Title: Adventures with Monte Carlo Simulations of the Self-Avoiding Walk

Date: Dec 12, 2012 02:00 PM

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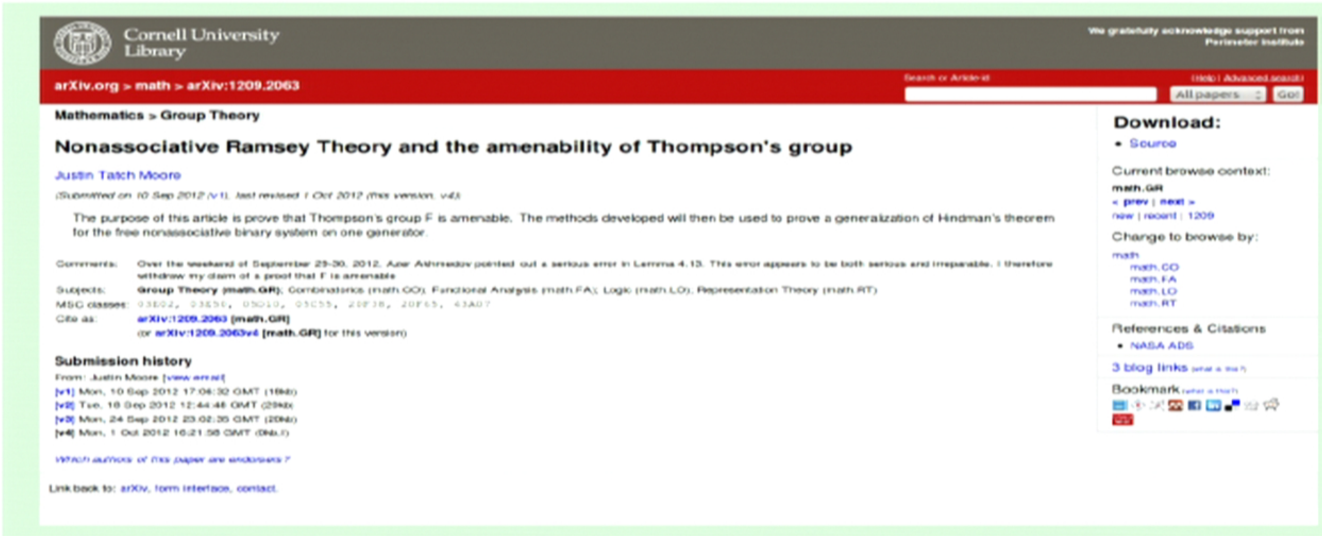
Abstract: The Rosenbluth Method is a classical kinetic growth Monte Carlo algorithm for growing a self-avoiding walk by appending steps to its endpoint.

This algorithm

can be generalised by the implementation of more general elementary moves (for example, BFACF elementary moves) to realise kinetic growth algorithms for lattice polygons.
This generalises the counting principle that underlies the Rosenbluth method and the result is a widely applicable class of algorithms which may be used for microcanonical sampling in discrete models. In addition to self-avoiding walks, several applications of kinetic growth and canonical Monte Carlo algorithms will be presented, including the sampling of trivial words in abstract groups, as well as knotted lattice polygons and discrete lattice spin systems such as the Potts model.

This is work was done in collaboration with Andrew Rechnitzer of the Mathematics Department at the University of British Columbia.

Thompson F-group



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Mathematics > Group Theory

Nonassociative Ramsey Theory and the amenability of Thompson's group

Justin Tatch Moore

(Submitted on 10 Sep 2012 (v1), last revised 1 Oct 2012 (this version, v4))

The purpose of this article is prove that Thompson's group F is amenable. The methods developed will then be used to prove a generalization of Hindman's theorem for the free nonassociative binary system on one generator.

Comments: Over the weekend of September 29-30, 2012, Azer Akhmedov pointed out a serious error in Lemma 4.13. This error appears to be both serious and irreparable. I therefore withdraw my claim of a proof that F is amenable

Subjects: **Group Theory (math.GR)**; Combinatorics (math.CO); Functional Analysis (math.FA); Logic (math.LO); Representation Theory (math.RT)

MSC classes: 03E02, 03E50, 05D10, 05C55, 20F38, 20F65, 43A07

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[v4] Mon, 1 Oct 2012 16:21:56 GMT (0kb,I)

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Thompson F-group

Some years ago, in 2010: On the website MathOverflow

"Last year [2009] a paper on the ArXiV (Akhmedov) claimed that Thompson's group F is not amenable, while another paper, published in the journal "Infinite dimensional analysis, quantum probability, and related topics" (vol. 12, p173-191) by Shavgulidze claimed the exact opposite, that F is amenable."

Thompson F-group

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On the other hand...

"I am told ...[Akhmedov's] paper was correct except for a lemma... Shavgulidze's paper(s) was much more readable [than Akhmedov's]. It has "Lemma 5" whose proof was found wrong by Matt Brin.... There are very nice notes of Matt Brin's seminar on Shavgulidze's proof." [Justin Moore]

Thompson F-group

Finitely presented group G on m generators $T = \{a, b, \ldots, z\}$.

Example: Abelian group on 2 generators

$$T = \{a, b\}$$
$$G = \langle a, b | [a, b] \rangle$$

A word w is *trivial* if $w \equiv e$

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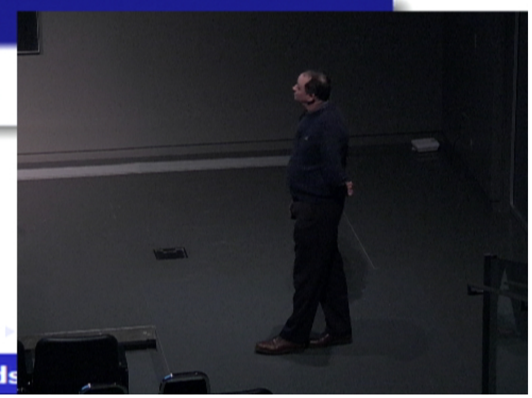
$S_n = \{$Set of freely reduced trivial words of length $n\}$

Theorem (Grigorchuk-Cohen)

$\mathrm{cogrowth}(G) = 2m - 1$ if and only if G is amenable.



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cogrowth$(G) = 2m - 1$ *if and only if* G *is amenable.*

If G is amenable:

$$|S_n| = (2m-1)^{n+o(n)}$$

Determine the growth rate of $|S_n|$.

Thompson F-group

Thompson's group F on m generators $S = \{a, b, c, d, f, \ldots\}$.

F-group on 2 generators

$$F = \langle a, b | [ab^{-1}, a^{-1}ba], [ab^{-1}, a^{-2}ba^2] \rangle$$

F-group on 4 generators

$$F = \langle a, b, c, d | a^{-1}bac^{-1}, a^{-1}cad^{-1}, [ab^{-1}, c], [ab^{-1}, d] \rangle$$

F-group on 5 generators

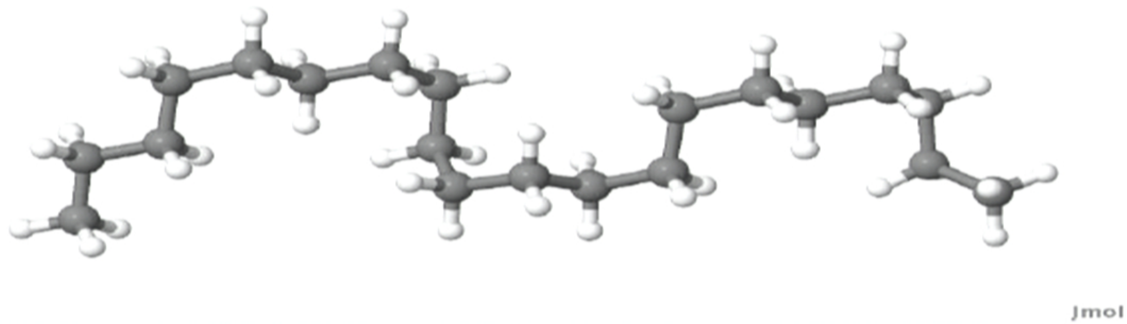
$$F = \langle a, b, c, d, f | a^{-1}bac^{-1}, a^{-1}cad^{-1}, ab^{-1} = f, [f, c], [f, d] \rangle$$

Trivial words are classes of lattice paths or polygons

Polymer Entropy

Basic Problem: Polymer Entropy

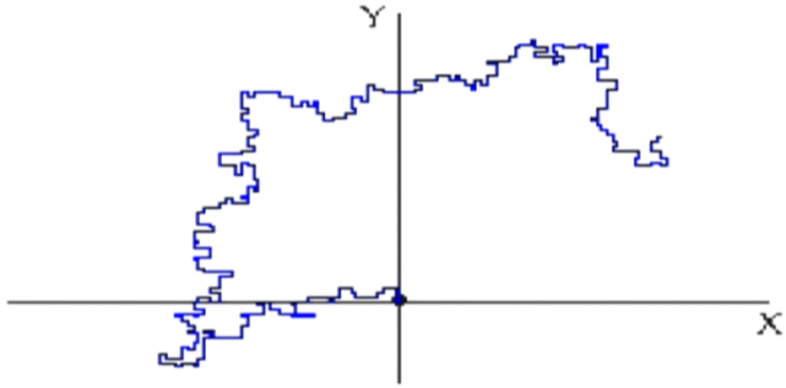
- Conformations of a Polymer Molecule:



- Problem: Determine the Conformational Entropy
- Models: Self-avoiding walks and polygons

Polymer Physics

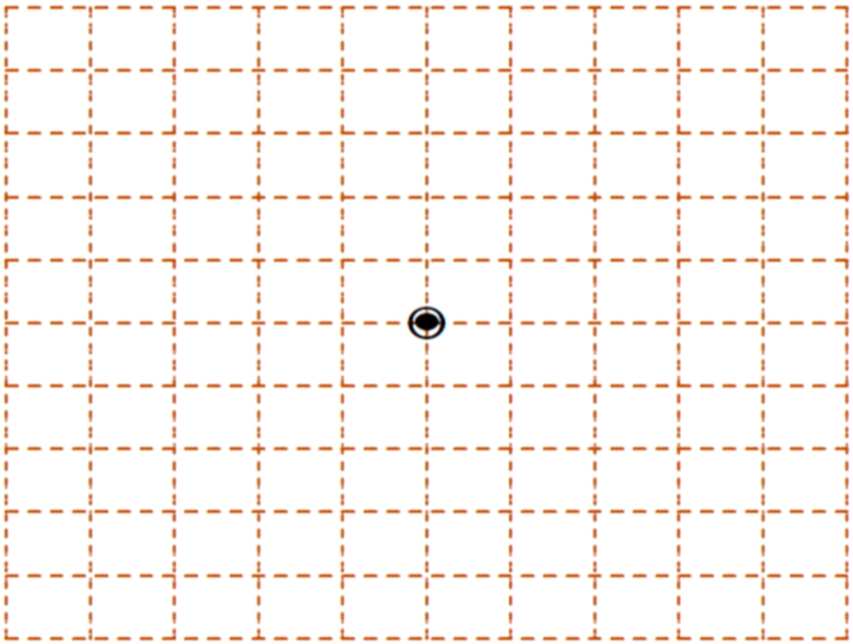
Polymer conformations – the self-avoiding walk



$c_n = \#\{$Self-avoiding walks of length $n\}$

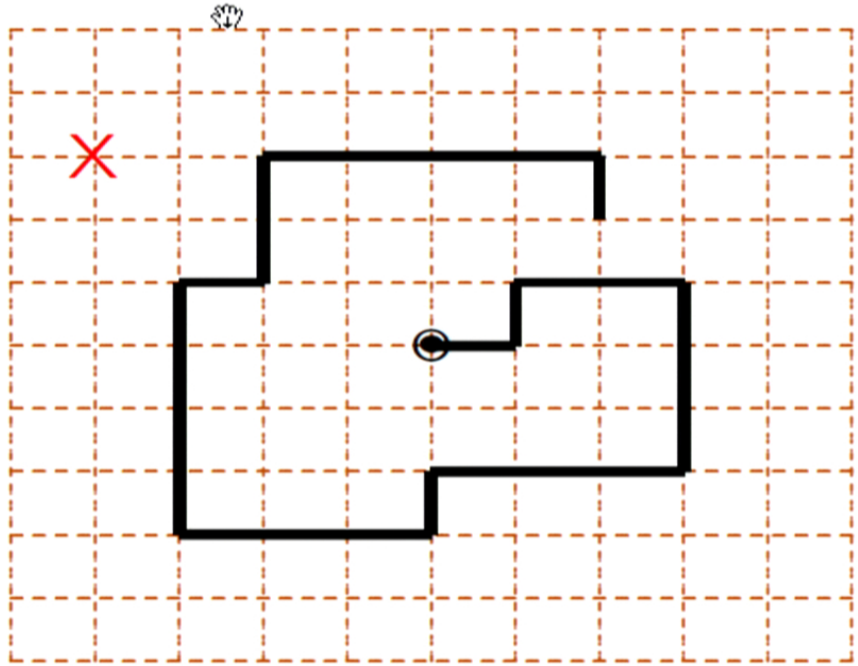
The prototype problem: Self-avoiding walk

$$c_0 = 1$$



The prototype problem

Non-Markovian.



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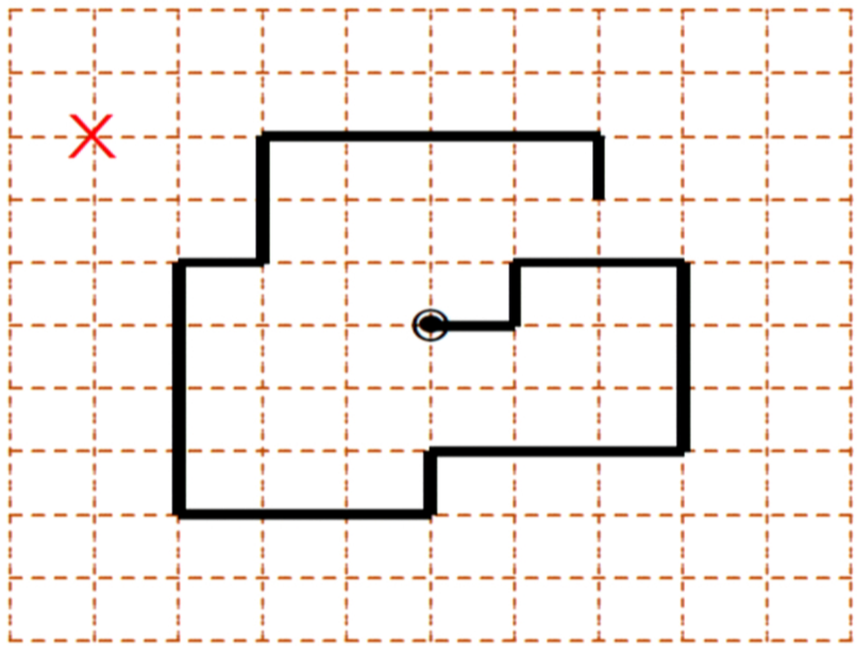


Self-Avoiding Walk

The most basic question

- What is c_n?
- $c_{71} = 4190893020903935054619120005916$. (Jensen 2004)
- Moore's law and better algorithms will give more terms...
- ...but CPU time grows exponentially

Self-Avoiding Walk

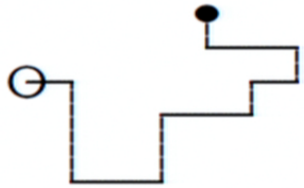
The most basic question

- What is c_n?
- $c_{71} = 4190893020903935054619120005916$. (Jensen 2004)
- Moore's law and better algorithms will give more terms...
- ...but CPU time grows exponentially
- Approximate Estimates?
- Monte Carlo sampling of walks?

The prototype problem

Submultiplicativity of self-avoiding walks

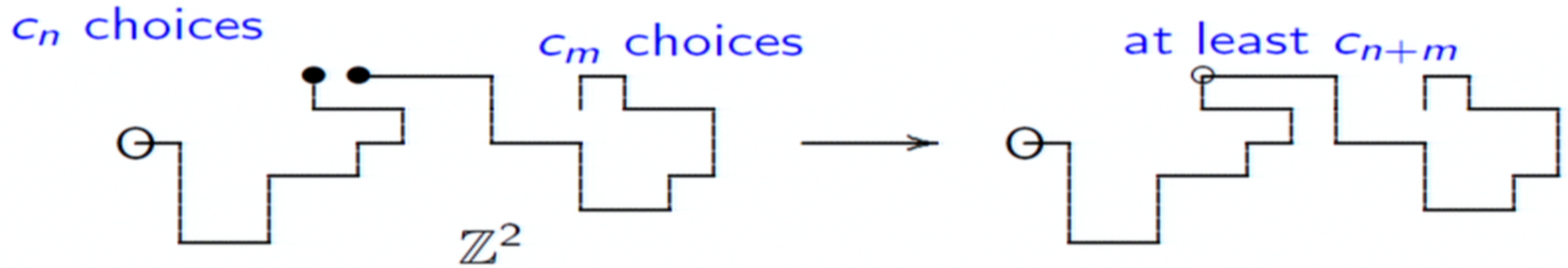
c_n choices



$\mathbb{Z}^2$

The prototype problem

Submultiplicativity of self-avoiding walks



- $c_n \, c_m \geq c_{n+m}$
- The Growth Constant: $\lim_{n\to\infty} c_n^{1/n} = \mu \Rightarrow c_n = \mu^{n+o(n)}$
- Scaling arguments (Entropic Exponent: γ $(=\frac{43}{32}$ in 2-d))

$$c_n \simeq C\, n^{\gamma-1} \mu^n$$

- $\mu \approx 2.6$ (2 dimensions)

MC Algorithms

Monte Carlo Sampling:

- Elementary moves
- A rule for implementing elementary moves (eg the Metropolis algorithm)

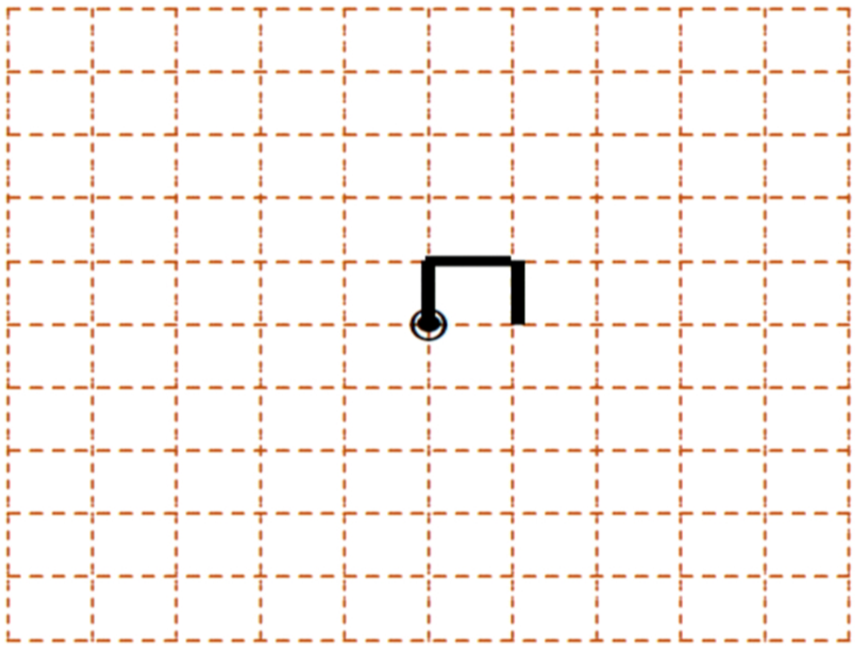
Monte Carlo and Polymers

Marshall and Arianna Rosenbluth

- Recruited by Edward Teller to work at Los Alamos
- Expert in Scattering, Plasma Physics, H-bomb development
- Metropolis Algorithm
- Hammersley and Morton: A static algorithm for walks

Rosenbluth Sampling

$$P_3 = \frac{1}{12} \times \frac{1}{3} = \frac{1}{36}$$



Rosenbluth Sampling

- Create walks by stepping from the origin
- Each step is chosen uniformly from those available
- Assign a weight to each walk ω:

$$W(\omega) = \frac{1}{P(\omega)}$$

Rosenbluth Sampling

- Create walks by stepping from the origin
- Each step is chosen uniformly from those available
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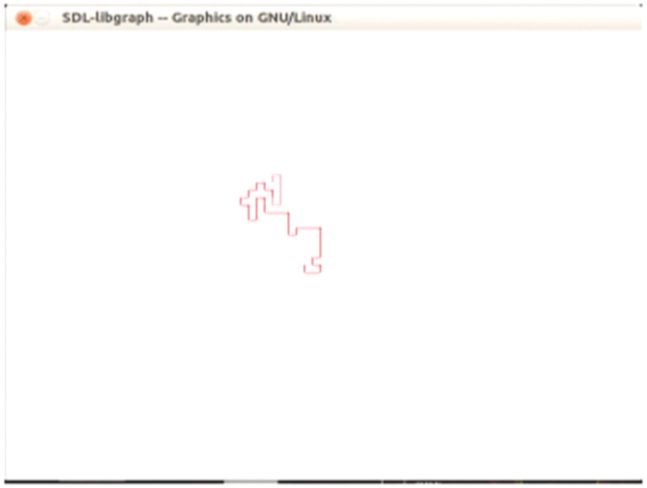
- If the walk is trapped, assign weight zero and start over
- Average weight at length n [Rosenbluth Counting theorem]:

$$\langle W \rangle_n = \sum_{|\omega|=n} P(\omega) W(\omega) = \sum_{|\omega|=n} \mathbf{1} = c_n .$$

Rosenbluth Sampling

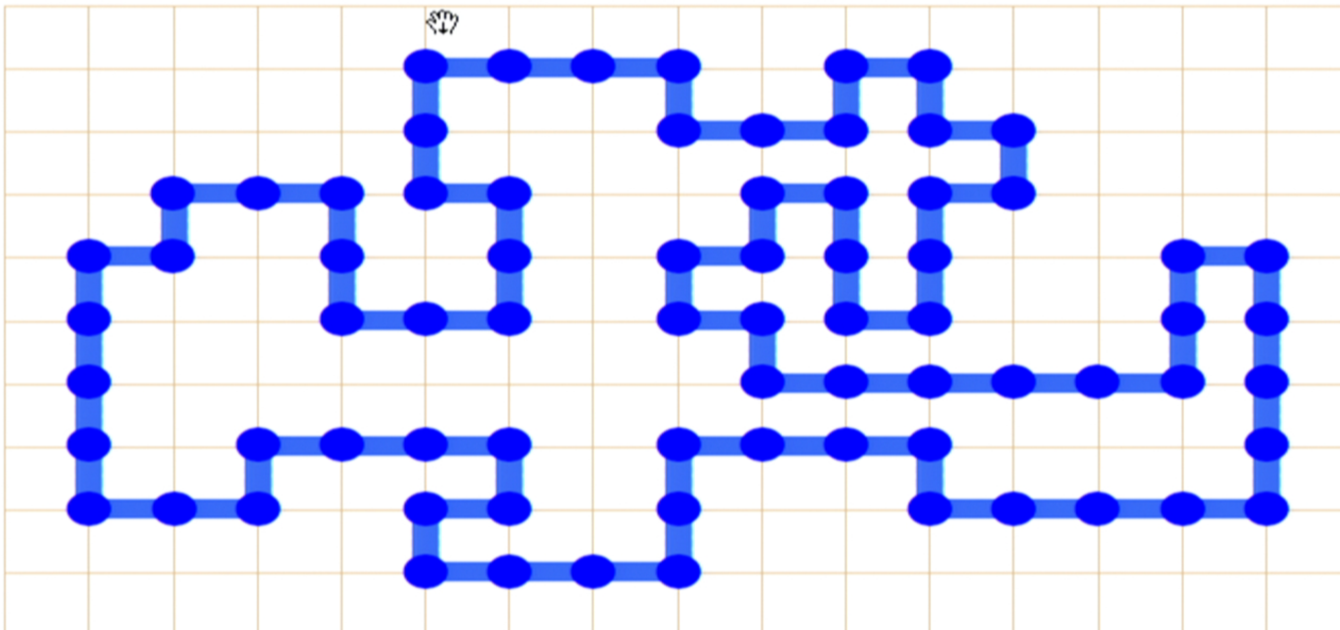


Rosenbluth Algorithm

Knotted Polygons of Minimal Length

n	c_n	$\langle W_n \rangle$	Completed Walks
1	4	4	100%
2	12	12	100%
3	36	36	100%
4	100	100.0	100%
5	284	284.0	100%
6	780	780.2	100%
7	2172	2172.9	100%
8	5916	5918.5	99.7%
9	16268	16276.8	99.5%
10	44100	44123.1	99.0%

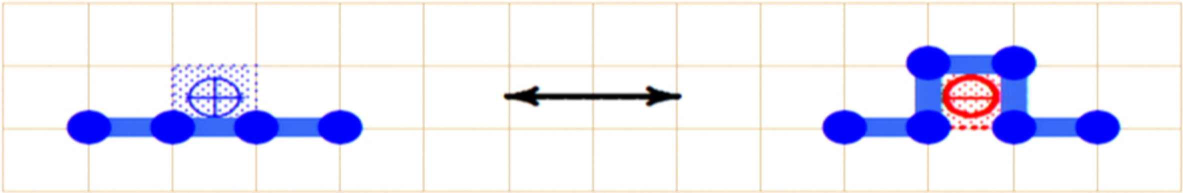
Lattice Polygons



BFACF elementary moves

Neutral BFACF moves

Positive/Negative BFACF moves



Berg-Foester 1981 and Aragaõ de Carvalho-Caracciolo-Fröhlich 1983

BFACF elementary moves

Neutral BFACF moves

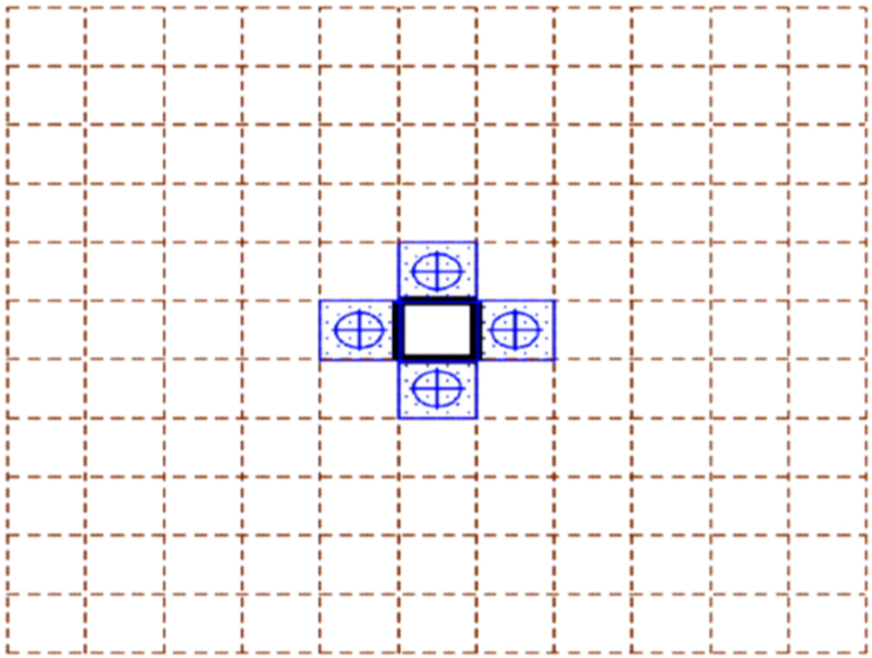
Positive/Negative BFACF moves

Berg-Foester 1981 and Aragaõ de Carvalho-Caracciolo-Fröhlich 1983

GARM for Polygons

$P = 1$ (Choose one of 4 moves)

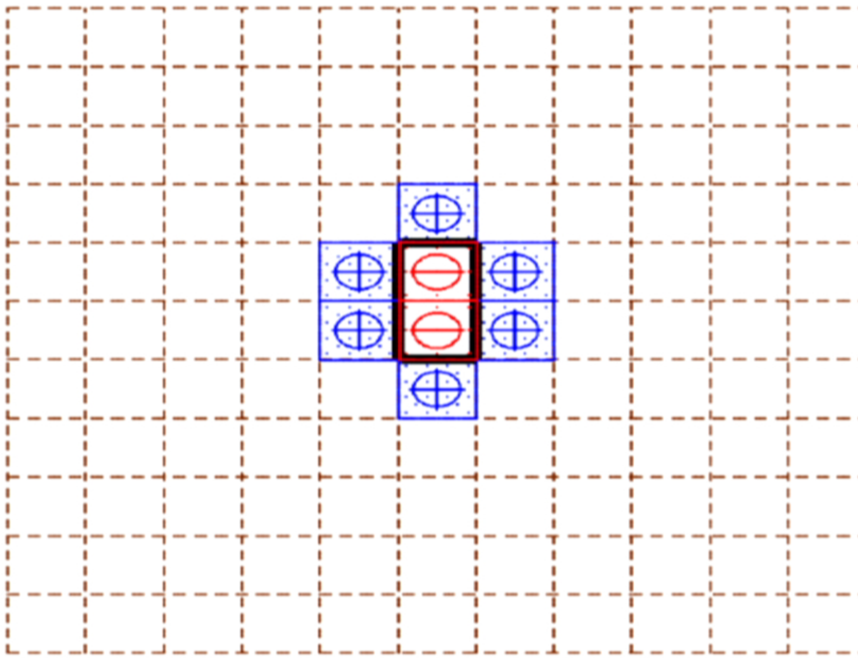
$$a_+ = 4$$



GARM for Polygons

$P = \frac{1}{4} = \frac{1}{a_+}$

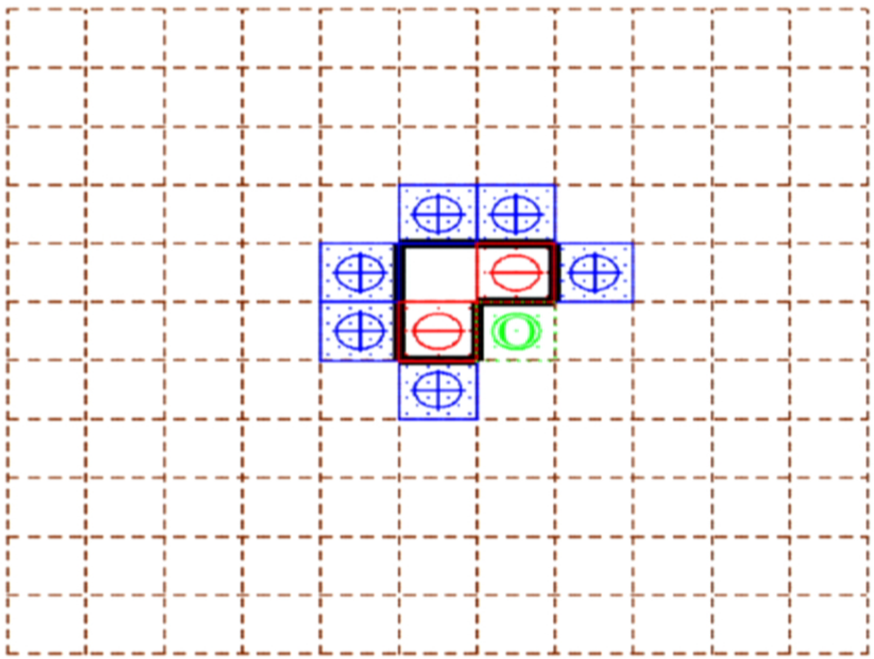
$$a_+ = 6,\ a_- = 2$$



GARM for Polygons

$P = \frac{1}{4} \times \frac{1}{6}$

$$a_+ = 6,\ a_- = 2,\ a_0 = 1$$



BFACF elementary moves

BFACF elementary moves for self-avoiding lattice polygons:

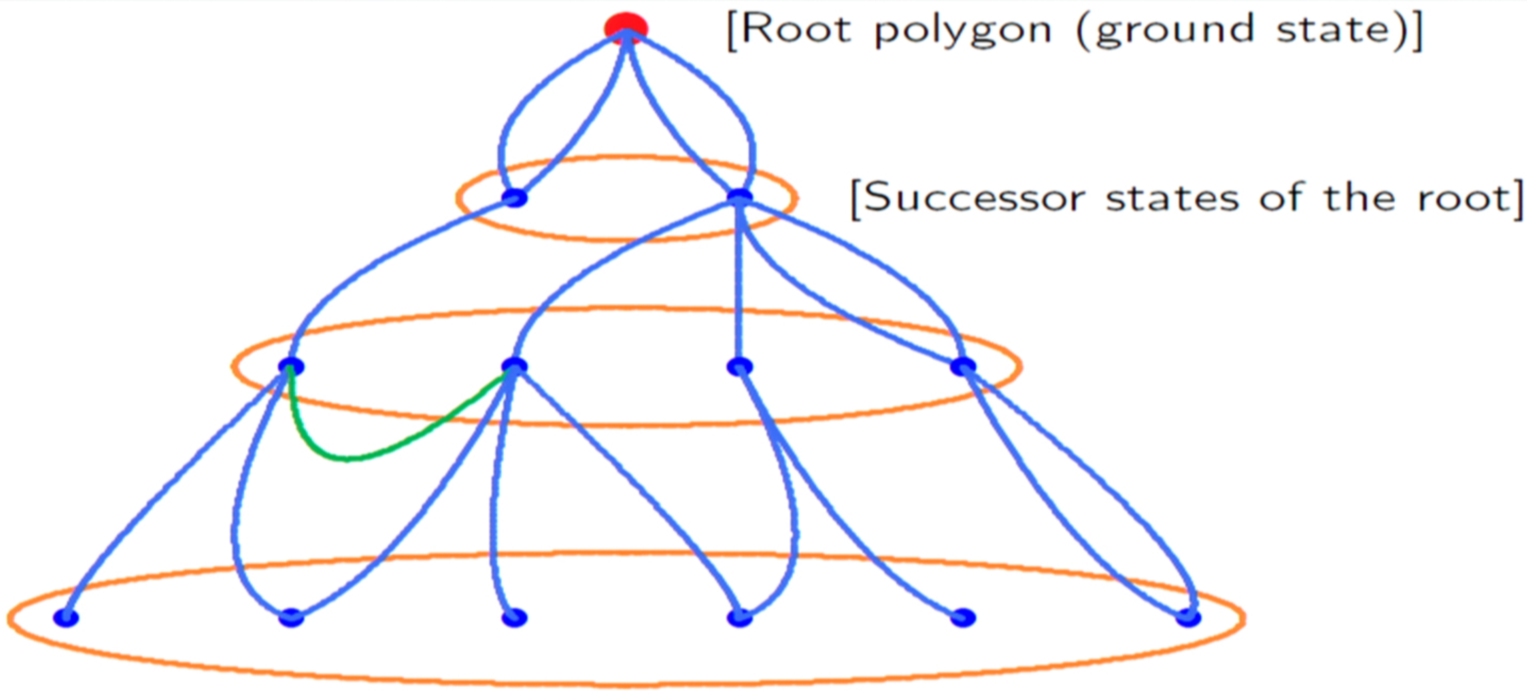
- Irreducible in the square lattice
- Not irreducible in the cubic lattice

Theorem (JvR and Whittington 1991)

The irreducibility classes of the BFACF moves for unrooted polygons in the cubic lattice coincide with the knot types of the polygons as closed simple curves in $\mathbb{R}^3$.

GARM

$P(\phi) =$



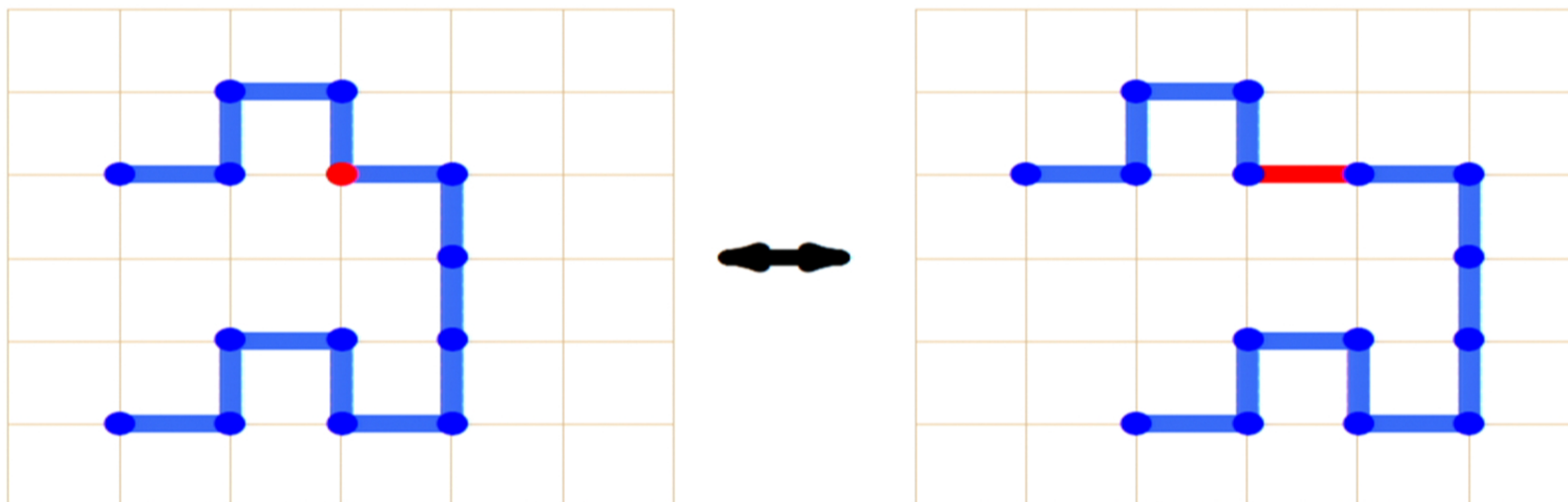
GARM Sampling

- The average weight of sequences ending in $\phi_\ell = \tau$ is

$$\langle W_\tau \rangle = \sum_{\phi \longrightarrow \tau} W(\phi) P(\phi|\phi_0) = \sum_{\phi \longrightarrow \tau} \prod_{i=0}^{|\phi|-1} \frac{1}{a_-(\phi_{i+1}) + a_0(\phi_{i+1})}.$$

- Time reverse the above. Start in state τ and end in state ϕ_0.

GARM Sampling of Self-avoiding Walks



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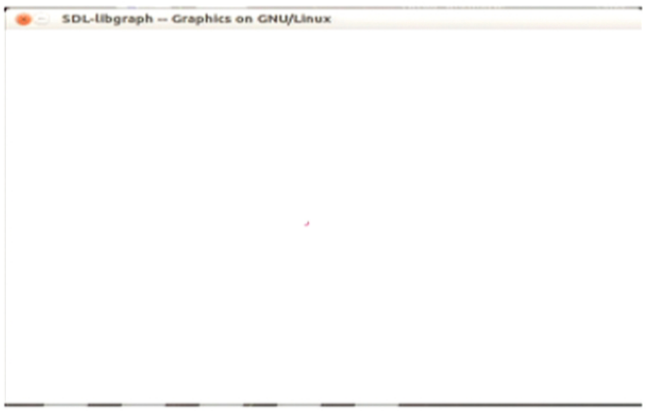


2×2 Ising Model

Microcanonical sampling of spin states: GARM

$a_+ = 4$, $a_- = 0$		$a_+ = 3$, $a_- = 1$		$a_+ = 2$, $a_- = 2$		$a_+ = 1$, $a_- = 3$		$a_+ = 0$, $a_- = 4$
σ: $\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$	$\longrightarrow$	$\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$	$\longrightarrow$	$\begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix}$	$\longrightarrow$	$\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$	$\longrightarrow$	$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$
$E = 0$		$E = 2$		$E = 2$		$E = 2$		$E = 0$

2×2 Ising Model

Microcanonical sampling of spin states: GARM

$a_+ = 4$, $a_- = 0$	$a_+ = 3$, $a_- = 1$	$a_+ = 2$, $a_- = 2$	$a_+ = 1$, $a_- = 3$	$a_+ = 0$, $a_- = 4$

$$\sigma: \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \longrightarrow \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \longrightarrow \begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

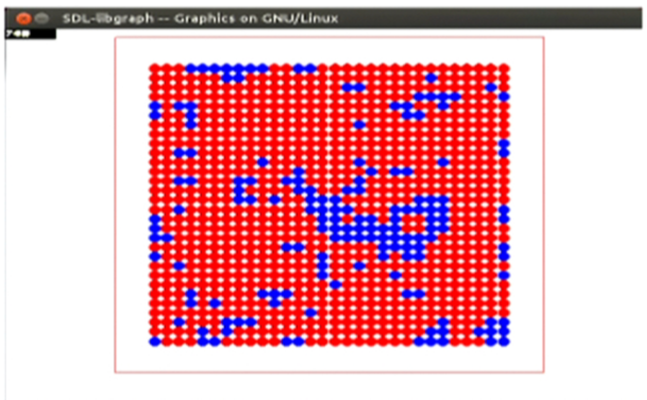
$E = 0$	$E = 2$	$E = 2$	$E = 2$	$E = 0$

$a_+ = 4$, $a_- = 0$	$a_+ = 3$, $a_- = 1$	$a_+ = 2$, $a_- = 2$	$a_+ = 1$, $a_- = 3$	$a_+ = 0$, $a_- = 4$

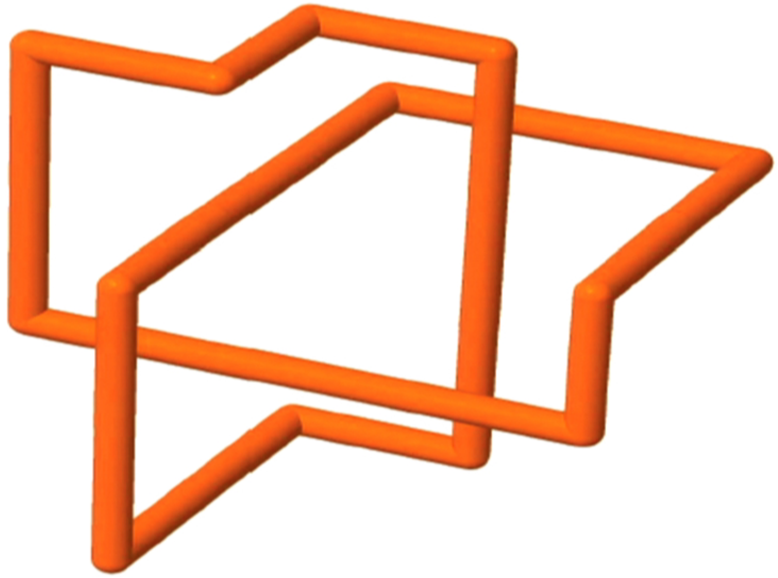
$$\tau: \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

$E = 0$	$E = 2$	$E = 4$	$E = 2$	$E = 0$

GARM Sampling of the Ising model



Knotted Polygons



Minimal conformation is not unique.

GAS Sampling of Lattice Polygons

- Generalise GARM sampling by including negative moves
- $\phi = \langle \phi_0, \phi_1, \phi_2, \ldots, \phi_k \rangle$ with $\ell_j = |\phi_j|$
- Introduce a set of parameters β_j along a sequence ϕ

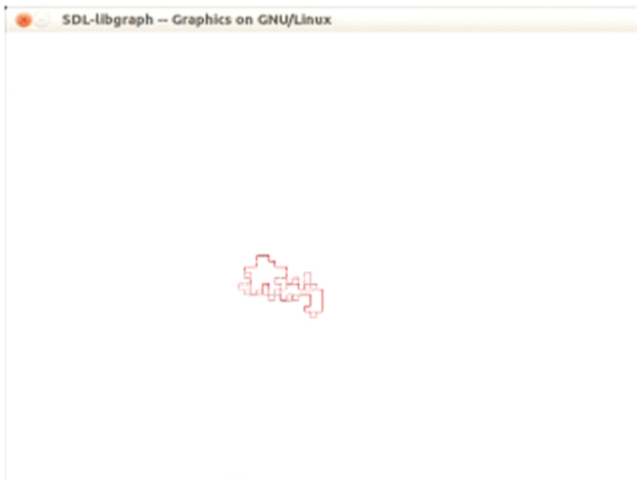
$$\mathrm{Pr[Pos.\ move]} = \frac{\beta_{\ell_j}\, a_+(\phi_j)}{a_-(\phi_j) + a_0(\phi_j) + \beta_{\ell_j}\, a_+(\phi_j)}$$

GAS Sampling of Lattice Polygons

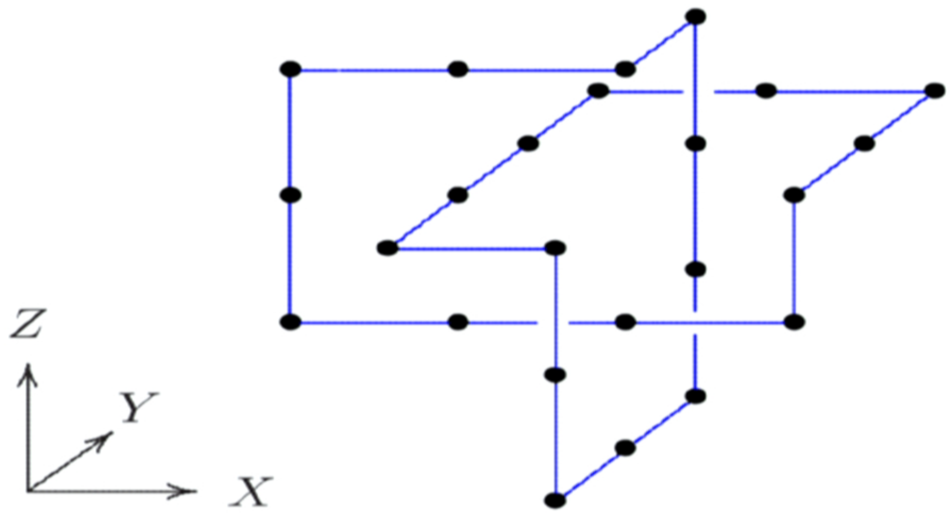
Assign a weight to each sequence ϕ:

$$W(\phi) = \left[\frac{a_-(\phi_0) + a_0(\phi_0) + \beta_{\ell_0} a_+(\phi_0)}{a_-(\phi_L) + a_0(\phi_L) + \beta_{\ell_L} a_+(\phi_L)} \right] \prod_{j=0}^{|\phi|-1} \beta_{\ell_j}^{\sigma(\phi_j, \phi_{j+1})}$$

GAS Sampling of Polygons



Knot Entropy



Knot type: Trefoil (3_1)
$p_n(3_1) = \#\{\text{Cubic lattice polygons of knot type } 3_1 \text{ and length } n\}$

Knot Entropy

$$p_n(K) = \#\{\text{Lattice polygons of knot type } K \text{ and length } n\}$$

Scaling arguments:

$$p_n(K) \simeq A_K \, n^{2-\alpha+N_K} \mu_0^n$$

where N_K = Number of prime components in K

Knot Entropy

$$p_n(K) = \#\{\text{Lattice polygons of knot type } K \text{ and length } n\}$$

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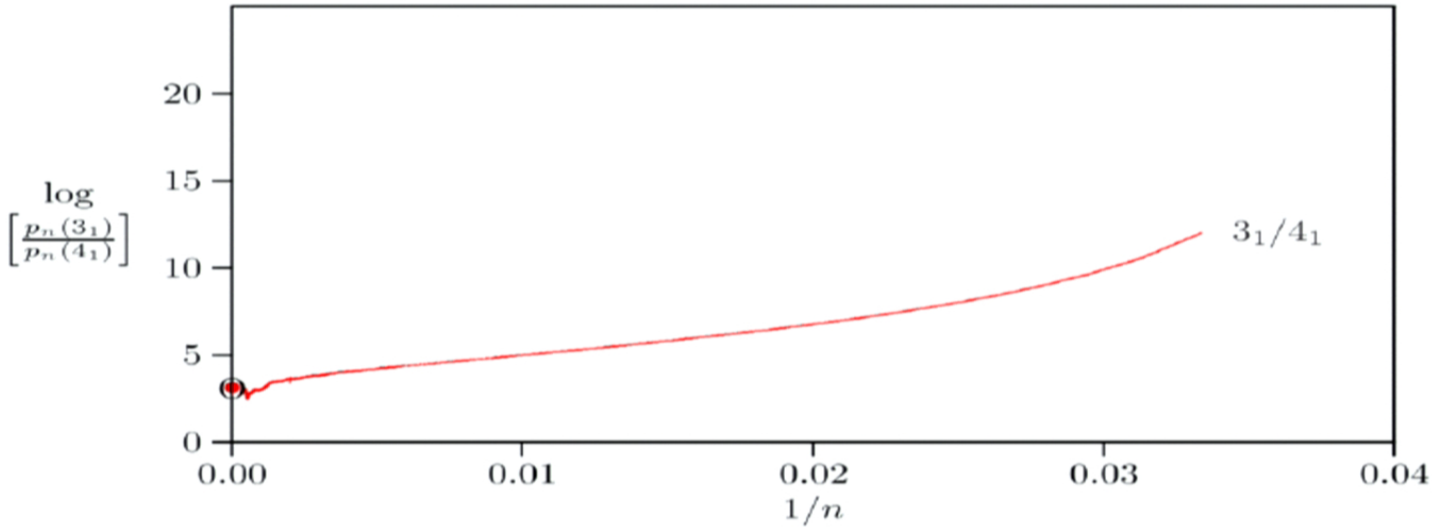
Knot Entropy



Asymptotically, about 22-27 trefoils for every figure eight knot.
Similar values on the fcc and bcc lattice.
Universal? [See also Baiesi + Orlandini 2012]

Thompson's group F

Elementary moves in analogy with BFACF elementary moves.

- Conjugation: With a generator $\mathbf{g}$:

$$ba^{-1}a^{-1}b^{-1}aab^{-1}a^{-1}ba \rightarrow \mathbf{g}\, ba^{-1}a^{-1}b^{-1}aab^{-1}a^{-1}ba\, \mathbf{g}^{-1}.$$

-

Thompson's group F

Conjugation and Left-insertions are uniquely reversible and irreducible on the state space of freely reduced trivial words S.

Metropolis-style sampling from a Boltzmann distribution on S.

Thompson's group F