Large Deviations of Convex Hulls of Self-Avoiding Random Walks

Hendrik Schawe   Alexander K. Hartmann   Satya N. Majumdar

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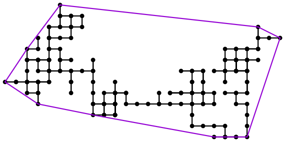
Self-Avoiding Walks

- Different constructions with different statistics
- Helpful for polymers, percolation clusters, spanning trees, ...
- End-to-end distance $r \propto T^{\nu}, \nu \geq 1/2$
  - in contrast to standard random walk $\nu = 1/2$

Random Walk (RW)



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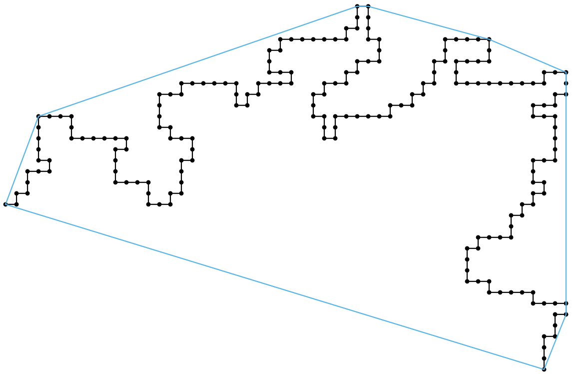
- SAW: Draw uniformly from all configurations

Self-Avoiding Walk (SAW), $\nu = 3/4$



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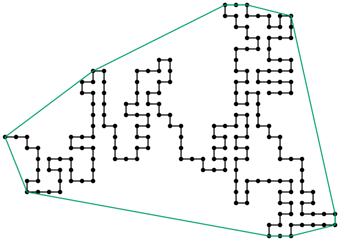
- End-to-end distance $r \propto T^{\nu}, \nu \geq 1/2$
  - in contrast to standard random walk $\nu = 1/2$
- SAW: Draw uniformly from all configurations
- SKSAW: Growth model, do not step on visited sites

Smart Kinetic Self-Avoiding Walk (SKSAW), $\nu = 4/7$



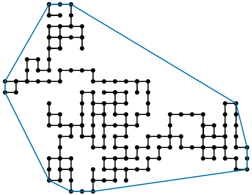
"True" Self-Avoiding Walk

- Record how often each site i is visited n_i
- Step on sites with probability

$$e^{-\beta n_i}/Z$$

  with $Z = \sum_{i \in \text{neighbors}} e^{-\beta n_i}$
- For large β, it will only step on itself if it is trapped
- Edge cases:
  - $\beta = 0$ is same as standard RW
  - $\beta \gg 1$ similar SKSAW

"True" Self-Avoiding Walk (TSAW), $\nu = 1/2$



D.J. Amit, G. Parisi, L. Peliti, Phys. Rev. B 27, 1635 (1983)

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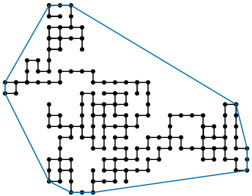

We are interested in the distribution of the area A of the convex hull.

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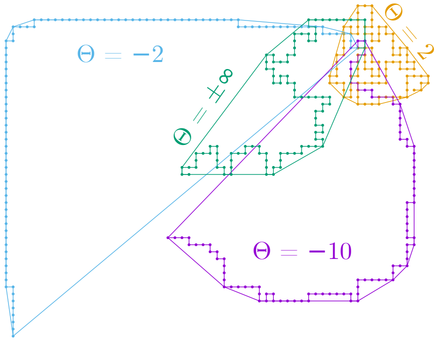
Large Deviation Sampling Scheme

- Use Metropolis algorithm with acceptance $p_{\text{acc}} = e^{-\Delta A/\Theta}$
- Treat area A of the convex hull as the “Energy”
- Simulate like a physical system at some “Temperature” Θ
- Markov chain of random number vectors $\vec{\xi}$



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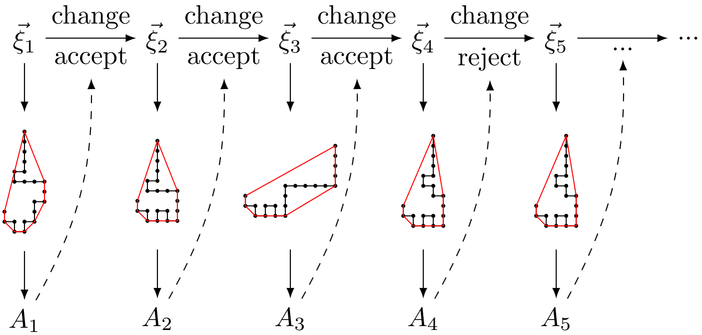
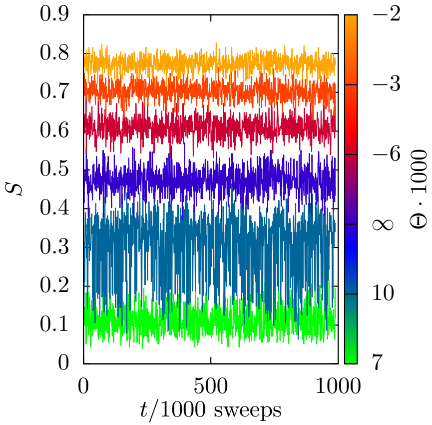


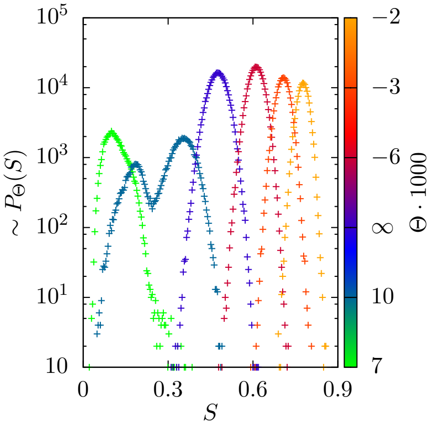
Large Deviation Sampling Scheme

- Standard MCMC using Metropolis algorithm to generate samples



Large Deviation Sampling Scheme

- Standard MCMC using Metropolis algorithm to generate samples
- Biased histograms $P_\Theta(A)$



Large Deviation Sampling Scheme

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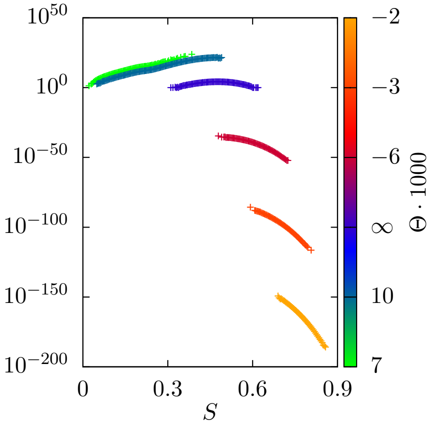
- Undo bias
  $P(A) = e^{A/\Theta} Z(\Theta) P_\Theta(A)$



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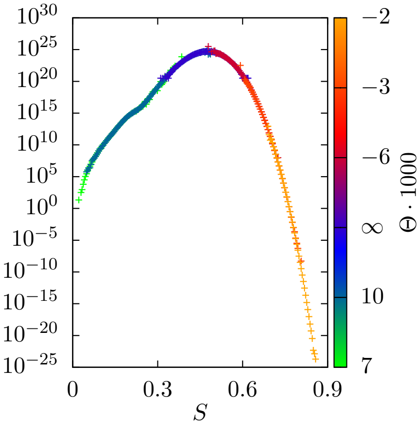

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- Biased histograms $P_\Theta(A)$
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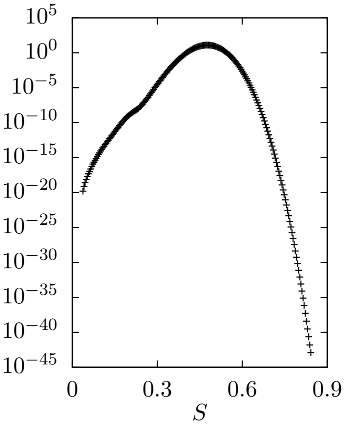
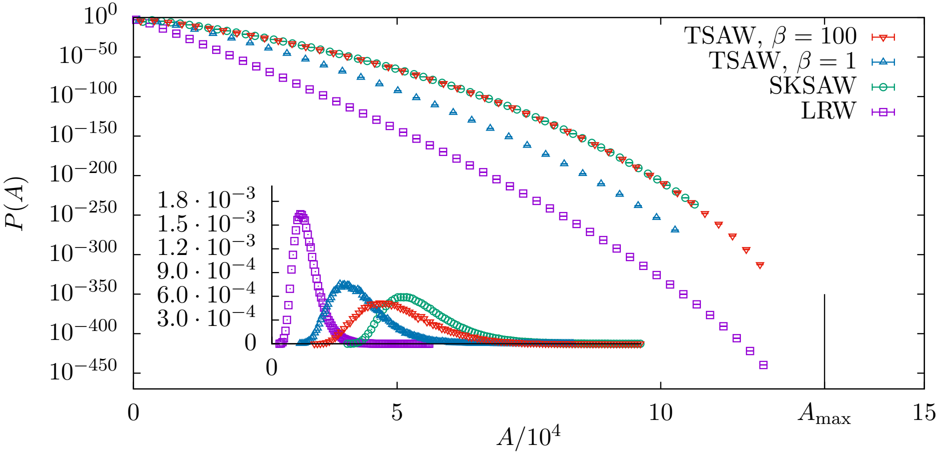
- Determine free parameter $Z(\Theta)$ by continuity
- Normalization for the actual distribution



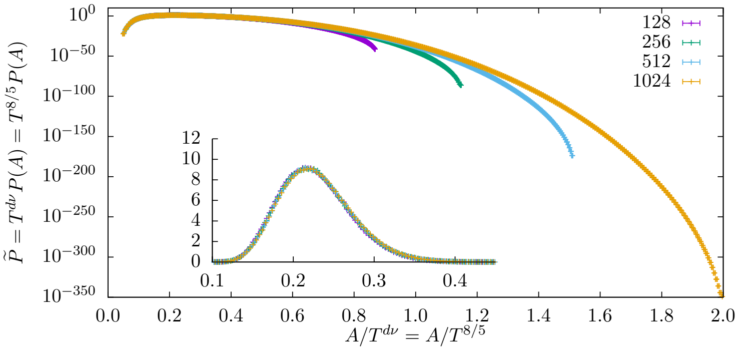
Full Distributions

- Large deviation tail is a region of extended walks $\rightarrow$ no trapping
- Without trapping TSAW with large values of β are basically the same as SKSAW
- Smaller values of β interpolate to standard RW case



Scaling

Usually the whole distribution scales like the end-to-end distance r and the dimension of the observable (not just the mean)



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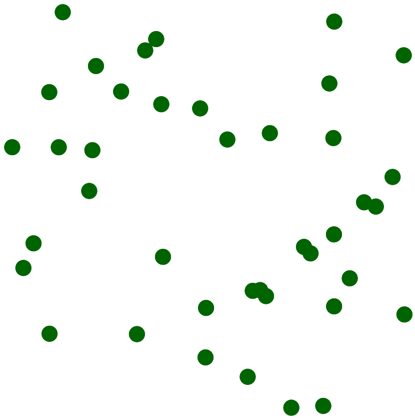
H. Schawe, A.K. Hartmann, S.N. Majumdar, Phys. Rev. E 96, 062101 (2017)
H. Schawe, A.K. Hartmann, S.N. Majumdar, Phys. Rev. E 97, 062159 (2018)

Further Results and Conclusion

- ν can be used to scale the whole distribution (not just the means)
- The tail behavior is given by $P_T(A) \approx e^{-T\Phi}$ with $\Phi(A) \propto A^{1/d(1-\nu)}$
- TSAW is the exception where the main part behavior does not predict the far tail behavior – at least for large β

Convex Hulls

- Characterizes point set
- Smallest convex polygon containing every point
- Home range of animals
- Spatial extend of epidemics
- Construction of Voronoi Diagrams / Delaunay Triangulations
- Look at area A, circumference L or volume V



E. Dumonteil, S.N. Majumdar, A. Rosso, A. Zoia, PNAS, 110, 4239 (2013)

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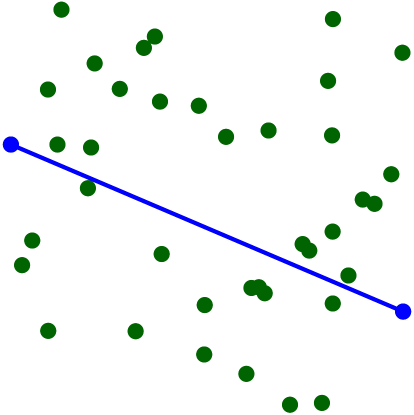

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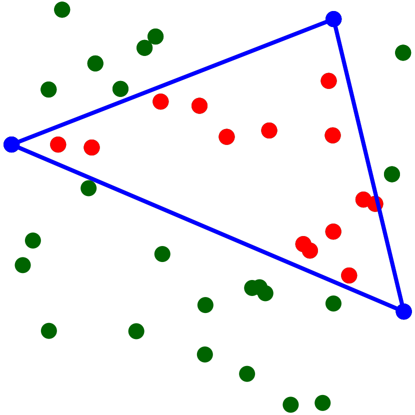

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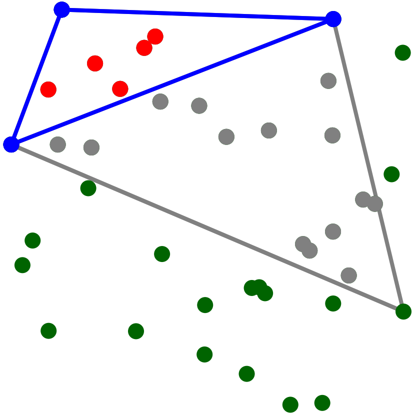

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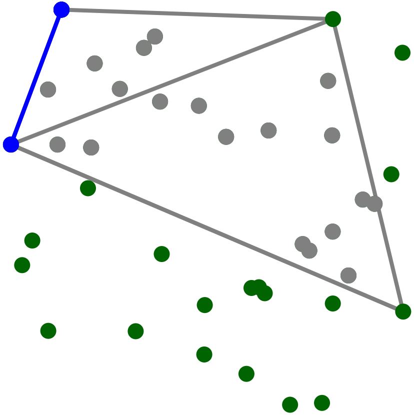

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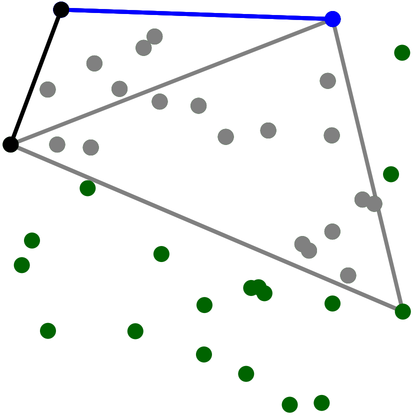

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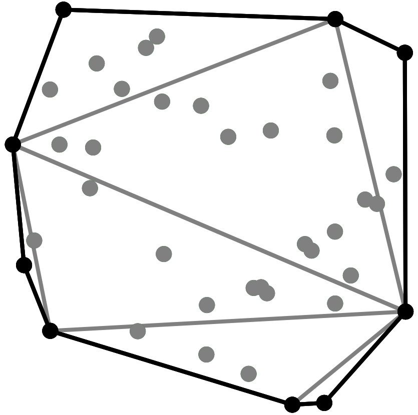

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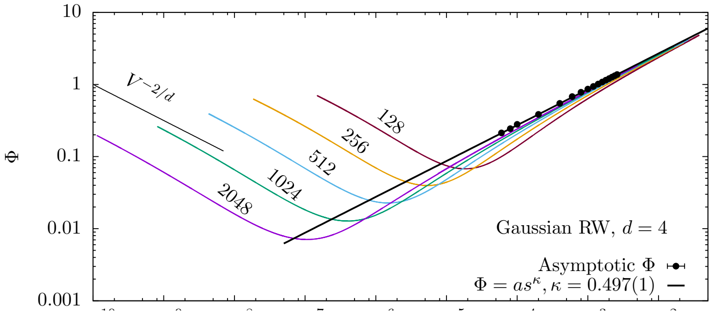
Large Deviation Principle and Rate Function Φ

- Assume Φ is a power law and simple scaling argument

$$\Phi = -\frac{1}{T} \ln P\left(S/S_{\max}\right) \propto \left(\frac{S}{S_{\max}}\right)^{1/d(1-\nu)}$$

- Works very well for off-lattice Gaussian walks
- Works reasonably well for SKSAW, SAW and LERW
- But does not work for TSAW with large β



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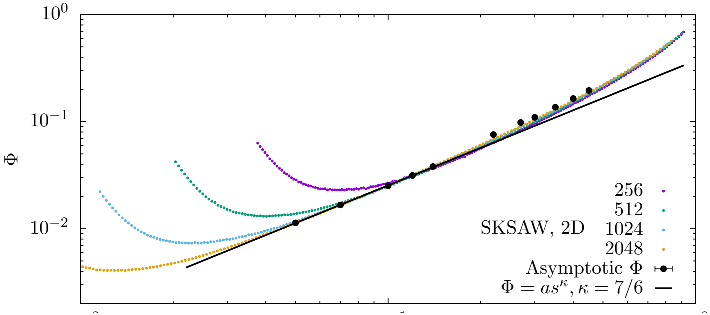

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