How to calculate the connective constant for self-avoiding walks really, really accurately

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Outline

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- Introduction
- Advances in algorithms for SAW
- Finding a suitable observable
- Advances in Monte Carlo “move sets”
- Minimizing statistical error
- Conclusion

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- 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.

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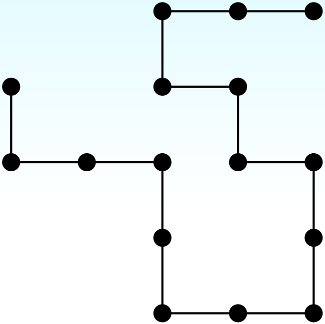
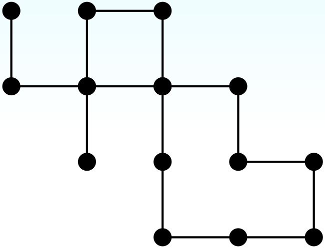


SAW



Not a SAW

Animation

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:

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

- γ is a universal exponent.
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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.
  - If walk is not self-avoiding: *reject* the pivot and keep the old configuration.
- Ergodic, samples SAWs uniformly at random.

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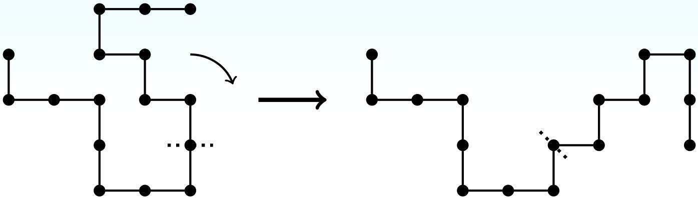

Example pivot move

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.
- Only need $O(1)$ successful pivots before we have an *essentially new* configuration.
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"For SAWs in planar geometry, the fastest known algorithm is the pivot algorithm - at least if one is not interested in mu"

As we'll see, the pivot algorithm does a pretty good job of calculating μ.

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- Define: $\widetilde{\tau}_{\mathrm{int}} = \tau_{\mathrm{int}} T(N)$, integrated autocorrelation time in CPU units.
- When estimating mean value of an observable, run for CPU time t: Error $\propto \sqrt{\widetilde{\tau}_{\mathrm{int}}/t}$.
- SAW-tree: $\widetilde{\tau}_{\mathrm{int}} = O(N^p \log N)$ for pivot algorithm (c.f. $O(N)^2$).
- Dramatic improvement for large N.
- Thus far $\nu = 0.587597(7)$[3] and $\gamma = 1.156957(9)$ (in preparation).

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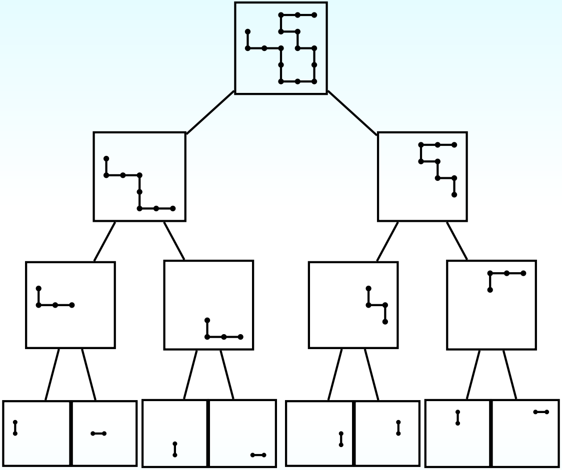

SAW-tree representation of a walk.

How to calculate μ?

- Effectively need to count SAW to determine μ.
- 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.
- 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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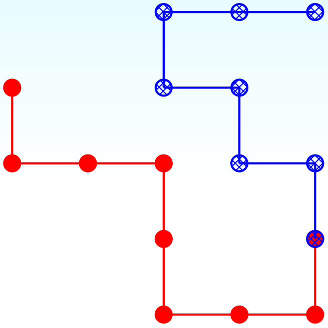
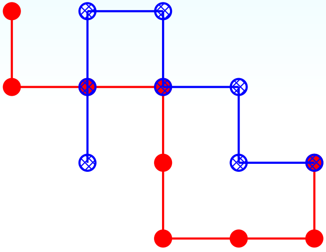


$B(\omega_1, \omega_2) = 1$



$B(\omega_1, \omega_2) = 0$

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

$$\langle B_{N,36} \rangle = \frac{c_{N+36}}{c_N c_{36}} = \frac{1}{c_{36}} \mu^{36} \left(1 + \frac{36(\gamma - 1)}{N} + \cdots \right)$$

- Direct calculation of μ, idea closely related to atmospheres[4].
- Effective, but can do better. Performance penalty due to large N, $\widetilde{\tau}_{\mathrm{int}} = O(N^p \log N)$.

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$$\langle B_{36,36} \rangle = \frac{c_{72}}{c_{36} c_{36}} = \frac{1}{c_{36}^2} \mu^{72} \left(1 + \frac{\gamma - 1}{72} + \cdots \right)$$

- Need a way to improve these estimates and approach the asymptotic regime.
- Use:

$$c_N = \frac{c_N}{c_{N/2}^2} \cdot \frac{c_{N/2}^2}{c_{N/4}^4} \cdots \frac{\cdots}{c_k^{N/k}}$$

where c_k is known.

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$$\langle B_{36,36} \rangle = \frac{c_{72}}{c_{36} c_{36}} = \frac{1}{c_{36}^2} \mu^{72} \left(1 + \frac{\gamma - 1}{72} + \cdots \right)$$

- Need a way to improve these estimates and approach the asymptotic regime.
- Use:

$$c_N = \frac{c_N}{c_{N/2}^2} \cdot \frac{c_{N/2}^2}{c_{N/4}^4} \cdots \frac{\cdots}{c_k^{N/k}}$$

where c_k is known.

- In terms of B:

$$\begin{aligned}
\log \mu_N &= \frac{1}{N} \log c_N \\
&= \frac{1}{k} \log c_k + \frac{1}{2k} \log \frac{c_{2k}}{c_k^2} + \frac{1}{4k} \log \frac{c_{4k}}{c_{2k}^2} + \cdots \\
&\qquad \cdots + \frac{1}{N} \log \frac{c_N}{c_{N/2}^2} \\
&= \frac{1}{k} \log c_k + \frac{1}{2k} \log \langle B_{k,k} \rangle + \frac{1}{4k} \log \langle B_{2k,2k} \rangle + \cdots \\
&\qquad \cdots + \frac{1}{N} \log \langle B_{N/2,N/2} \rangle \\
&= \log \mu + \frac{(\gamma - 1) \log N}{N} + \frac{\log A}{N} + \text{corrections}
\end{aligned}$$

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.
- Now: $\widetilde{\tau}_{\mathrm{int}} = N^p \log^2 N$.

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Error estimate

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

$$\log \mu_N = \frac{1}{k} \log c_k + \frac{1}{2k} \log\langle B_{k,k}\rangle + \cdots + \frac{1}{N} \log\langle B_{N/2,N/2}\rangle$$

- Choose N high enough so that corrections to scaling are completely negligible.
- Partition CPU time amongst different terms to minimize overall statistical error (short test run).

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

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

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Conclusion

- For $\mathbb{Z}^3$ we have:
- PERM: $\mu = 4.684038(6)$ (Hsu and Grassberger, "Polymers confined between two parallel plane walls")
- Series: $\mu = 4.68404(1)$ (Clisby, Liang, and Slade, "Self-avoiding walk enumeration via the lace expansion")
- Series: $\mu = 4.684040(5)$ (Schram, Barkema, and Bisseling, "Exact enumeration of self-avoiding walks")
- Pivot: $\mu = 4.6840xxxx(4)$, 100 times more accurate than previous best.
- Power law improvement in error from each of: SAW-tree, move set, and choice of observable.
- $\sigma = 4 \times 10^8$, 35000 CPU hours.
- Computer experiment to start soon.

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