Convex Hulls of Self-Avoiding Random Walks: A Large-Deviation Study

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Random Walks

1

A random walk is a tuple of T d-dimensional steps.

- Random Walk (RW): Single coordinates of steps are drawn from a Gaussian distribution $G(0,1)$.
- Lattice Random Walk (LRW): Every step moves to an adjacent lattice site. It may only traverse one site per step. Here, the lattice is a square lattice. Immediate reversals are allowed.
- Self-Avoiding Walk (SAW): A LRW but steps may not visit already visited sites.
- Loop-Erased Random Walk (LERW): A LRW but loops are erased from the walk such that there are no intersections.

One-dimensional properties scale like T^{ν}.

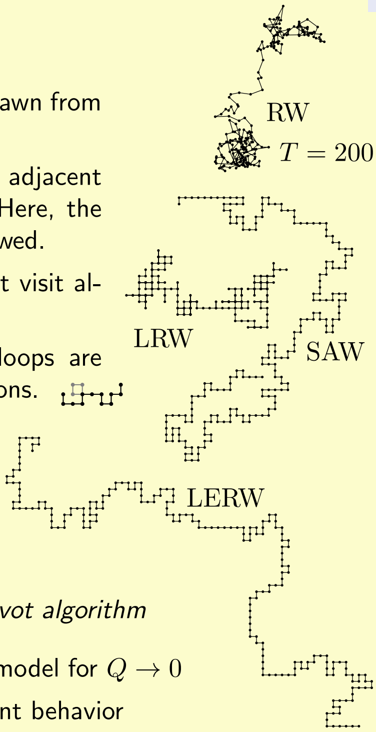
- $1/2 = \nu_{\mathrm{RW}} \le \nu_{\mathrm{SAW}} \le \nu_{\mathrm{LERW}}$, equality for $d \ge 4$.

SAW: Model for polymers [1]

- not trivial to generate uniformly distributed instances
- use Markov chain to generate new realizations, i.e., *pivot algorithm*

LERW: Connected to uniform spanning trees and the Potts model for $Q \to 0$

- intended as an easy version of SAW, but shows different behavior

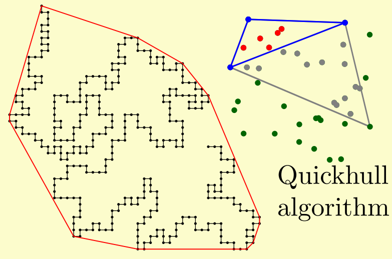


Convex Hulls

2

The convex hull of a set of points is the smallest convex polygon enclosing all T points.

- area A and perimeter L characterize the point set
- well researched in the context of computer graphics
- fast: $\sim \mathcal{O}(T \log T)$
- easy generalization to points in d dimensions



Large Deviation Simulation

3

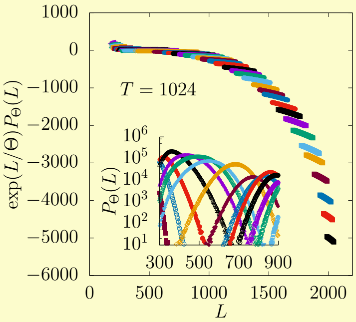
Using sophisticated sampling methods [2], the large deviation tails of the distributions, here with probabilities below $P(L) = 10^{-800}$, can be obtained.

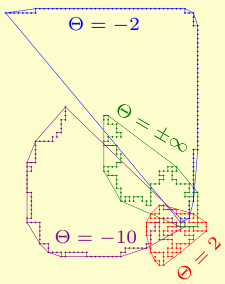
- Markow chain Monte Carlo sampling using a "Temperature" Θ based Metropolis algorithm
- propose a change of the configuration $c_t \to c_{t+1}$, accept depending on "energy" difference ΔS (here: S is either area A or perimeter L)

$$p_{\mathrm{acc}} = \min\left[1, \mathrm{e}^{-\Delta S/\Theta}\right]$$

- after equilibration: sample S
- biased distributions $P_{\Theta}(S)$ can be transformed into the true distribution

$$P(S) = \mathrm{e}^{S/\Theta} Z(\Theta) P_{\Theta}(S)$$





- calculate $Z(\Theta)$ by matching overlaps
- can be applied to a wide range of problems and enhancements like parallel tempering are applicable [3]
- alternative: Wang Landau sampling

Distributions of Area and Perimeter

4

Distribution for SAW and LERW over whole support

- decent system sizes up to $N = 2048$
- no small L and A because of excluded volume effects

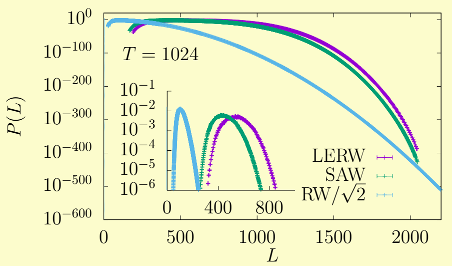
Whole distribution scales well with T^{ν}, as in the RW case [4]

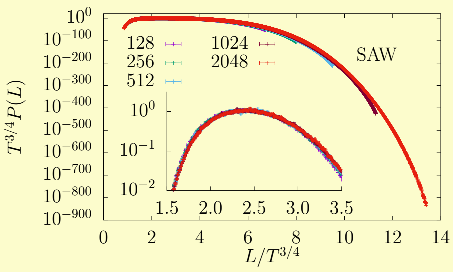
- deviations near $S_{\max}$ due to lattice structure
- excellent at the peak region

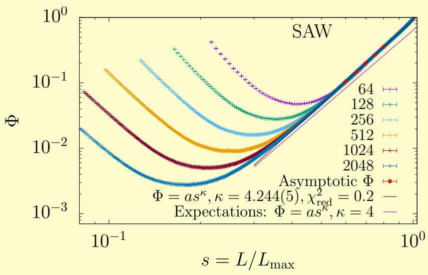
Empirical rate function

$$\Phi\left(S/S_{\max}\right) = -\frac{1}{T}\log P(S)$$

- extrapolated from the large S tail for $T \to \infty$ by a power law
- shows slight deviations from prediction $\kappa = \frac{1}{d(1-\nu)}$.
- fits better for L than for A
- A shows stronger effects of the lattice structure







Bibliography

[1] N. Madras and G. Slade, "The Self-Avoiding Walk" (2013)
[2] A.K. Hartmann, Phys. Rev. E **65**, 056102 (2002)
[3] P. Fieth, A.K. Hartmann, Phys. Rev. E **94**, 022127 (2016)
[4] G. Claussen, A.K. Hartmann, and S.N. Majumdar. Phys. Rev. E **91**, 052104 (2015)