Compressed random and self-avoiding walks

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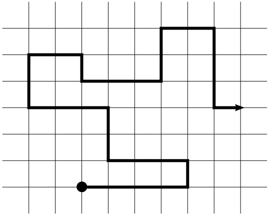
Introduction

A self-avoiding walk (SAW) is a walk on a lattice which cannot revisit vertices.



For a given lattice, c_n is the number of n-step SAWs (up to translation).
eg. square lattice:

$$c_0 = 1$$
$$c_1 = 4$$
$$c_2 = 12$$
$$c_3 = 36$$
$$c_4 = 100, \ldots$$

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Any SAW of length $m+n$ can be split into two smaller SAWs, of lengths m and n. So

$$c_{m+n} \leq c_m c_n.$$

So $\{c_n\}$ is a sub-multiplicative sequence. Then

$$\log c_{m+n} \leq \log c_m + \log c_m,$$

so $\{\log c_n\}$ is a sub-additive sequence. It follows that the limit

$$\log \mu = \lim_{n\to\infty} \frac{1}{n} \log c_n$$

exists. $\log \mu$ is called the connective constant of the lattice. Then

$$c_n \sim \theta_n \mu^n,$$

where μ is called the growth constant (sometimes connective constant) and $\theta_n = e^{o(n)}$. By submultiplicativity, we know that $\theta_n \geq 1$.

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Conjecture (Nienhuis 1982)

$$c_n \sim A n^{\gamma - 1} \mu^n$$

for A, μ, γ *constant.* A *and* μ *are lattice-dependent,* γ *depends only on dimension. In two dimensions,* $\gamma = 43/32$*.*

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In high dimensions, can do a bit better:

Theorem (Hara and Slade 1992)

On the hypercubic lattice in five or more dimensions,

$$c_n \sim A\mu^n.$$

Also interested in the size and shape of SAWs. eg. let $\langle R_e^2 \rangle_n$ be the mean-squared end-to-end distance of SAWs of length n.

Conjecture (Nienhuis 1982; Lawler, Schramm and Werner 2004)

$$\langle R_e^2 \rangle_n \sim C n^{2\nu}$$

with C lattice-dependent and ν dimension-dependent. In two dimensions, $\nu = 3/4$.

The exponents γ and ν are also connected to the scaling limit of SAWs:

Conjecture (Lawler, Schramm and Werner 2004)

Self-avoiding walks have a conformally invariant scaling limit, namely $SLE_{8/3}$.

Generating functions

The (ordinary) generating function for $\{c_n\}$ is

$$C(z) = \sum_{n\geq 0} c_n z^n$$

Then $z_c = 1/\mu$ is the radius of convergence of $C(z)$. In general, expect the behaviour near z_c to be

$$C(z) \sim \text{const.}(1 - z/z_c)^{-\gamma},$$

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Because $c_n \geq \mu^n$,

$$C(z) \geq \sum_{n\geq 0} \mu^n z^n = \frac{1}{1 - z\mu}$$

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Expect that $C(z)$ is non-D-finite, ie. does not satisfy a linear ODE with polynomial coefficients.

Polymer models

SAWs are an important model in statistical mechanics of linear polymers in a solvent: chains of monomers, connected by bonds of fixed length and at fixed angles.

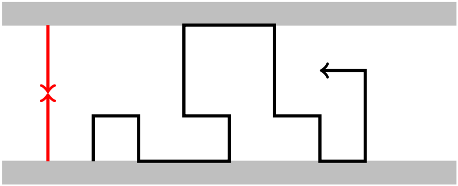
Unlike random walks (another, simpler model), SAWs encapsulate the excluded volume principle: two different monomers can't occupy the same point in space.

Monomers in a polymer can interact with each other, other polymers, surfaces (both penetrable and impenetrable) or with other external agents. Usually, these interactions are either attractive or repulsive.

Can also model forces applied to the polymer at various points/directions.

Compressive force

The model we are interested in here is a polymer between two impenetrable plates, being compressed together.



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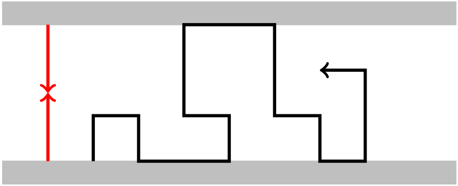

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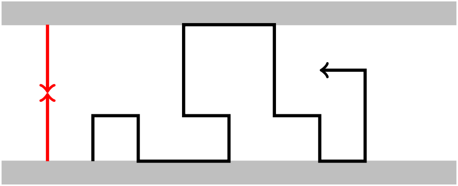

Take walks in the upper half-plane, starting at the origin. For a walk γ which reaches maximum height $h(\gamma)$ above the surface, associate a Boltzmann weight $e^{-f \cdot h(\gamma)}$.

So the walk above receives weight e^{-3f}.

The partition function of walks of length n is then

$$Z_n(f) = \sum_{|\gamma|=n} e^{-f \cdot h(\gamma)}$$

and the free energy is

$$\lambda(f) = \lim_{n\to\infty} \frac{1}{n} \log Z_n(f)$$

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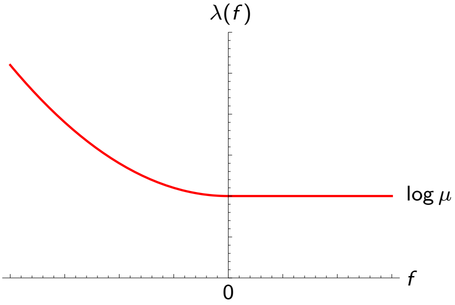
$f > 0$ represents a force pushing down towards the surface. $f < 0$ represents a force pulling away from the surface. When f is large and positive, walks with small $h(\gamma)$ dominate the partition function. When f is large and negative, walks with large $h(\gamma)$ dominate.

$\lambda(f)$ is a continuous, convex function of f, and is almost-everywhere differentiable.

It has been proven [NRB 2015] that $\lambda(f)$ has a point of non-analyticity at $f = 0$: it is strictly decreasing for $f < 0$, but $\lambda(f) = \log \mu$ for $f \geq 0$:



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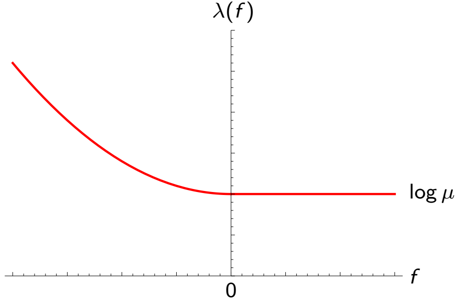

This indicates a phase transition at $f = 0$.

However, this behaviour is slightly puzzling. No matter how large we make f (favouring walks which stay close to the surface, and punishing those which wander away), $\lambda(f)$ remains constant and equal to its value at $f = 0$.

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Conjecture

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For $f < 0$, expect that $\theta_n(f)$ does not depend on n.

Random walks

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Easy to show

Theorem

$$R_n(0) \sim \frac{2}{\sqrt{\pi}} n^{-1/2} 4^n$$

In a horizontal strip of height $h-2$, let $c_n(h,r,s)$ be the number of n-step walks which start at height r and end at height s, with $0 \le r,s \le h-2$. Then, because random walks are Markovian, $c_n(h,r,s) = K_h^n(r,s)$, where K_h is the $(h-1)\times(h-1)$ symmetric matrix with

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Let $J_h = \frac{1}{4}K_h$. J_h is tridiagonal and Toeplitz, so it is (with a change of variables) the Jacobi matrix for Chebyshev polynomials.

Lemma

$$\det(J_h - \lambda I) = 4^{-h+1} U_{h-1}(1-2\lambda),$$

where $U_i(x)$ are Chebyshev polynomials of the second kind:

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The roots of $U_i(x)$ are well known:

$$x_k = \cos\left(\frac{k\pi}{i+1}\right) \qquad \text{for } k = 1,\dots,i.$$

Eigenvalues and eigenvectors:

$$J_h \mathbf{v}_j = \lambda_j \mathbf{v}_j$$

with

$$\lambda_j = \frac{1}{2} + \frac{1}{2}\cos\left(\frac{j\pi}{h}\right) \qquad \text{and} \qquad \mathbf{v}_j = \left\{\sin\left(\frac{j(k+1)\pi}{h}\right)\right\}_{k=0,\ldots,h-2}$$

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Eigendecomposition:

$$J_h^n(r,s) = \frac{2}{h}\sum_{j=1}^{h-1} \sin\left(\frac{j(r+1)\pi}{h}\right)\left[\frac{1}{2} + \frac{1}{2}\cos\left(\frac{j\pi}{h}\right)\right]^n \sin\left(\frac{j(s+1)\pi}{h}\right)$$

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If $n, h \to \infty$ with $h^2 \ll n$, then $j = 1$ term dominates, so

$$\begin{aligned} J_h^n(r,s) &\sim \frac{2}{h}\left[\frac{1}{2} + \frac{1}{2}\cos\left(\frac{\pi}{h}\right)\right]^n \sin\left(\frac{(r+1)\pi}{h}\right)\sin\left(\frac{(s+1)\pi}{h}\right) \\ &\sim \frac{2}{h}\exp\left\{-\frac{n\pi^2}{4h^2}\right\}\sin\left(\frac{(r+1)\pi}{h}\right)\sin\left(\frac{(s+1)\pi}{h}\right) \end{aligned}$$

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In particular, we want walk to start at height 0, so

$$J_h^n(0,s) \sim \frac{2\pi}{h^2}\exp\left\{-\frac{n\pi^2}{4h^2}\right\}\sin\left(\frac{(s+1)\pi}{h}\right)$$

Can end at any height between 0 and $h-2$, so define

$$F_n(h) = \sum_{s=0}^{h-2} J_h^n(0,s) \sim \frac{4}{h} \exp\left\{-\frac{n\pi^2}{4h^2}\right\} \qquad \text{for } h^2 \ll n$$

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So the partition function $R_n(f)$ is

$$\begin{aligned} R_n(f) &= 4^n \sum_{h=0}^{\infty} e^{-fh} \left[F_n(h+2) - F_n(h+1)\right] \\ &= 4^n e^{2f}(1-e^{-f}) \sum_{h=2}^{\infty} e^{-fh} F_n(h) \\ &\sim 4^{n+1} e^{2f}(1-e^{-f}) \sum_{h=2}^{\infty} e^{-fh} h^{-1} \exp\left\{-\frac{n\pi^2}{4h^2}\right\} \end{aligned}$$

Convert sum to integral:

$$\sim 4^{n+1} e^{2f} (1 - e^{-f}) \int_0^\infty x^{-1} \exp\left\{ -\left(\frac{n\pi^2}{4x^2} + fx \right) \right\} dx$$

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The asymptotics of this integral can be computed (with care). Get

Theorem

$$R_n(f) \sim A \cdot 4^n \cdot n^{-1/6} \cdot f^{-1/3} e^f (e^f - 1) \cdot \exp\left\{B \cdot n^{1/3} \cdot f^{2/3}\right\} \qquad \text{for } f > 0$$

for known constants A and B.

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This matches series analysis.

Back to SAWS

Can use SLE to estimate the probability that a SAW stays in a strip of height h. Get a similar integral, and use the same method to compute the asymptotics.

Conjecture

$$Z_n(f) \sim A \cdot \mu^n \cdot n^{3/16} \cdot f^{5/16} \cdot \exp\left\{B \cdot n^{3/7} \cdot f^{4/7}\right\} \qquad \text{for } f > 0$$

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A term like $\exp\{c \cdot n^{1/2}\}$ has also now been observed in the asymptotics of 1324-avoiding permutations [Conway & Guttmann 2014].

Unusual asymptotics

Similar results are conjectured for compressed self-avoiding bridges and polygons.

These asymptotics are unusual for models like this. Something similar is conjectured to occur in a model of polymer collapse, with a subexponential term like $\exp\{c \cdot n^{1/2}\}$. [Owczarek, Prellberg & Brak 1993]

A term like $\exp\{c \cdot n^{1/2}\}$ has also now been observed in the asymptotics of 1324-avoiding permutations [Conway & Guttmann 2014].

Unclear why such terms appear for some models but not others.

Reference:

NRB, A J Guttmann, I Jensen and G F Lawler, *Compressed self-avoiding walks, bridges and polygons*, submitted, preprint at arXiv:1506:00296

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Thank you!