}.$$

Define the generating functions

$$\chi(z) = \sum_{n=0}^{\infty} c_n z^n, \quad \Pi(z) = \sum_{m=2}^{\infty} \pi_m z^m.$$

The recursion relation gives

$$\chi(z) = \frac{1}{1 - 2dz - \Pi(z)}.$$

The radius of convergence of $\chi(z)$ is $z_c = \mu^{-1}$, and $\chi(z_c) = \infty$, so

$$1 - 2dz_c - \Pi(z_c) = 0.$$

$1/d$ expansions: truncation

The critical point is given implicitly by

$$z_c = \frac{1}{2d}[1 - \Pi(z_c)] = \frac{1}{2d}\left[1 - \sum_{m=2}^{\infty}\sum_{M=1}^{\infty}(-1)^M \pi_m^{(M)} z_c^m\right].$$

Hara–Slade used this to prove that there exist $a_i \in \mathbb{Z}$ such that

$$z_c \sim \sum_{i=1}^{\infty} \frac{a_i}{(2d)^i} \quad \text{as } d \to \infty.$$

An old estimate gives (in high d)

$$\sum_{m=2}^{\infty}\sum_{M=N}^{\infty} m\pi_m^{(M)} z_c^m \leq C_N d^{-N}$$

and we prove (in high d)

$$\sum_{m=j}^{\infty} m\pi_m^{(M)} z_c^m \leq C_{M,j} d^{-j/2}.$$

$1/d$ expansions: results

Upshot: Knowledge of $\pi_m^{(M)}$ for $m \leq 2N$ and $M \leq N$ permits the recursive calculation of a_i for $i = 1, \ldots, N+1$.

Using $\pi_m^{(M)}$ for $m \leq 24$ and $M \leq 12$ gives

$$\mu = 2d - 1 - \frac{1}{2d} - \frac{3}{(2d)^2} - \frac{16}{(2d)^3} - \frac{102}{(2d)^4} - \frac{729}{(2d)^5} - \frac{5533}{(2d)^6} - \frac{42229}{(2d)^7} - \frac{288761}{(2d)^8} - \frac{1026328}{(2d)^9} + \frac{21070667}{(2d)^{10}} + \frac{780280468}{(2d)^{11}} + O\left(\frac{1}{(2d)^{12}}\right).$$

Presumably the full asymptotic series is divergent. Note sign change at order $(2d)^{-10}$.

Similar expansions result for the amplitudes A and D, using e.g.,

$$\frac{1}{A} = 2dz_c + \sum_{m=2}^{\infty} m\pi_m z_c^m$$

Future work

- Complete series analysis: μ, γ, ν.
- Attempt to extend the two-step method to the k-step method, to extend series for $d = 3$.
- We find that π_m is alternating in sign whenever its values are known ($m \leq 71$ for $d = 2$). Can this be proved? Relate to antiferromagnetic singularity of $\chi(z)$.