Enumeration of self-avoiding walks via the lace expansion

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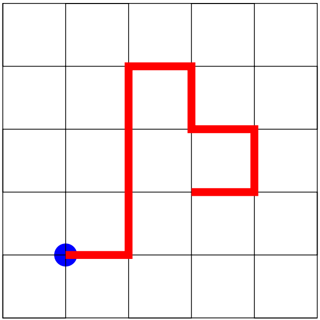
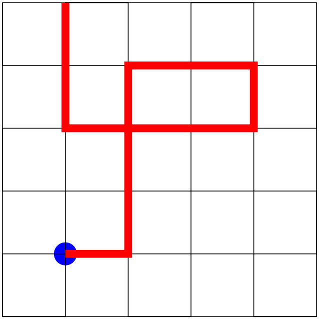
The self-avoiding walk model

- A self-avoiding walk (SAW) is a path on a lattice, which starts at the origin and hops successively to neighbouring lattice sites without intersecting itself.
- We count the number of SAWs of length n, c_n, and in particular study the critical behaviour of the generating function
$$C(x) = \sum_{n=0}^{\infty} c_n x^n$$
- For the simple cubic lattice $c_0 = 1$, $c_1 = 6$, $c_2 = 30$, $c_3 = 150$, $c_4 = 726$, $c_5 = 3534, \ldots$

SAW example



- SAW!



- Not a SAW, due to self intersection.

Known results

- For the square lattice c_n has been enumerated to very high order via the finite lattice method by Iwan Jensen:

$$c_{71} = 4190893020903935054619120005916$$

- Best results for $d > 2$ are via direct enumeration.
- MacDonald et al., simple cubic lattice

$$c_{26} = 549493796867100942$$

- For $d = 4$, c_n is known to c_{19}, for $d = 5$ to c_{15}, and for $d = 6$ to c_{14}.

Known results

- It is universally believed (but not proven) that for dimensions $d < 4$ asymptotically

$$c_n \sim A\, n^{\gamma-1} \mu^n \, [1 + \text{corrections}]$$

  and the mean-square end-to-end distance behaves asymptotically as

$$\bar{\rho}_n \sim D\, n^{2\nu} \mu^n \, [1 + \text{corrections}]$$

- Improved enumerations allow better estimation of A, μ, γ, D and ν.

Known results for $d \geq 3$

- For the cubic lattice, no exact results available; best estimates $\mu = 4.68404(9)$ (from exact series), $\gamma = 1.1575(6)$, $\nu = 0.5874(2)$ (from Monte-Carlo).
- $\gamma = 1$ for $d = 4$, but with logarithmic corrections.
- For $d \geq 5$ it has been proven that $\gamma = 1$ using the lace expansion.

The two-step method

- For brute force enumeration of SAWs of length n expect

$$\tau(n) \sim c_n \approx \mu^n$$

- Reduce the time taken by reducing the complexity.
- Take two steps at once, and represent walks which have the same endpoint by a single configuration.
- Sequence of endpoints defines a 2-step walk, Ω.

Two step method for SAWs

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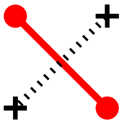
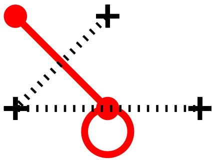
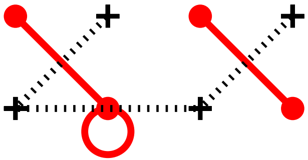
Two step method for SAWs



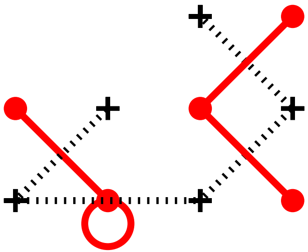
Two step method for SAWs



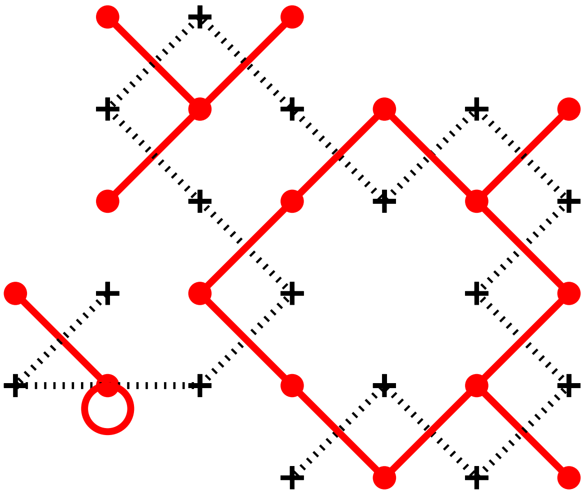
Two step method for SAWs



Two step method for SAWs



Two step method for SAWs



The two-step method

- Weight of a 2-step walk can be calculated in linear time in the size of the allocation graph.
- By counting many configurations at once, the two-step method reduces the complexity.
- Straightforward to prove this for $d \geq 3$ (also true for $d = 2$, but no proof yet).

The lace expansion

- The lace expansion, originally due to Brydges and Spencer, is a method that has been used to study the critical behavior of SAWs and related models above their critical dimension.
- Has not been applied to an enumeration problem before.

The lace expansion

- The number of SAWs of length n may be obtained from the following recursion relation,

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

where π_m can be expressed in terms of the number of lace graphs of length m with N loops:

$$\pi_m = \sum_N (-1)^N \pi_m^{(N)}$$

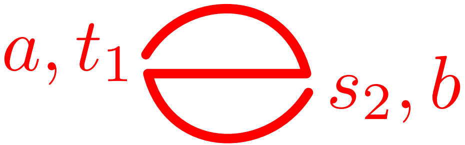
- Lace graphs are less numerous, and therefore easier to count!

The lace expansion

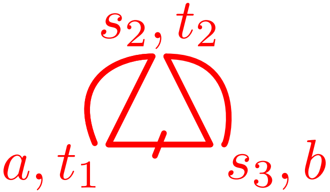
- First of these graphs are paths that avoid themselves until they return to the origin, i.e. graphs which form a single loop.
- Then graphs with $2, 3, 4, \ldots$ loops, represented by the following diagrams.

- $\pi^{(1)}$: start at the origin, must return to the origin.

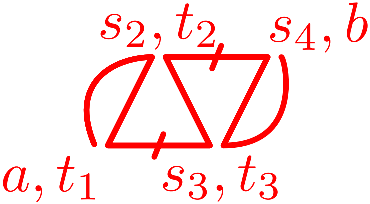
- $\pi^{(2)}$: start at the origin, return to the origin, continue until the first loop is intersected.



- $\pi^{(3)}$:



- $\pi^{(4)}$:



Why are there fewer lace graphs?

- Lace graphs can be thought of as generalised polygons; there are less of them because they are less spatially extended than SAWs.
- But only by a polynomial factor! Algorithmic complexity is unchanged, and is still given by the connective constant μ. i.e. for any N

$$\pi_m^{(N)} \sim \mu^m$$

- For $d = 3$, $n = 30$,

$$c_{30} \approx 525\pi_{30}$$

Enumeration results

- Simple cubic lattice

$$
\begin{aligned}
c_{30} &= 270569905525454674614 \\
c_{26} &= 549493796867100942 \\
c_{30}/c_{26} &= 492.3\cdots
\end{aligned}
$$

- Hypercubic lattice, $d = 4$

$$
\begin{aligned}
c_{24} &= 124852857467211187784 \\
c_{19} &= 8639846411760440 \\
c_{24}/c_{19} &= 14450.8\cdots
\end{aligned}
$$

Enumeration results

- Hypercubic lattice, $d = 5$

$$\begin{aligned} c_{24} &= 6374252557029958121009\,0 \\ c_{15} &= 192003889675210 \\ c_{24}/c_{15} &= 3.3 \times 10^8 \end{aligned}$$

- Hypercubic lattice, $d = 6$

$$\begin{aligned} c_{24} &= 868926509216790410173153\,2 \\ c_{14} &= 37329225326269\,2 \\ c_{24}/c_{14} &= 2.3 \times 10^{10} \end{aligned}$$

- Our enumerations for $n = 24$ allow us to calculate c_{24} for any dimension.

$1/d$ expansion for μ

- $1/d$ asymptotic expansion for the connective constant, with error estimate,

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

- Similar formulae for A and D.

Analysing the series

- Complicated, because series are far from the asymptotic regime, and the corrections to scaling are large.
- Used differential approximants and direct fitting of the asymptotic form.
- For $d = 3$, we obtain the most accurate value available for $\mu = 4.684043(12)$ (c.f. $\mu = 4.68404(9)$). Estimates of critical exponents of comparable accuracy to the best available Monte-Carlo estimates.
- Estimates of μ for $d \geq 4$ are competitive with those obtained via the PERM algorithm by Owczarek and Prellberg.

- Significantly extended SAW series for $d \geq 3$ by combining two algorithmic improvements, the lace expansion and the two-step method.
- Obtained improved estimates of critical parameters through detailed series analysis.
- Both the lace expansion and the two-step method can be reformulated and applied to enumeration problems on arbitrary graphs.

- Preprint available at `http://www.math.ubc.ca/~slade/se.pdf` (submitted to J. Phys. A).
- All enumeration data at `http://www.math.ubc.ca/~slade/lacecounts`