Enumeration of SAWs via the lace expansion

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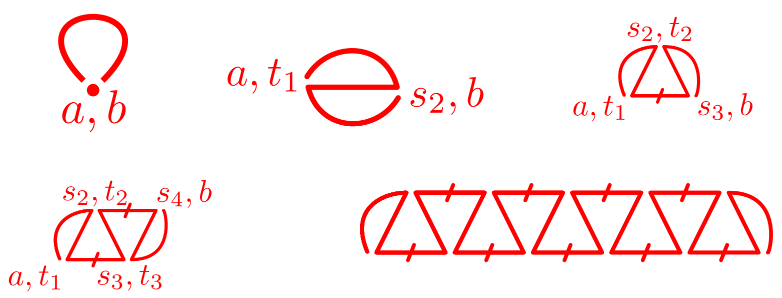
The self-avoiding walk model (SAW)

- A SAW is a path on a lattice, which starts at the origin and hops successively to neighbouring grid points, but without intersecting itself.
- We count all the SAWs of length n, c_n, and wish to know how c_n grows as the length increases.
- Enumeration gives exact answers for relatively small values of n; difficult because c_n grows exponentially.
- Very impressive results have been achieved via the finite lattice method for the square lattice, up to $n = 71$.
- For higher dimensions the best literature values for $d = 3, 4, 5, 6$ are $n = 26, 19, 15, 14$ respectively.
- We improve on existing enumerations for $d \geq 3$ via the lace expansion and the two-step method.

Lace expansion

- Instead of counting SAWs, the lace expansion allows us to count other, less numerous, graphs, and then use this information to obtain c_n.
- The first of these graphs are paths that avoid themselves until they return to the origin, i.e. graphs which form a single loop. Then there are graphs with $2, 3, 4, \ldots$ loops, which are represented by the following diagrams:



- We enumerate $\pi_m^{(N)}$ ($r_m^{(N)}$), which gives us π_m (r_m) via:

$$\pi_m = \sum_{N=1}^{m-1} (-1)^N \pi_m^{(N)} \quad \text{and} \quad r_m = \sum_{N=1}^{m-1} (-1)^N r_m^{(N)}.$$

- From the π_m and r_m we recursively determine c_n and ρ_n:

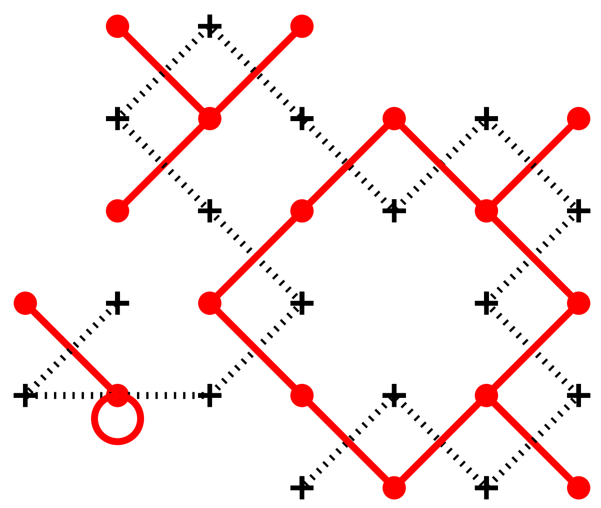
$$c_n = 2dc_{n-1} + \sum_{m=2}^{n} \pi_m c_{n-m}$$

$$\rho_n = 2dc_{n-1} + 2d\rho_{n-1} + \sum_{m=2}^{n} r_m c_{n-m} + \sum_{m=2}^{n} \pi_m \rho_{n-m}.$$

- For the square lattice there are approximately 36 times as many 30 step SAWs as there are lace graphs.
- For the cubic lattice this ratio is approximately 525.
- For $d = 4$, $n = 24$ it is 1700, for $d = 5$, $n = 24$, it is 6200, while for $d = 6$, $n = 24$, it is 20000.

Two-step method

- This additional algorithmic improvement allows us to count many SAW configurations simultaneously.
- A 2-step walk, Ω, is a sequence of endpoints from taking two steps at once; the allocation graph corresponding to Ω is in red.



- For the allocation graph of Ω we define: $\mathcal{T}_\Omega$ is the set of connected components of $\mathcal{G}_\Omega$ which are trees; $\mathcal{C}_\Omega$ is the set of connected components of $\mathcal{G}_\Omega$ which contain exactly one cycle but no loop; $\mathcal{L}_\Omega$ is the set of connected components of $\mathcal{G}_\Omega$ which contain exactly one loop but no cycle.
- The weight of a two-step walk Ω is then given by

$$W(\Omega) = I_\Omega 2^{|\mathcal{C}_\Omega|} \prod_{T \in \mathcal{T}_\Omega} N_T$$

where I_Ω is an indicator function which is zero if any connected component has multiple loops and/or cycles.

- Weight can be calculated in linear time in the size of the allocation graph.
- Time to enumerate SAWs of length n, $\tau(n) \sim \kappa^n$, where $\kappa < \mu$. Therefore the complexity is reduced!
- For $d = 3$, $\kappa \approx 4.0$ c.f. $\mu \approx 4.684$.

Results

- Enumerated SAWs in $d = 3$ to $n = 30$; $c_{30} = 270569905525454674614$.
- SAWs in all dimensions $d \geq 4$ to $n = 24$.
- Self-avoiding polygons in $d = 3$ to $n = 32$ (single loops).
- Dramatically increased length of the $1/d$ expansion for the connective constant:

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

Analysis

- Analysed series using the method of differential approximants. Estimates for critical exponents were slow to converge due to strong confluent corrections.
- Direct fitting, where one fits a presumed asymptotic form to the higher order coefficients was more effective.
- For the simple cubic lattice the asymptotic form used was:

$$c_n \sim \mu^n n^{\gamma-1}\left(A + \frac{a_1}{n^\theta} + \frac{a_2}{n} + \frac{a_3}{n^{1+\theta}} + \frac{a_4}{n^2} + \cdots\right) + \mu^n(-1)^n n^{\alpha-2}\left(b_0 + \frac{b_1}{n^\theta} + \frac{b_2}{n} + \frac{b_3}{n^{1+\theta}} + \frac{b_4}{n^2} + \cdots\right).$$

- A range of values for the correction to scaling exponent, θ, were used. It was a large source of uncertainty.
- Fitted asymptotic forms for $\log c_n$, c_n/c_{n-1}, and c_n/c_{n-1}.
- Estimates of μ, γ and ν for $d = 3$ (estimates of the amplitudes A and D also available).

	μ	γ	ν
$0.47 \leq \theta \leq 0.5$	4.684044(11)	1.1566(6)	0.5874(2)
$0.47 \leq \theta \leq 0.56$	4.684043(12)	1.1568(8)	0.5876(5)
MacDonald et al.	4.68404(9)	1.1585	0.58755
Prellberg			0.5874(2)
Caracciolo et al.		1.1575(6)	

- Higher dimensional results for μ, compared with the Monte-Carlo work of Owczarek and Prellberg.

$d = 4$	$d = 5$	$d = 6$	$d = 7$
6.774168(32)	8.8385451(90)	10.8780919(21)	12.9028174(53)
6.774043(5)	8.838544(3)	10.878094(4)	12.902817(3)

Further Reading

- Preprint at `http://www.math.ubc.ca/~slade/se.pdf`
- All enumeration data at `http://www.math.ubc.ca/~slade/lacecounts`
- Gordon Slade, The Lace Expansion and its Applications, for the Summer School on Probability at UBC, 2005.
- D. MacDonald, S. Joseph, D. L. Hunter, L. L. Moseley, N. Jan and A. J. Guttmann, *J. Phys. A*, **33**, 5973–5983 (2000).
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- S. Caracciolo, M.S. Causo, and A. Pelissetto, *Phys. Rev. E*, **57**:1215–1218, (1998).
- A.L. Owczarek and T. Prellberg, *J. Phys. A: Math. Gen.*, **34**:5773–5780, (2001).