Endless self-avoiding walks

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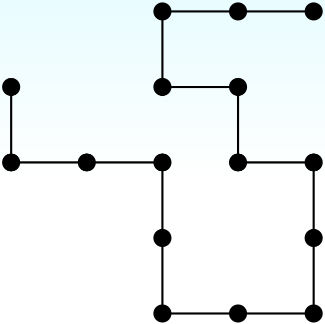
Outline

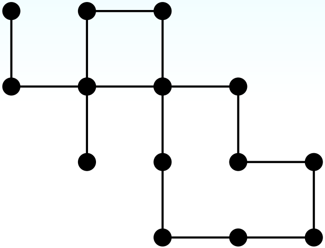
- Introduction
- Why?
- The eSAW model
- Series
- Series analysis
- Future work

Self-avoiding walk model

- A walk on a lattice, step to neighbouring site provided it has not already been visited.
- n-step SAW on $\mathbb{Z}^d$ is a mapping $\omega : \{0, 1, \ldots, n\} \to \mathbb{Z}^d$ with $|\omega(i+1) - \omega(i)| = 1$ for each i ($|x|$ denotes the Euclidean norm of x), and with $\omega(i) \neq \omega(j)$ for all $i \neq j$.
- For uniqueness, choose $\omega(0) = 0$.
- Models polymers in good solvent limit.
- *Exactly* captures universal properties such as critical exponents.
- Important both for theoretical understanding of critical phenomena, and real polymers.
- WOS: more than 1800 articles with SAW in title / abstract.



SAW



Not a SAW

Critical phenomena

- The number of SAW of length N, c_N, tells us about how many conformations are available to SAW of a particular length:

$$c_N \sim A\ N^{\gamma-1}\mu^N\,[1+\mathrm{corrections}]$$

- Mean square end to end distance tells us about the size of a typical SAW:

$$\langle R_{\mathrm{e}}^2\rangle_N \sim D_e N^{2\nu}\,[1+\mathrm{corrections}]$$

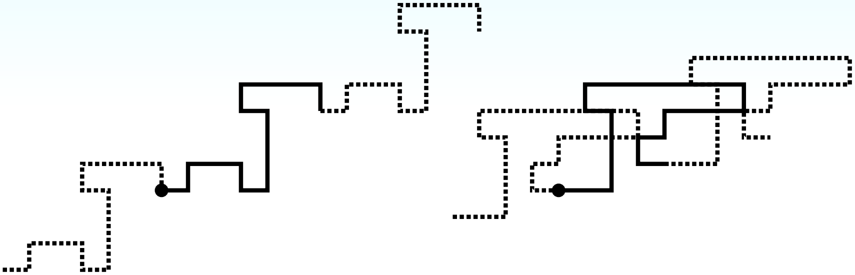
- By *universality* we expect that the critical exponents γ and ν do not depend on the model used. i.e. same for real polymers, SAWs on a lattice, SAWs in a continuum (strong evidence supports this hypothesis).
- μ is the connective constant; lattice dependent.
- Thus far, SAW unsolved, although much progress has been made for $d = 2$, $d \geq 4$.

Why?

- SAW is a model of fundamental importance, any generalisation interesting.
- Making progress in finding solvable models of walks which are ‘closer’ to SAW: directed, partially directed, prudent (1 sided, 2 sided, 3 sided), quasi-prudent.
- This idea goes in other direction, creating a ‘simpler’ model from SAW.
- Similar models: self-avoiding polygons, bridges.

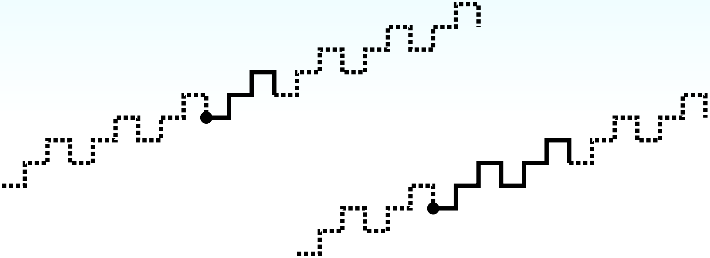
The key idea

- Idea: extend SAW by concatenating head to tail ad infinitum. If result is self-avoiding then it is an eSAW.



Example eSAW on the left; on the right is a SAW which is not an eSAW.

- More natural definition of an endless SAW (to us) is related to a SAW in the same way that a self-avoiding polygon is related to a self-avoiding return – “unrooted” configurations.
- Only interested in equivalence classes of eSAW which correspond to the same ‘shape’, regardless of the root point, or the direction of traversal.
- Additional complication for eSAW which does not occur for SAR / SAP: eSAW can have repeating sub-units which makes the infinite chain corresponding to a given eSAW non-unique.
- See next figure where it can be seen that the same infinite chain results for the two eSAW shown.



Examples of two eSAW which correspond to the same infinite chain. The eSAW on the left is irreducible.

Thus eSAW can also be thought of as infinite chains, where the length n of an eSAW is identified as that of the smallest repeating sub-unit.

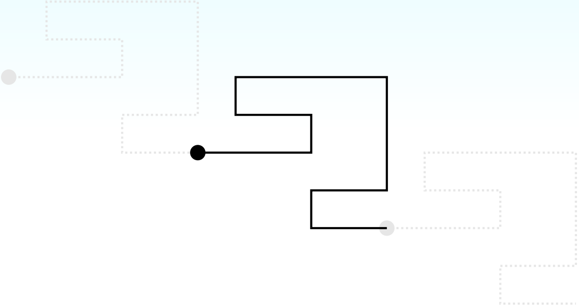
eSAW of 1-4 steps

Alternative definition: words which avoid forbidden subwords (loops).

- On $\mathbb{Z}^d$ the steps in the positive axes directions as $1, 2, \cdots, d$, and the steps in the negative axes directions as $\bar{1}, \bar{2}, \cdots, \bar{d}$.
- SAW of n steps correspond to the set of words which contain no loops, i.e. for which there are no sub-words with equal numbers of 1 and $\bar{1}$, 2 and $\bar{2}$, $\cdots$, d and $\bar{d}$.
- E.g. $12\bar{1}\bar{2}$ is a square loop.

- eSAW if infinite word from repeated concatenation has no loops.
- E.g., if we have a SAW, $1221\bar{2}$, then the corresponding eSAW is $\cdots 1221\bar{2}\ 1221\bar{2}\ 1221\bar{2} \cdots$.

Bridge: a SAW for which the x coordinate of the first site lies to the left of all others, and the last site is at least as far to the right as others.



- Bridges $\subseteq$ eSAW $\subseteq$ SAW. Since bridges and SAW have growth constant μ, eSAW must also have growth constant μ.
- In fact expect that

$$e_n = A\mu^n n^{\gamma_{eSAW}-1}(1 + o(1))$$

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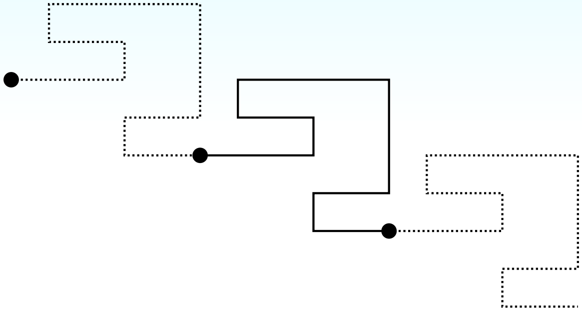

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- For SAW, *gamma* > 1 from direct renormalization arguments, because ends have more freedom than interior (true for $d < 4$).
- Expect that eSAW have $\gamma_{eSAW} = 1$ due to complete absence of end effects.
- $\Rightarrow$ Growth of eSAW purely exponential, $e_n \sim A\mu^n(1 + o(n))$.
- No effect on ν (average shape unaffected, end-effect is small)
- Identical amplitude for leading non-analytic correction to scaling?? (Reasoning: short distance physics inside chain is unaltered by global 'endless' condition)

- eSAW have genuine knots, unlike SAW.
- No end-effects may mean that data are cleaner for other observables.
- In some sense a generalisation of directed walks: walks which are endless as they are grown incrementally correspond to directed walks.

Enumeration method

- Enumerate walks to obtain information about eSAW.
- For the moment, using simplest approach: direct enumeration via backtracking.
- Don't need to generate full set of SAW, for end vector v use congruence $x/v = y/v$ to determine self-intersections.
- Utilise lattice symmetry, factor of 8 for $\mathbb{Z}^2$, 48 for $\mathbb{Z}^3$ (could get factor of n from lexicographic ordering)

n	e_n	r_n	irreducible eSAW	i_n
1	4	4	4	2
2	12	32	8	2
3	28	156	24	4
4	76	640	64	8
5	204	2380	200	20
6	540	8304	504	42
7	1404	27580	1400	100
8	3724	89216	3648	228
9	9748	280980	9720	540
10	25772	869360	25560	1278
11	67940	2649284	67936	3088
12	179068	7967808	178464	7436
...	...	...	...	...
34	331633319500804	70954363887188496	331633296639192	4876960244694
35	874875502020444	195525476447120540	874875502018840	12498221457412

n	e_n	r_n	irreducible eSAW	i_n
1	6	6	6	3
2	30	72	24	6
3	126	558	120	20
4	606	3744	576	72
5	2766	23070	2760	276
6	13134	135288	12984	1082
7	60990	764862	60984	4356
8	286014	4214784	285408	17838
9	1333926	22773798	1333800	74100
10	6235950	121158840	6233160	311658
11	29160390	636821526	29160384	1325472
12	136280046	3312601632	136266336	5677764
...	...	...	...	...
23	3213444320539710	172198320473193822	3213444320539704	69857485229124
24	15042778398965358	848672945442198144	15042778262399904	313391213799998

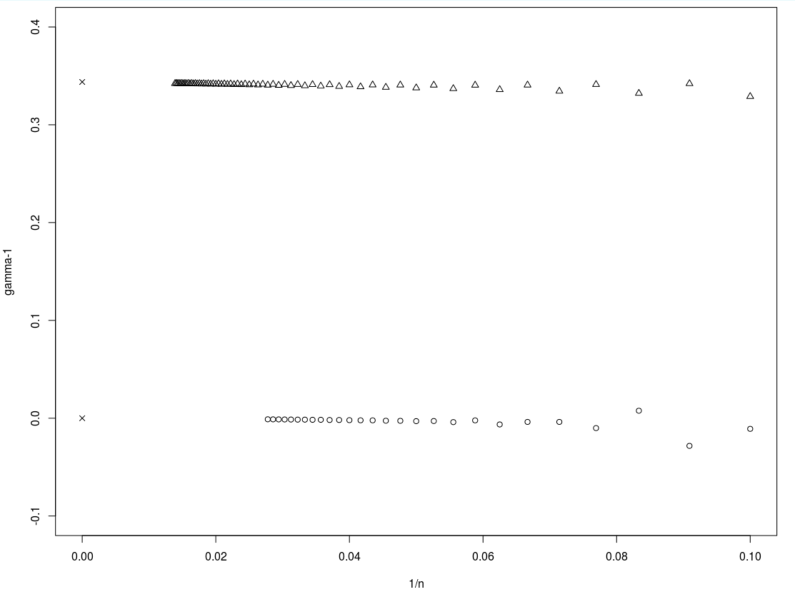
Analysis

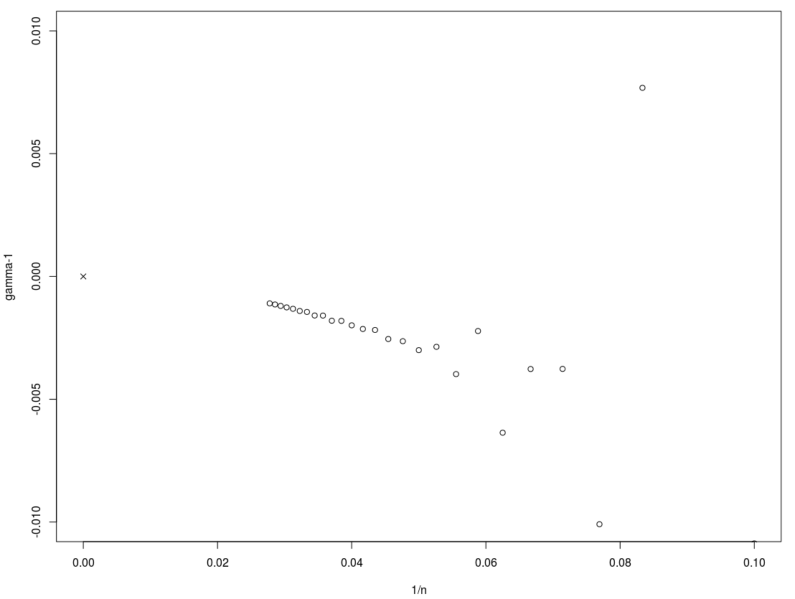
- Use method of *direct fitting* to determine asymptotic behaviour. Trick is to fit consecutive terms from series with asymptotic form.
- For short series, essentially equivalent to ratio method.
- Have advantage that μ, γ, ν are known with high precision from other work (numerical and exact results).

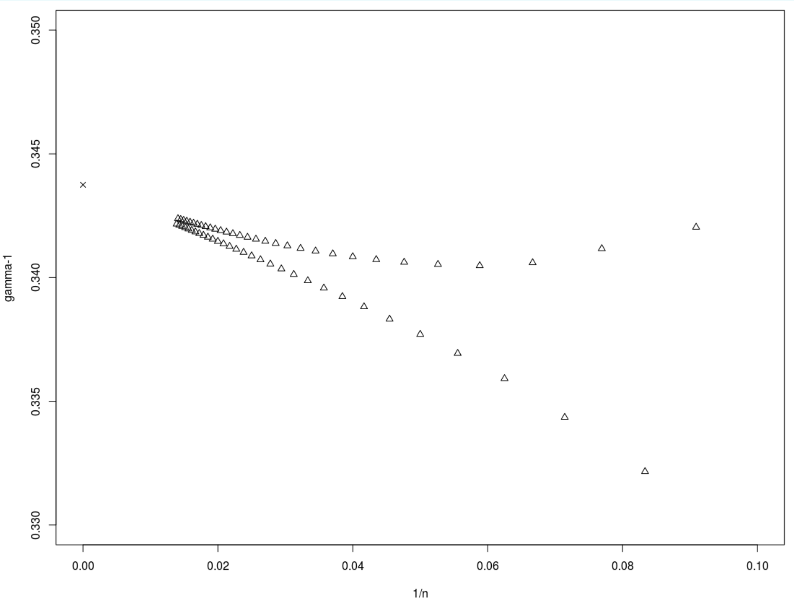
Estimates of γ for $\mathbb{Z}^2$, via

$$\frac{c_n}{c_{n-2}} \sim \frac{A\mu^n n^{\gamma-1}(1+\cdots)}{A\mu^{n-2}(n-2)^{\gamma-1}(1+\cdots)}$$

$$\sim \mu^{-2}\left(1-\frac{2}{n}\right)^{1-\gamma}(1+\cdots)$$

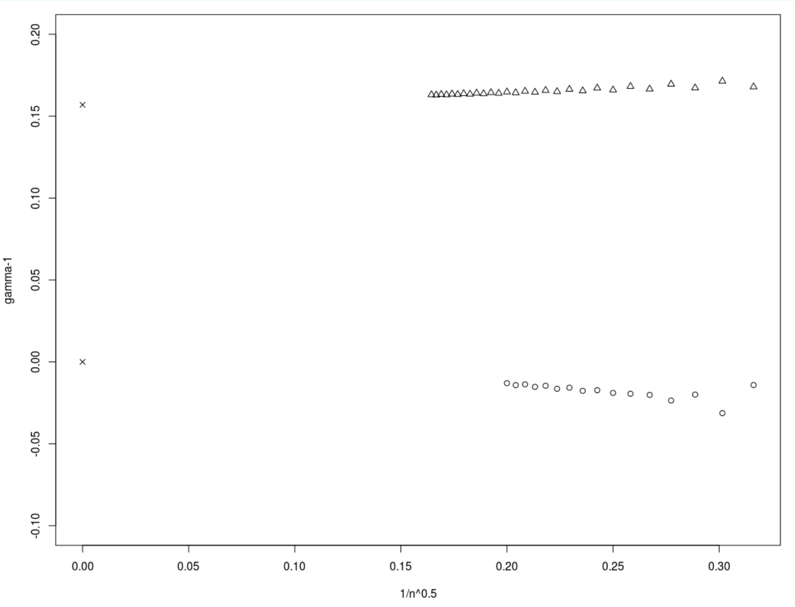

gamma-1
1/n
0.00
0.02
0.04
0.06
0.08
0.10
-0.1
0.0
0.1
0.2
0.3
0.4

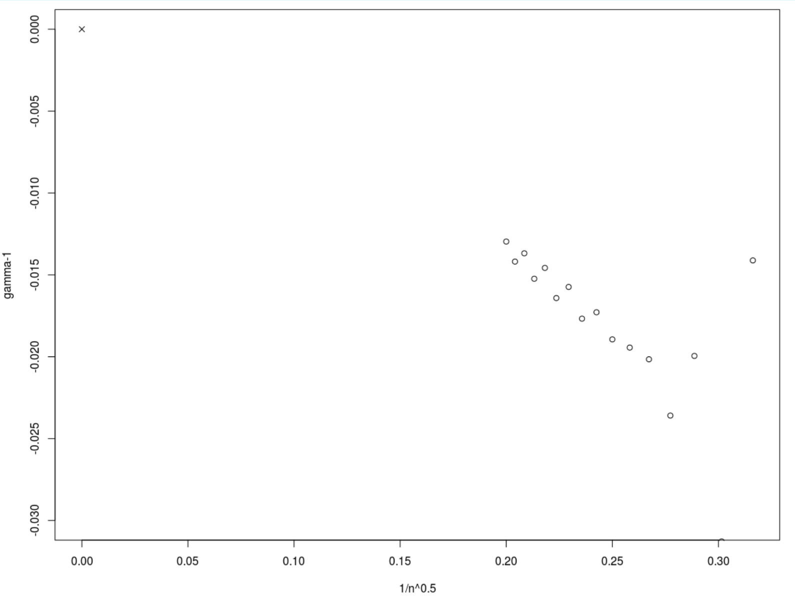

gamma-1
0.010
0.005
0.000
-0.005
-0.010
0.00
0.02
0.04
0.06
0.08
0.10
1/n


0.350
0.345
0.340
0.335
0.330
gamma-1
0.00
0.02
0.04
0.06
0.08
0.10
1/n

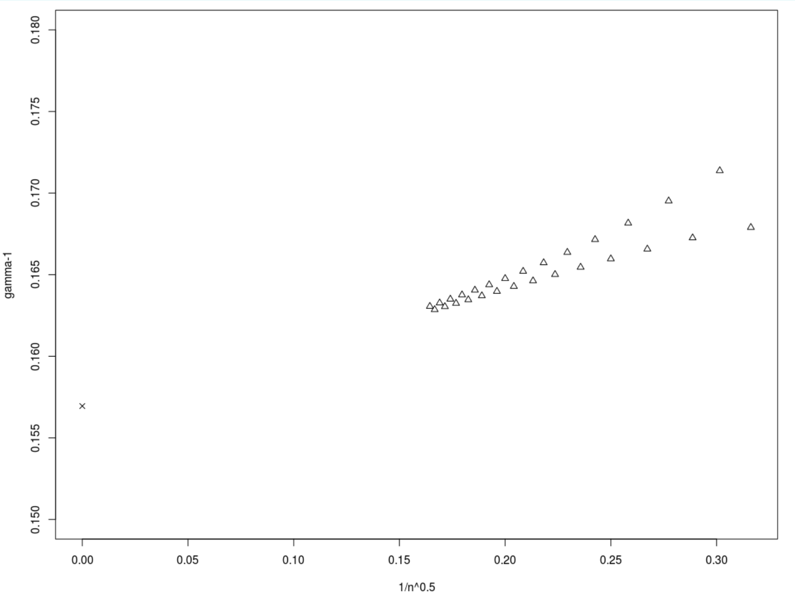
Estimates of γ for $\mathbb{Z}^3$, via

$$\frac{c_n}{c_{n-2}} \sim \frac{A\mu^n n^{\gamma-1}(1+\cdots)}{A\mu^{n-2}(n-2)^{\gamma-1}(1+\cdots)}$$
$$\sim \mu^{-2}\left(1-\frac{2}{n}\right)^{1-\gamma}(1+\cdots)$$

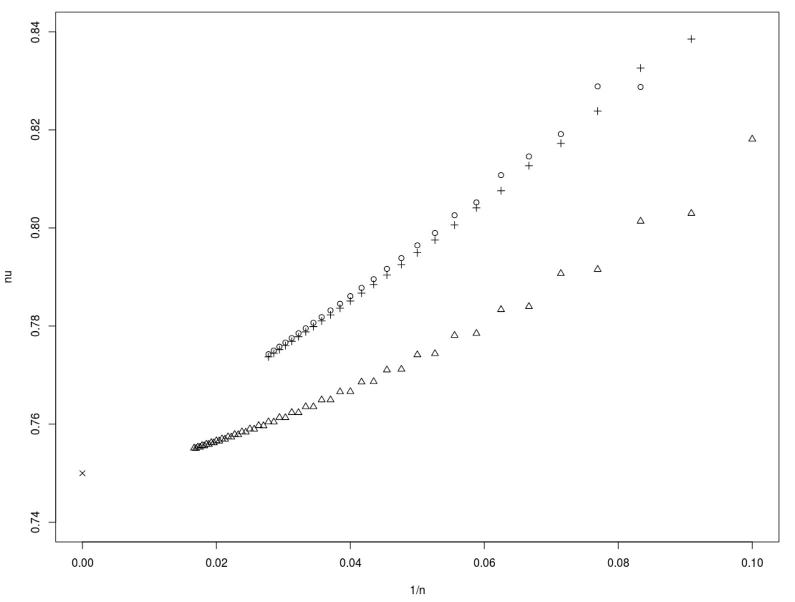

gamma-1
0.20
0.15
0.10
0.05
0.00
-0.05
-0.10
0.00
0.05
0.10
0.15
0.20
0.25
0.30
1/n^0.5



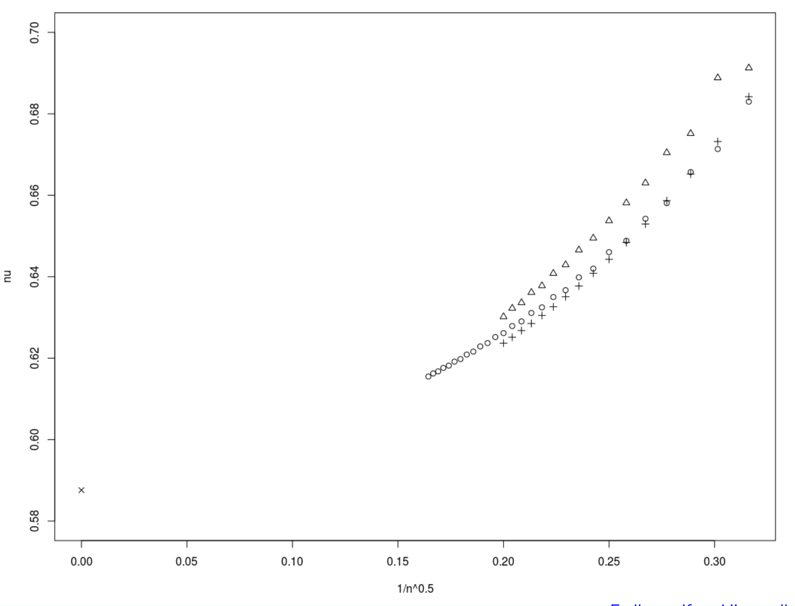
gamma-1
0.000
-0.005
-0.010
-0.015
-0.020
-0.025
-0.030
0.00
0.05
0.10
0.15
0.20
0.25
0.30
1/n^0.5


gamma-1
1/n^0.5
0.150
0.155
0.160
0.165
0.170
0.175
0.180
0.00
0.05
0.10
0.15
0.20
0.25
0.30

Estimates of ν for $\mathbb{Z}^2$



Estimates of ν for $\mathbb{Z}^3$



Results

- $\gamma = 1$ to fair precision.
- ν same as for SAW, to fair precision.
- No clear result (yet) for corrections to scaling.

Questions

- Is the pivot algorithm ergodic on eSAW?
- Are the (leading order) corrections to scaling really the same as for SAW? (test with Monte Carlo)
- Are there any other interesting properties of eSAW?

Future

- Will allow significant improvement in estimate of γ for $d = 3$ via Monte Carlo. (Estimate probability that a SAW is eSAW)
- Nail down corrections to scaling.
- Adapt FLM enumeration method to eSAW?
- Apply to other models: ISAW, self-avoiding trails.
- Self-avoiding networks? (repeated star polymers)
- Generalisations? (if eSAW is an analogue of directed walk, is there an analogue to partially directed walks?)