There are $7 \times 10^{26\,018\,276}$ self-avoiding walks of 38 797 311 steps on $\mathbb{Z}^3$

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The University of Ballarat
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Outline

- Self-avoiding walks
- Enumeration
- Direct sampling and weighted sampling (PERM)
- Ingredients for efficiently estimating c_N
  - Global move (pivot)
  - Efficient data structure (SAW-tree)
  - Clever choice of observable
  - Minimizing statistical error
- Results and conclusion

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Self-avoiding walk model

- A walk on a lattice, step to neighbouring site provided it has not already been visited.
- Models polymers in good solvent limit.
- Exactly captures universal properties such as critical exponents.
- 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 $i \neq j$.
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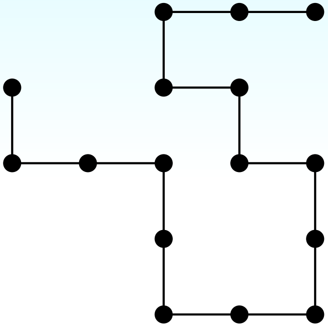
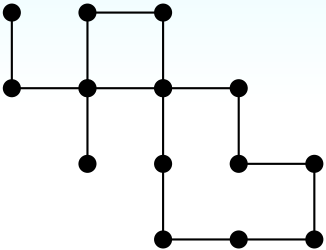


SAW



Not a SAW

Asymptotic behaviour

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

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

- For $\mathbb{Z}^2$, $c_N = 1, 4, 12, 36, 100, 284, 780, 2172, \cdots$
- For $\mathbb{Z}^3$, $c_N = 1, 6, 30, 150, 726, 3534, \cdots$
- γ is a *universal* exponent.
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- So, transform problem and count something else.
- For 2d lattices: finite lattice method extremely powerful. Count boundary states instead of walks, $O(1.3^n)$ (unfortunately, still exponential). Recently, Iwan Jensen found $c_{79} = 10194710293557466193787900071923676$ for $\mathbb{Z}^2$!
- For 3d lattices: most powerful method "length-doubling algorithm", combines brute force enumeration with inclusion-exclusion. $O(\mu^n) \to O((\sqrt{2\mu})^n)$[1].
- I think there are strong prospects to apply length-doubling algorithm to other problems, and improve its efficiency.
- $c_{36} = 2941370856334701726560670$ for $\mathbb{Z}^3$.
- Series analysis used to extract information about asymptotic behaviour.

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- Obvious approach: simple sampling. Generate a simple random walk of length N, calculate probability that RW is self-avoiding. Probability $= c_N/(2d)^N \approx 4.68^N/6^N$ for $\mathbb{Z}^3$.
- Can improve slightly: forbid immediate reversals in the walk. Probability $= c_n/2d/(2d-1)^{N-1} \approx 4.68^N/6/5^{N-1}$ for $\mathbb{Z}^3$.
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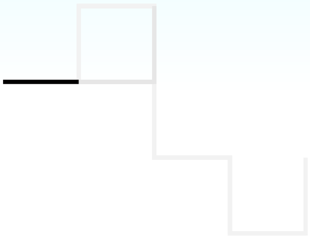

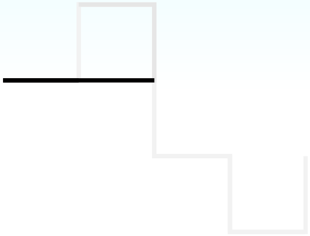

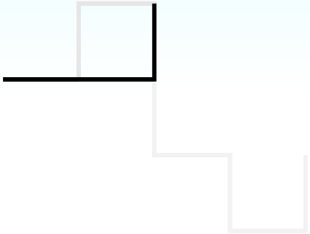

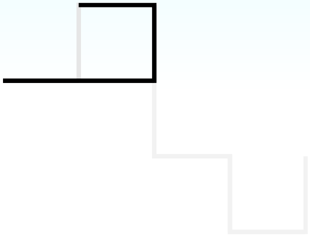

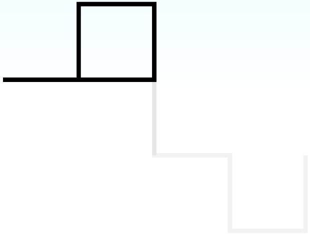

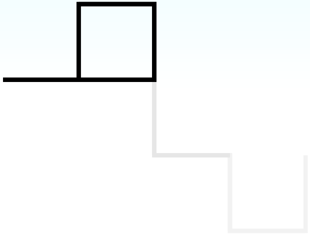

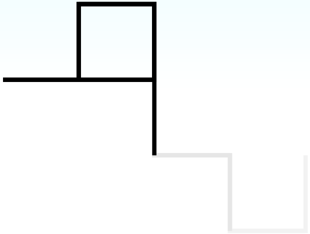

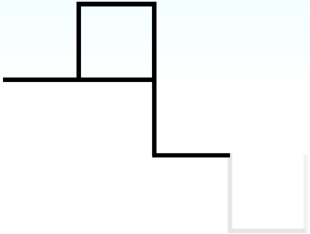

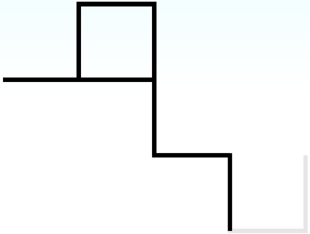

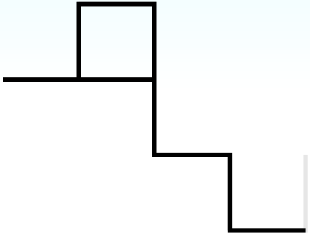

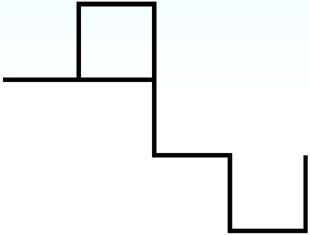

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- This introduces bias: compact walks which have few choices available are preferred.
- Correct bias by weighting walks.
- Weights provide an estimator of c_N, $c_N = \langle W_N \rangle$.
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Factors limiting the efficiency of PERM.

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- Variance of sample is reduced, but not eliminated. (In practice, variance can be essentially eliminated, at the expense of stronger correlation.)
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Pivot algorithm

- Sample from the set of SAWs of a particular length.
- Markov chain:
  - Select a pivot site *uniformly at random.*
  - Randomly choose a lattice symmetry g (rotation or reflection).
  - Apply this symmetry to one of the two sub-walks created by splitting the walk at the pivot site.
  - If walk is self-avoiding: *accept* the pivot and update the configuration.
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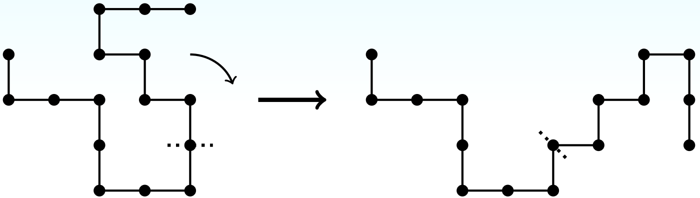

Example pivot move

Why is it so effective?

- Pivots are rarely successful, $\Pr = O(N^{-p})$, $p \approx 0.11$ for $\mathbb{Z}^3$.
- Every time a pivot attempt *is* successful there is a large change in global observables.
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An efficient data structure for SAW

- Represent SAW as a binary tree.
- Enables global moves like pivots to be performed in CPU time $T(N) = O(\log N)$.
- c.f. $O(N^{1-p})$ for hash table implementation[2].
- Dramatic improvement for large N.

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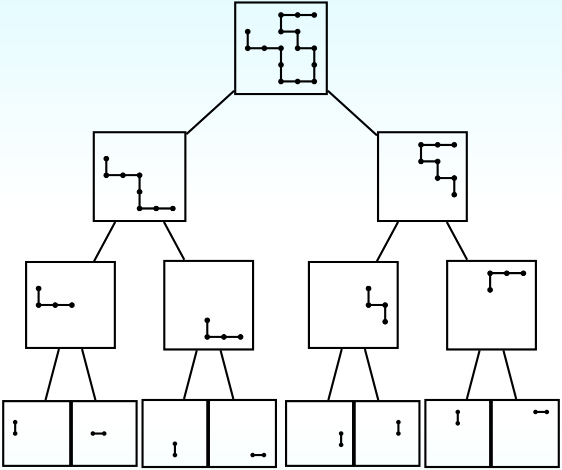

SAW-tree representation of a walk.

How to calculate c_N?

- Would like to apply pivot algorithm in canonical ensemble.
- Approach: measure probability that object from larger set is a SAW, $|S| = P(x \in S | x \in T)|T|$, with $|T|$ known.
- Obvious choice: concatenating pairs of SAWs. Every $M + N$-step walk can be split into M and N step subwalks $\Rightarrow c_{M+N} \leq c_M c_N$ for all M, N.
- S_N set of walks of length N.
- $|S_{M+N}| = P(\omega_1 \circ \omega_2 \in S_{M+N} | (\omega_1, \omega_2) \in S_M \times S_N)|S_M||S_N|$
- Indicator function for successful concatenation is our observable, and

$$B(\omega_1, \omega_2) = \begin{cases} 0 & \text{if } \omega_1 \circ \omega_2 \text{ not self-avoiding} \\ 1 & \text{if } \omega_1 \circ \omega_2 \text{ self-avoiding} \end{cases}$$

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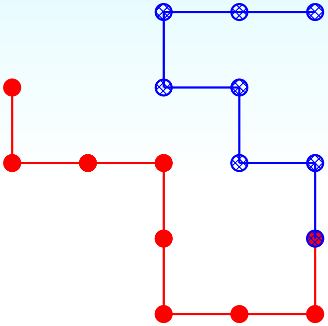

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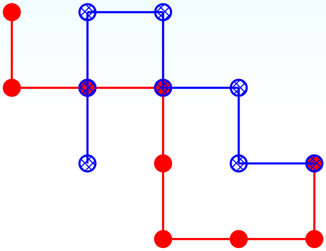

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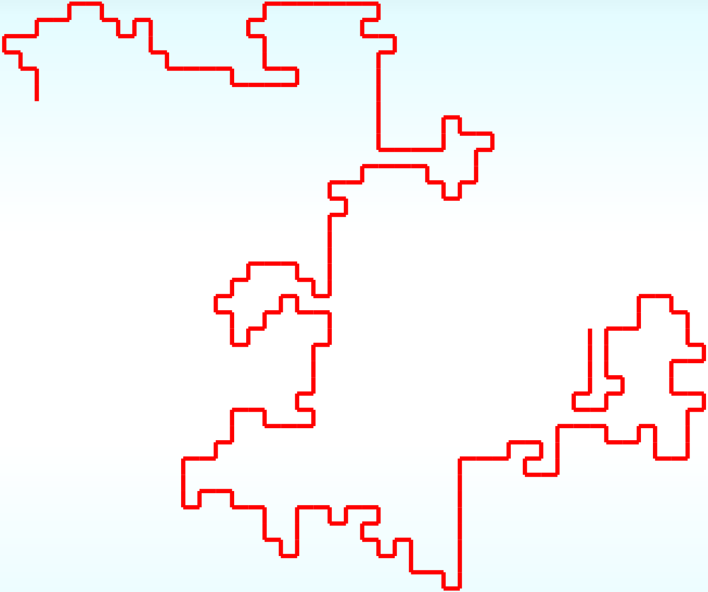
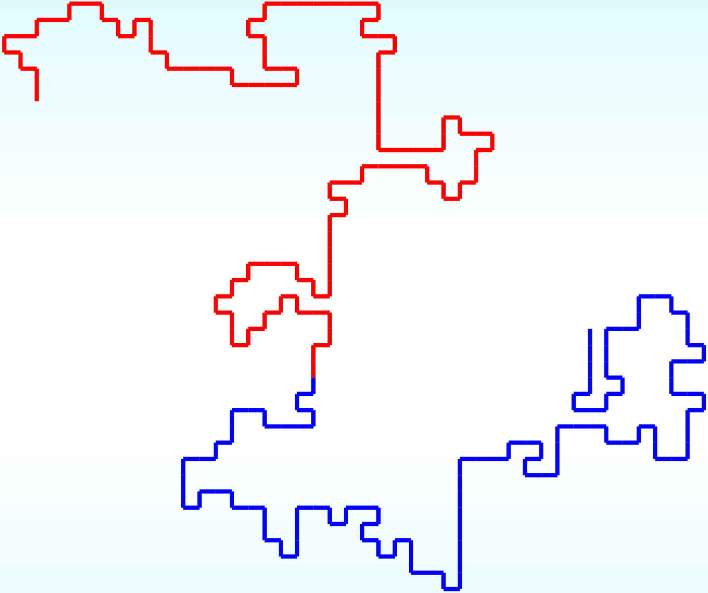
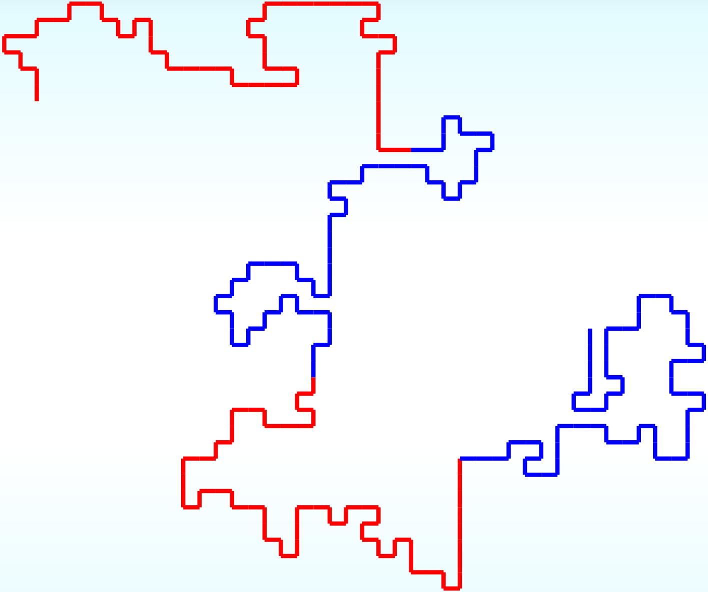
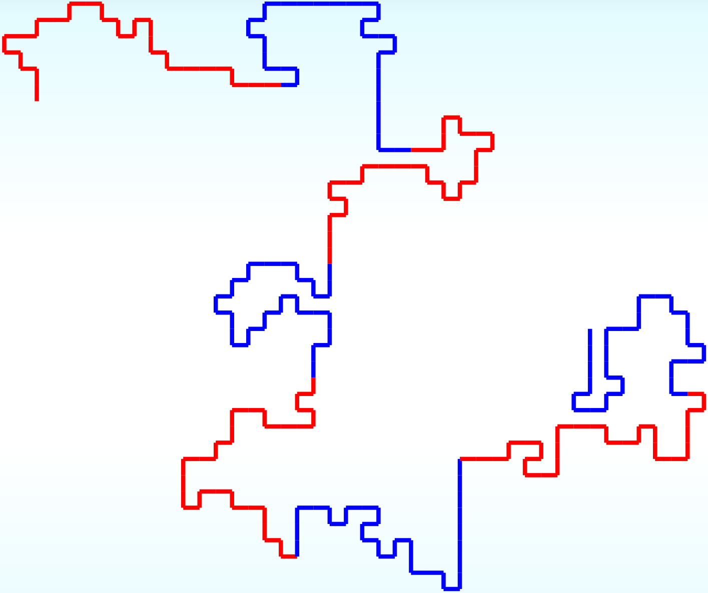
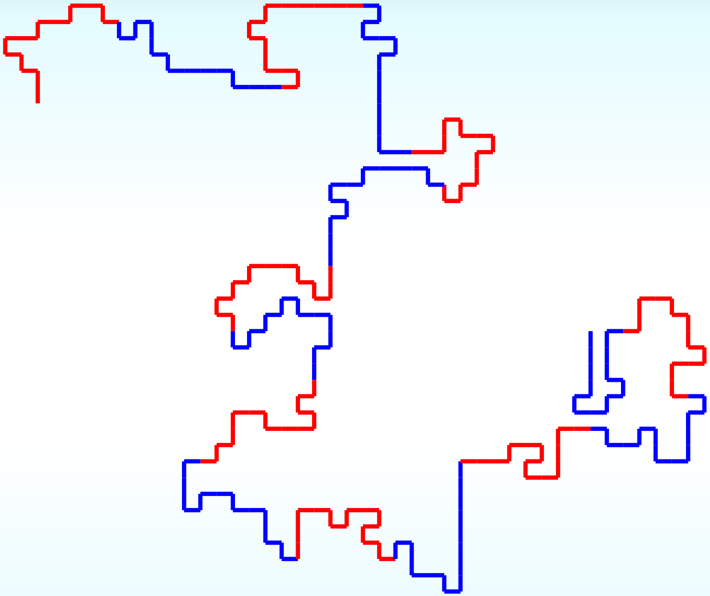
A long N step walk can be successively subdivided into smaller pieces.

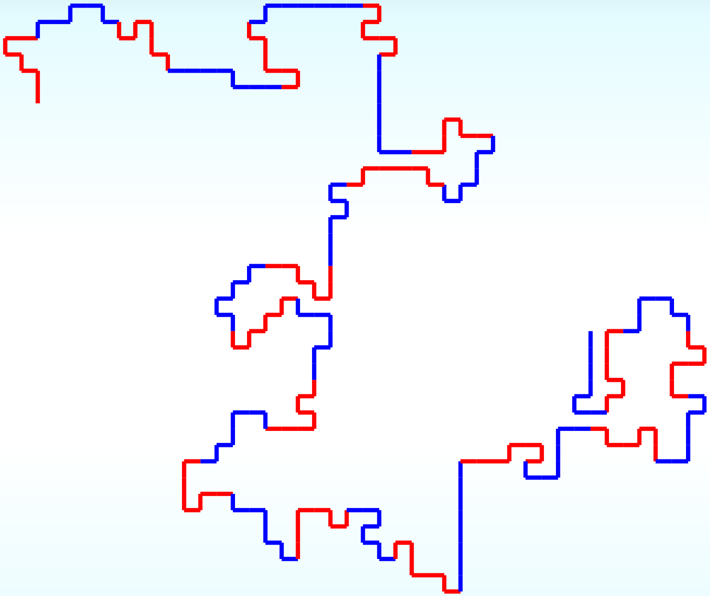


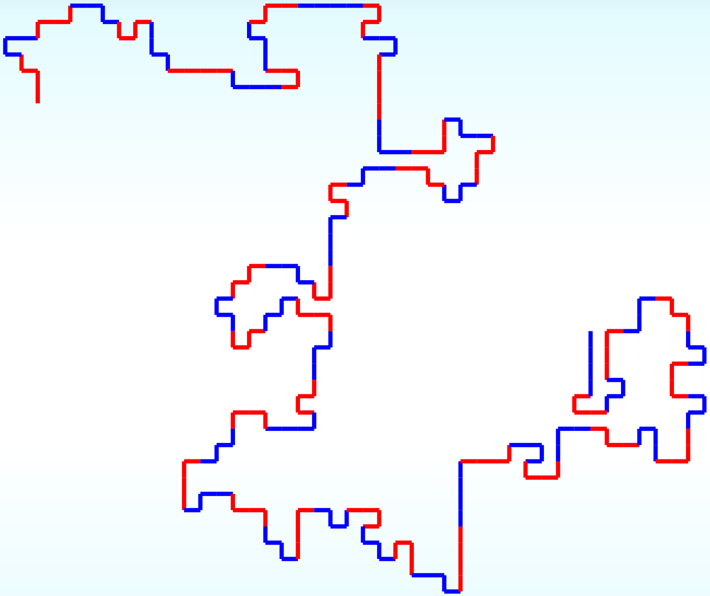


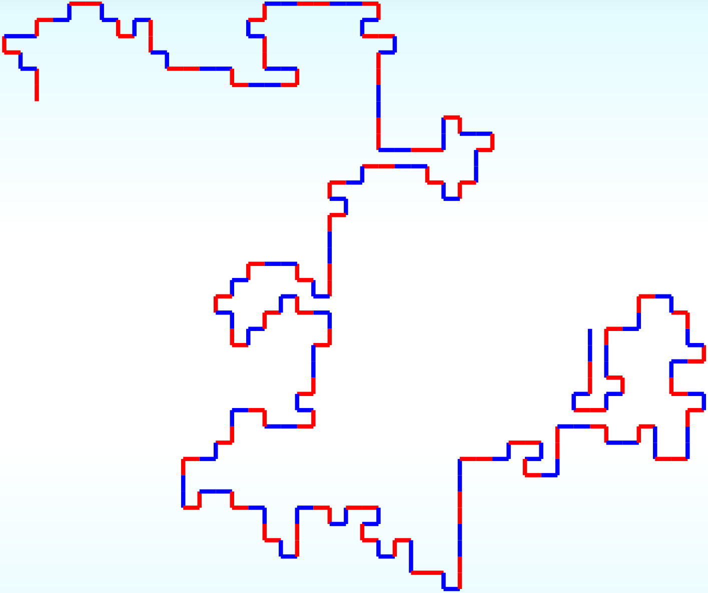


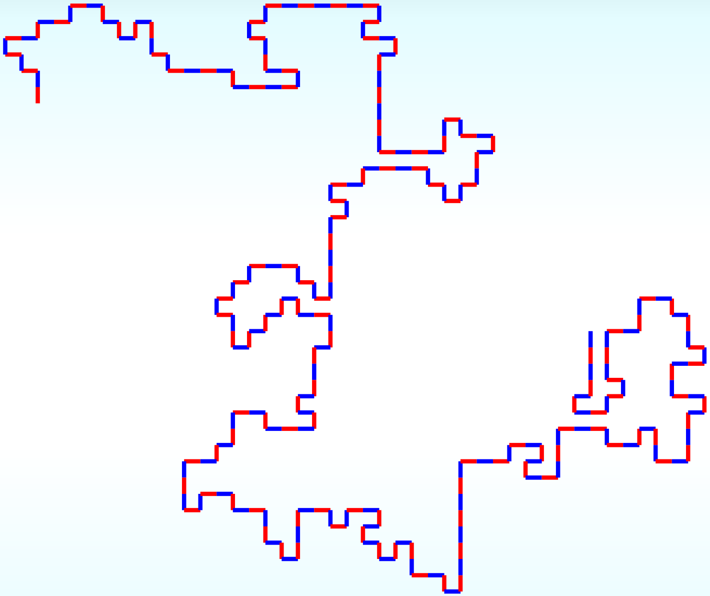












- Could choose $m, n = 36$ (longest known for $\mathbb{Z}^3$):

$$\langle B_{36,36} \rangle = \frac{c_{72}}{c_{36} c_{36}}$$

- Iterate to obtain estimates for c_N for longer walks.

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$$= \log\mu + \frac{(\gamma-1)\log N}{N} + \frac{\log A}{N} + \text{corrections}$$

- Corrections vanish with increasing N! In limit of large N systematic error of estimator $\to 0$.

- Can also use $c_N \sim A\mu^N N^{\gamma-1}$ to estimate μ:

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$$\cdots + \frac{1}{N}\log\langle B_{N/2,N/2}\rangle$$
$$= \log\mu + \frac{(\gamma-1)\log N}{N} + \frac{\log A}{N} + \text{corrections}$$

- Corrections vanish with increasing N! In limit of large N systematic error of estimator $\to 0$.

Scale free moves

- Need to calculate $\langle B_{k,k} \rangle$, $\langle B_{2k,2k} \rangle$, $\cdots$
- Use pivot algorithm / SAW-tree.
- How many pivots must be completed before two walks are "essentially new" configurations with respect to observable B?
- Shape of walks close to the joint clearly important.
- Uniform pivot sites: $\widetilde{\tau}_{\mathrm{int}} = \Omega(N)$.
- Choose distance from joint uniformly from all distance scales, i.e. $u = \log(\text{distance})$ chosen uniformly at random.
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Error estimate

- Expected error, for same CPU time, diminishes as a power law for higher order terms in the sum!

$$\log c_N = \frac{N}{k} \log c_k + \frac{N}{2k} \log\langle B_{k,k}\rangle + \cdots + \log\langle B_{N/2,N/2}\rangle$$

- Partition CPU time amongst different terms to minimize overall statistical error (short test run).

$$\sigma^2 = \sum \frac{a_i^2}{t_i} \qquad \text{Total time } t = \sum t_i$$

$$\Rightarrow t_i = \frac{a_i}{\sum a_i} t, \qquad \sigma = \frac{\sum a_i}{\sqrt{t}}$$

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Results

- Calculated $\log c_N$ with relative error of approximately 4×10^{-9} up to $N = 38797311$ (about 60000 CPU hours).
- Concentrated on $\mathbb{Z}^3$ because asymptotic behaviour for $\mathbb{Z}^2$ well understood from series.
- $c_{9471} = 1.43323(8) \times 10^{6352}$
- $c_{38797311} = 7 \times 10^{26018276}$. Confidence interval of mantissa is $(6.6, 8.2)$.
- For comparison, see[3]. Relative error from PERM and related algorithms of the order of 10^{-3} for short walks of 100 steps. Not a fair comparison:
  - Not much CPU time used, i.e. not serious computer experiments.
  - Estimates would degrade for large N. Best case: error increasing as $O(\sqrt{N})$.

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- Different ingredients fit together to produce extremely accurate estimates.
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