SAW in a box: proof via Monte Carlo moves

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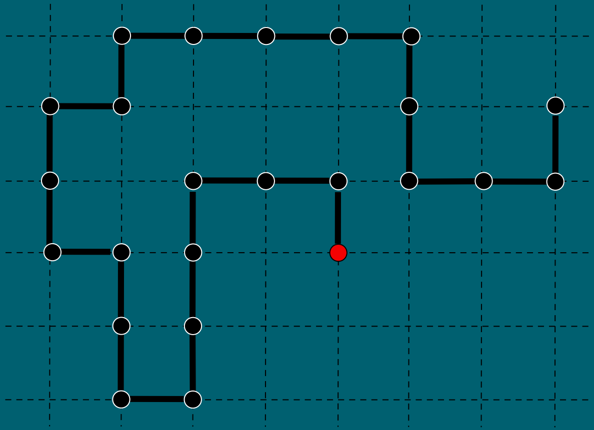
Square lattice Self-avoiding walks (SAW)

A square lattice SAW



A SERIES OF SAW PROBLEMS

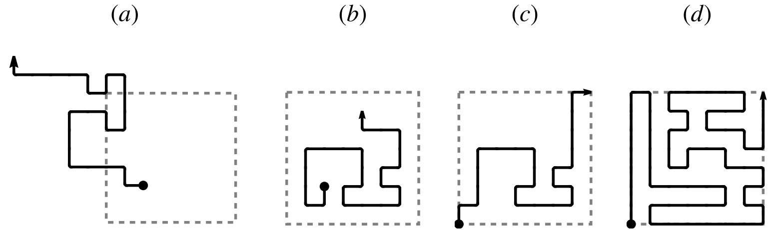


Figure: Example SAWs with increasing degree of confinement to a box of side length $L = 8$. (a) Unconfined, (b) confined to the box (our model), (c) crossing a square and (d) a Hamiltonian path crossing a square.

SAW without any restriction

- Let the number of them be denoted $w(n)$
- It is known that the growth constant exists (Hammersley 1957)

$$\mu = \lim_{n\to\infty} w(n)^{1/n}$$

- with a best estimate of μ most recently $\mu = 2.63815853032790(3)$ (Jacobsen, Scullard and Guttmann, 2016)
- It is expected that

$$w(n) \sim A\mu^n n^{\gamma-1}$$

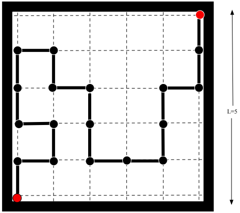
where $\gamma = 43/32$.

SAW crossing a Square I

- Now consider SAWs with end points fixed at two opposing vertices of a square of side L bonds and all sites of the walk lie within or on the boundary of the square where

$$2L \leq n \leq L^2 + 2L$$

- This problem has a long history too: Whittington and Guttmann 1990, Madras 1995 and Bousquet-Mélou, Guttmann and Jensen 2005 and Knuth 1976 introduced a similar problem



SAW crossing a Square II

Let the number of such SAW be s_L .
It has been proven (Abbott and Hanson 1978 and Whittington and Guttmann 1990) that the limit

$$\lambda_S = \lim_{L\to\infty} s_L^{1/L^2}$$

exists so that $s_L = \lambda_S^{L^2+o(L^2)}$
The best estimate of this growth constant until recently was (Bousquet-Mélou, Guttmann and Jensen 2005) $\lambda_S = 1.744550(5)$
For unconstrained SAW (or critical fugacity) the average number of steps $n(L)$ is expected to scale as

$$n(L) \sim CL^{4/3}$$

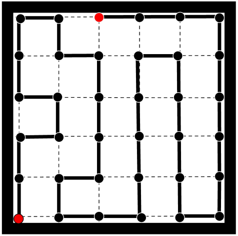
HAMILTONIAN WALKS

Walks that visit every vertex of a finite patch of lattice are known as Hamiltonian

Let the number of such walks be h_L and the limit

$$\mu_H = \lim_{L\to\infty} h_L^{1/L^2}$$

exists and has been estimated as $\mu_H = 1.472801(1)$ (Bousquet-Mélou, Guttmann and Jensen 2005)



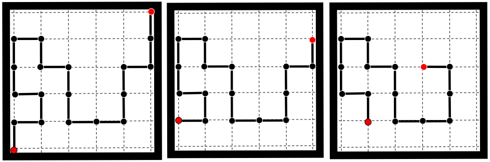
SIMULATING HAMILTONIAN WALKS

Monte Carlo Backbite Algorithm (clisby.net)

- Moves go back to ”Monte Carlo studies of polymer chain dimensions in the melt” by Marc L. Mansfield, J. Chem. Phys. 77, 1554 (1982)
- “Secondary structures in long compact polymers” by Richard Oberdorf, Allison Ferguson, Jesper L. Jacobsen and Jané Kondev, Phys. Rev. E 74, 051801 (2006)
- An aside: no proof of ergodicity
- Let’s use the moves for a different purpose ...

SAW in a Box with Three Endpoint Conditions

1. walks whose endpoints lie at opposing corners of the square counted as s_L;
2. walks whose endpoints lie on opposing sides of the square counted as d_L;
3. walks whose endpoints lie anywhere inside the square (or on the boundary) counted as a_L.



THE LIMIT OF INTEREST

We are interested in the existence of the limit

$$\lambda_A = \lim_{L \to \infty} a_L^{1/L^2} \; .$$

and comparing its value to the previously considered

$$\lambda_S = \lim_{L \to \infty} s_L^{1/L^2} = 1.744550(5) \; .$$

One can in fact prove that

$$\lambda_A = \lambda_S$$

START OF THE PROOF

Let us further define the number of walks whose endpoints lie anywhere inside a square of side ℓ that span the square in at least one direction: in this way they are walks whose minimal bounding box is of side ℓ and these have cardinality m_ℓ with the convention $m_0 = 1$. Denote by $\widehat{m}_L$ the union of the sets counted by m_ℓ for $0 \le \ell \le L$. Hence

$$\widehat{m}_L = \sum_{\ell=0}^{L} m_\ell$$

and

$$s_L \le d_L \le m_L \le \widehat{m}_L \le a_L \ .$$

Importantly can also argue that

$$a_L \le (L+1)^2 \widehat{m}_L \le (L+1)^3 m_L \ .$$

Our comparisons

So

$$m_L \leq a_L \leq (L+1)^3 m_L \ .$$

Hence, if we can show that

$$\lambda_M = \lim_{L\to\infty} m_L^{1/L^2}$$

exists then λ_A exists and $\lambda_A = \lambda_M$
Moreover if we can also prove

$$\lambda_M = \lambda_S$$

we will have our result

$$\lambda_A = \lambda_S$$

So need to compare

walks with end points anywhere to those at opposite corners where the bounding box is a square of side L

STRATEGY

- Start with walks whose end points are anywhere inside the box
- Move the endpoints to the sides of the box
- bound the number of configurations that lead to a unique configuation with endpoints on the sides of the box

Backbite moves

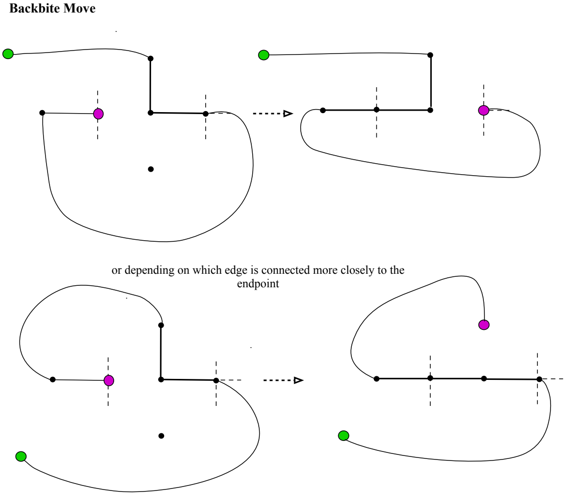


Figure: The backbite move from the Hamiltonian walk algorithm

END ATTACK MOVES

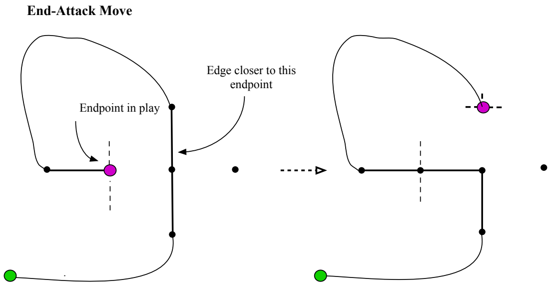


Figure: The end-attack move

CHANGING THE LENGTH MOVES

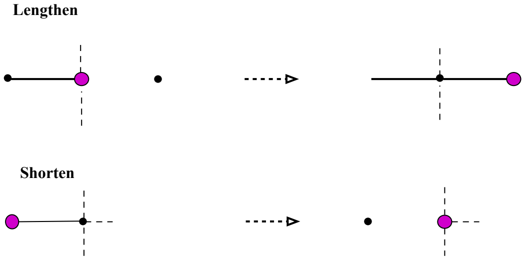


Figure: The lengthening and shortening moves.

Antecedents

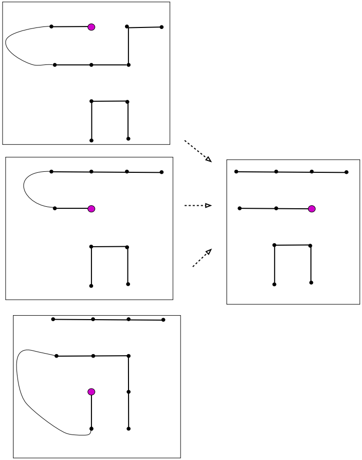


Figure: On the left are the three possible antecedents of the configuration on the right when moving the endpoint to the right

Final bounds

Consider the antecedents whose left endpoint reach the boundary after b moves, then the total is a sum over values of $b \leq L$. Hence the total number of antecedents is bounded for $L \geq 2$ by

$$\sum_{b=0}^{L} 3^b \sum_{r=0}^{L-b} 3^r = \frac{1}{2} \sum_{b=0}^{L} 3^b (3^{L-b+1} - 1) < \frac{1}{2}(L+1)3^{L+1} .$$

Hence we have

$$s_L \leq m_L \leq \frac{1}{2}(L+1)3^{L+1} s_L$$

and the results (λ_M exists and $\lambda_M = \lambda_S$) follow by raising each to the power $1/L^2$ and taking the limit $L \to \infty$. Hence

$$\lambda_A = \lambda_S$$

Full asymptotics

From series analysis we conjecture that the number of such walks A_L, for both problems, behaves as

$$A_L \sim \lambda_A^{L^2+bL+c} \cdot L^g,$$

where $\lambda_A = 1.7445498 \pm 0.0000012$, $b = -0.04354 \pm 0.0005$, $c = -1.35 \pm 0.45$, and $g = 3.9 \pm 0.1$.

FURTHER AND RELATED RESULTS

- Adding a length fugacity connects the box problem to free SAW
- From Monte Carlo and scaling theory of this expanded problem with a length fugacity can estimate exponents associated with the model in a box (Bradly and AO)
- Polygons (Guttmann and Jensen)
- Links (Janse van Rensburg and Orlandini)
- Honeycomb lattice (Guttmann and Jensen)
- Proving subdominant factors (Whittington)
- Higher dimensions (Whittington)