Solvable models of self-avoiding walks

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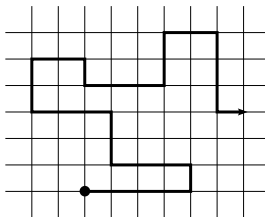
Collaborators
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Outline

Introduction I: SAWs

Walks 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:

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

For regular lattices in $d \geq 2$, no known expression for c_n. But we still know something! Because $\log c_n$ is a sub additive sequence,

$$c_n = \exp(\kappa n + o(n))$$

κ is the connective constant, $\mu = e^{\kappa}$ is the growth constant.

In general, κ and μ are not known exactly. Honeycomb lattice is special:

Theorem (Duminil-Copin and Smirnov 2012)

On the honeycomb (hexagonal) lattice, $\mu = \sqrt{2 + \sqrt{2}}$.

For other lattices, have numerical estimates based on series data (eg. 70 terms for square lattice)

$$\mu_{\text{square}} \approx 2.63815853031 \qquad \mu_{\text{triangular}} \approx 4.150797226$$

Subexponential factors unproven, but

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, $\gamma = 43/32$.

In high dimensions, can do a bit better:

Theorem (Hara and Slade 1992)

On the hypercubic lattice in five or more dimensions,

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

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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)

$$\langle R_e^2 \rangle_n \sim Cn^{2\nu}$$

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 $SLE_{8/3}$.

The 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 $C(z)$, and

$$C(z) \to \infty \qquad \text{as } z \to z_c^-.$$

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

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Previously solved models – Partially directed walks

There are lots of things we don't know about SAWs! Instead, we can look at simpler models.

Partially directed walks (on the square lattice) avoid stepping in a certain direction.
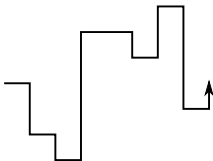
Easy to solve the generating function (construct column by column):

Theorem

The generating function of PDWs on the square lattice is

$$G_{PDW}(z) = \frac{1+z}{1-2z-z^2} = 1 + 3z + 7z^2 + 17z^3 + 41z^4 + 99z^5 + 239z^6 + \ldots$$

The number of PDWs of length n is asymptotically

$$c_n^{PDW} \sim \frac{2+\sqrt{2}}{2\sqrt{2}}(1+\sqrt{2})^n.$$

Prudent walks

These are walks which never take a step towards a vertex they have previously visited. They always end on the boundary of their bounding box.

This provides a sub-classification: 1-sided must end on one chosen side (eg. east) of box (= PDWs), 2-sided must end on one of two chosen sides (eg. north or east), 3-sided on one of three chosen sides, and 4-sided can end anywhere on box. 2- and 3-sided have been solved, using the kernel method (more later) and its variants.
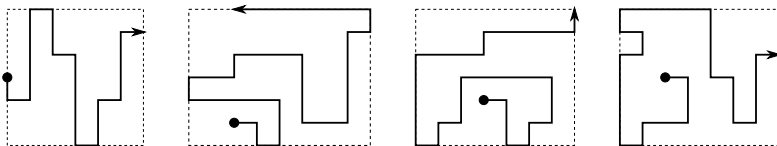
Theorem (Duchi 2005)

The generating function of 2-sided prudent walks is

$$G_{2\text{-}pru}(z) = \frac{1}{1 - 2z - 2z^2 + 2z^3}\left(1 + z - z^3 + z(1-z)\sqrt{\frac{1-z^4}{1-2z-z^2}}\right).$$

Theorem (Bousquet-Mélou 2010)

The generating function of 3-sided prudent walks is

$$G_{\text{3-pru}}(z) = [\text{big sum of algebraic functions}]$$

$G_{\text{3-pru}}(z)$ *is non-D-finite.*

From these two results,

Corollary (Duchi 2005; Bousquet-Mélou 2010)

*The numbers of 2-sided and 3-sided prudent walks of length n are asymptotically*

$$c_n^{\text{2-pru}} \sim a\tau^n \qquad \text{and} \qquad c_n^{\text{3-pru}} \sim b\tau^n$$

where a, b, τ *are positive constants. In particular,* $\tau \approx 2.48$ *is a root of*
$2 - 2\tau - 2\tau^2 + 2\tau^3 = 0.$

Numerical evidence also suggests that the number of 4-sided prudent walks has the same asymptotic form as 2- and 3-sided.

Weakly directed walks

These are walks which are partially directed between any two visits to the same horizontal line.

They can be constructed by concatenating partially directed bridges.

A self-avoiding bridge is a SAW whose starting point has (strictly) minimal y-coordinate, and whose endpoint has (not strictly) maximal y-coordinate.

Bridges can be freely concatenated without creating intersections (unlike SAWs). Any bridge can be decomposed into a sequence of irreducible bridges, which cannot be decomposed any further. A row of the lattice is a split row of a bridge ω if ω crosses it precisely once. Irreducible bridges have only one split row: $0 \leq y \leq 1$.
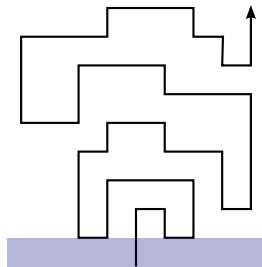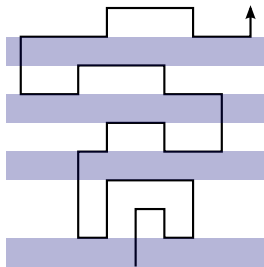
Easy to show bridges have the same exponential growth rate as SAWs.

Weakly directed walks are (except for funny stuff at the start and end) composed of a sequence of irreducible partially directed bridges. (Any two visits to the same horizontal line must occur in the same irreducible bridge.)

Theorem (Bacher and Bousquet-Mélou 2011)

The generating function of weakly directed walks is

$$G_{WDW}(z) = [big \ sum \ of \ algebraic \ functions].$$

$G_{WDW}(z)$ is non-D-finite. The number of weakly directed walks of length n is asymptotically

$$c_n^{WDW} \sim c\omega^n,$$

where c is a positive constant and $\omega \approx 2.54$.

Unknown if ω is algebraic or not. Decimal expansion suggests no.

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To recap, the growth constant μ for SAWs on the square lattice is ≈ 2.63815. These solvable models have growth rates

- partially directed walks: $1 + \sqrt{2} \approx 2.414$
- 2- and 3-sided prudent walks: $\tau \approx 2.48$
- weakly directed walks: $\omega \approx 2.54$.

Can get higher growth rates by computing the generating function $\mathcal{I}_n(z)$ of irreducible bridges up to length n, and then taking

$$B(z) = \frac{\mathcal{I}_n(z)}{1 - \mathcal{I}_n(z)}.$$

But it doesn't seem fair to call this "solvable", since it's limited only by computing power...

Weakly prudent bridges – Definition

Say a SAW w is co-prudent if its reversal $\bar{w}$ is prudent.

A bridge is weakly prudent if each of its irreducible components is prudent or co-prudent. A weakly prudent bridge is k-sided if each of its irreducible components is too. (So 1-sided weakly prudent bridge = weakly directed bridge.)

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This is not the same as "prudent between any two visits to a line" – an irreducible bridge may satisfy that property without being prudent itself.

Our construction method, like that of Bacher and Bousquet-Mélou, depends on the bridge decomposition, so it's unclear if that model can be solved.

Construction

A ramp is a bridge whose endpoint has (not strictly) maximal x-coordinate.

Using symmetry arguments (eg. prudent and co-prudent bridges have same generating function) and inclusion-exclusion, can show that we need two new generating functions:

- 2-sided (north and east) irreducible prudent ramps $\rightarrow$ gf $\mathcal{P}(z)$
- irreducible partially directed (no west steps) ramps $\rightarrow$ gf $\mathcal{D}(z)$

Bacher and Bousquet-Mélou already calculated $\mathcal{D}$.

For $\mathcal{P}$, the irreducibility is what makes this complicated. Can calculate it directly, but the resulting function is very complicated. Instead, there is another way:

Lemma

$$\mathcal{P}(z) = \frac{\mathcal{R}(z) - \tilde{\mathcal{R}}(z)}{1 + \mathcal{R}(z)}$$

where

- $\mathcal{R}$ is gf of 2-sided (north and east) prudent ramps
- $\tilde{\mathcal{R}}$ is gf of 2-sided (north and east) prudent ramps which
  - start with pair of steps north-west, and
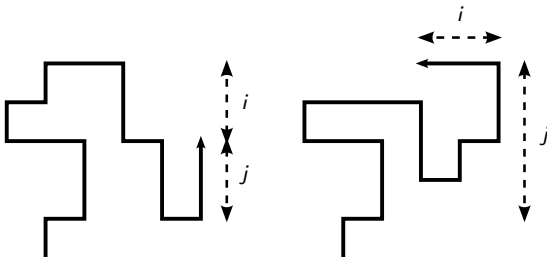 - have $1 \leq y \leq 2$ as a split row

Generating functions

$$E(z; u, v) \equiv E(u, v) = \sum_{n,i,j} e_{n,i,j} z^n u^i v^j$$

$$N(z; u, v) \equiv N(u, v) = \sum_{n,i,j} n_{n,i,j} z^n u^i v^j$$

where $e_{n,i,j}$ (resp. $n_{n,i,j}$) is the number of 2-sided (north and east) prudent walks of length n which end on the east (resp. north) side of their bounding box, starting with a north step and never returning to $y = 0$.

- i is distance from endpoint to north-east corner of box
- j is distance from endpoint to the line $y = 1$.

Then $\mathcal{R}(z) = E(z; 0, 1) = N(z; 0, 1)$.

Lemma

The generating functions E and N satisfy the functional equations

$$\left(1 - \frac{zu}{u-zv} - \frac{z^2 u}{v-zu}\right) E(u,v) = z - \frac{z^2 v}{u-zv} E(zv,v)$$
$$- \frac{z^2 u}{v-zu} E(u,zu) + zvN(z,v)$$

$$\left(1 - \frac{zuv}{u-z} - \frac{z^2 uv}{1-zu}\right) N(u,v) = \frac{z}{1-zu} - \frac{z^2 v}{u-z} N(z,v) + zE(zv,v).$$

Construct walks according to last inflating step – last step which moved the north or east side of the bounding box.

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These equations (and the ones for $\tilde{\mathcal{R}}$, which are similar) can be solved with the iterated kernel method. $\mathcal{R}$ and $\tilde{\mathcal{R}}$ end up having the same asymptotic growth rate as 2-sided prudent walks (cf. Duchi and Bousquet-Mélou).

Lemma

The gf $\mathcal{I}(z)$ of irreducible weakly prudent bridges is

$$\mathcal{I}(z) = 4\mathcal{P}(z) - 2\mathcal{D}(z) - z$$

An irreducible prudent or co-prudent bridge can take four possible forms: (north and east) or (north and west), or the reversal of (south and east) or (south and west). All these have the same gf.

But some bridges are both (north and east) prudent and (south and west) co-prudent! These are partially directed bridges. Likewise for (north and west) prudent and (south and east) co-prudent.

The bridge of a single step is still counted twice, so subtract z.

Theorem

The gf $G_{WPB}(z)$ of weakly prudent bridges is

$$G_{WPB}(z) = \frac{\mathcal{I}(z)}{1 - \mathcal{I}(z)}$$

Asymptotics

The dominant singularity of $G_{WPB}(z)$ is the smallest root of $\mathcal{I}(z) = 1$. Can't solve it exactly, but have good numerical bounds:

$$z_{lower} < z_c < z_{upper}$$

where

$z_{lower} = 0.38787171534830376203597305306343719377725417206085039570$
$\qquad\qquad 64093675449931517842499455633171275906253711439593918,$

$z_{upper} = 0.38787171534830376203597305306343719377725417206085039570$
$\qquad\qquad 64093675449931517842499455633171275906253711461907434.$

So z_c is, correct to 101 digits,

$z_c \approx 0.38787171534830376203597305306343719377725417206085039570$
$\qquad\qquad 64093675449931517842499455633171275906253711464.$

Corollary

The number of weakly prudent bridges of length n is asymptotically

$$c_n^{WPB} \sim c\zeta^n,$$

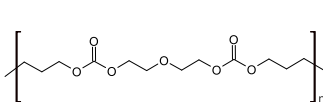*where $\zeta = z_c^{-1} \approx 2.57817201$ and c is a positive constant.*

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z_c and ζ are almost certainly not algebraic.

The gf is almost certainly non-D-finite. (Unable to prove!)

The mean-squared end-to-end distance is $O(n^2)$, like all other solved models (except spiral walks) but unlike SAWs.

Introduction II: Polymer adsorption - SAWs

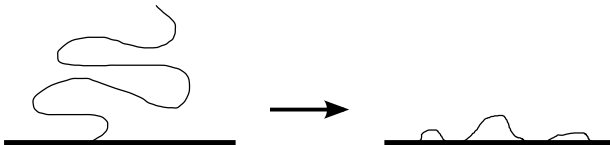A polymer is a large molecule made of many repeated parts.
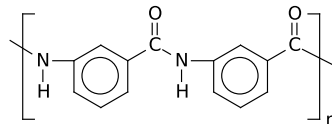
Polymers in solution interact with one another, themselves and their environment.

These interactions depend on solvent quality, temperature, pressure, etc.

Polymer adsorption is the interaction with a surface:
- impenetrable
- penetrable

and this interaction can be attractive or repulsive. At an impenetrable surface, sometimes observe a phase transition: as temperature is decreased, polymers transition from a desorbed to an adsorbed state:

To model polymer adsorption, restrict SAWs to a half-space. Interactions occur when walks visit the boundary. (A visit could be a vertex or an edge.)

Define $c_n^+(\nu)$ to be number of n-step SAWs which visit boundary ν times.

Then associate a fugacity (Boltzmann weight) y with each visit. Define the partition function

$$Z_n^+(y) = \sum_\nu c_n^+(\nu) y^\nu$$

Physically, $y = \exp(\epsilon/kT)$, where

- ϵ is energy gain per contact (determined experimentally?)
- k is Boltzmann's constant, $1.38 \times 10^{-23}\,\mathrm{JK}^{-1}$
- T is absolute temperature

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When y is small (large T), walks with few contacts dominate the partition function, but when y is large (small T), walks with lots of contacts dominate. So

- small $y \Rightarrow$ surface is repulsive
- large $y \Rightarrow$ surface is attractive

Like c_n, can prove

$$Z_n^+(y) = \exp(\kappa(y)n + o(n))$$

For $y > 0$, $\kappa(y)$ is

- convex in $\log y$ ($\Rightarrow$ continuous)
- non-decreasing

By comparison with walks which never touch the surface, can show

$$\kappa(y) = \kappa \qquad \text{for } 0 \leq y \leq 1.$$

By comparison with the walk which never leaves the surface, can show

$$\kappa(y) \geq \log y$$

So there must be a critical point y_c with

$$\kappa(y) \begin{cases} = \kappa & \text{if } y \leq y_c \\ > \kappa & \text{if } y > y_c \end{cases}$$
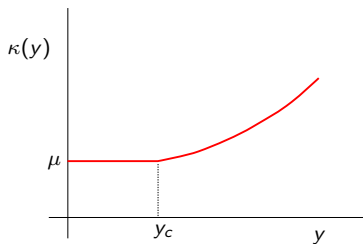
This is the location of the phase transition:

$$T_c = \frac{\epsilon}{k \log y_c}$$

In the limit of polymer length:

- $y < y_c$ ($T > T_c$) $\Rightarrow$ polymers are desorbed
- $y > y_c$ ($T < T_c$) $\Rightarrow$ polymers are adsorbed

Define the bivariate generating function

$$C^+(t, y) = \sum_{n, \nu} c_n^+(\nu) t^n y^\nu = \sum_n Z_n^+(y) t^n.$$

Then if $\mu(y) = e^{\kappa(y)}$, the radius of convergence of $C^+(x, y)$ for a given y is $t_c(y) = \mu(y)^{-1}$.

What does this really mean?

Put a Boltzmann distribution on the walks of length n by setting

$$\mathbb{P}(\gamma) = \frac{y^{c(\gamma)}}{Z_n^+(y)}$$

where $c(\gamma)$ is the number of γ's surface contacts.

Then the mean density of contacts for walks of length n is

$$\frac{1}{n} \frac{\sum_\nu \nu c_n^+(\nu) y^\nu}{Z_n^+(y)} = \frac{y}{n} \frac{\partial \log Z_n^+(y)}{\partial y}.$$

As $n \to \infty$, this becomes

$$y \frac{\partial \kappa(y)}{\partial y} \begin{cases} = 0 & \text{if } y < y_c \\ > 0 & \text{if } y > y_c. \end{cases}$$

Since the general SAW model has not been solved, finding exact results (like the value of y_c) is difficult. The honeycomb lattice is special:

Theorem (NRB, Bousquet-Mélou, de Gier, Duminil-Copin and Guttmann 2013)

For the honeycomb lattice oriented with edges perpendicular to the surface,

$$y_c = 1 + \sqrt{2}$$

Theorem (NRB 2013)

For the honeycomb lattice with edges oriented parallel to the surface,

$$y_c = \sqrt{\frac{2 + \sqrt{2}}{1 + \sqrt{2} - \sqrt{2 + \sqrt{2}}}}$$

Methods for the honeycomb lattice can be used to compute estimates for other lattices [NRB, Guttmann and Jensen 2012]:

- Square lattice: $y_c^{\text{vertex}} \approx 1.77564$, $y_c^{\text{edge}} \approx 2.040135$
- Triangular lattice: $y_c^{\text{vertex}} \approx 2.144181$, $y_c^{\text{edge}} \approx 2.950026$

Another strategy: subclasses of SAW for which the model is solvable.

Previously solved models

Previously the subclasses of SAW which have been solved all have a directedness constraint:

Dyck paths

Motzkin paths

Partially directed walks
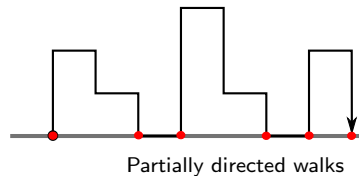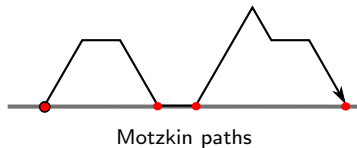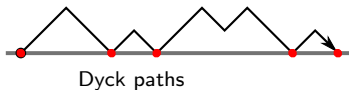
Adsorbing prudent walks

Prudent walks are (in general) not directed. We consider 2-sided prudent walks on the square lattice above an impenetrable surface, and 1- and 2-sided walks on the triangular lattice, with a weight associated with steps along the surface.
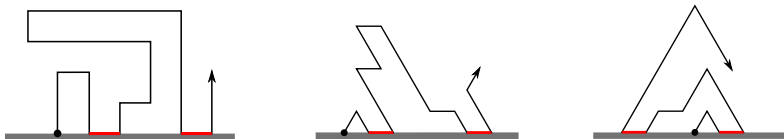
Note: 1-sided square walks are just PDWs, which are already solved. 3- and 4-sided square walks are the same thing, as are 2- and 3-sided triangular walks. We are unable to solve 3-sided square walks above a surface.

2-sided square walks and 2-sided triangular walks are non-directed – they can take steps in all directions on the lattice.

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Construction - 2-sided square walks

Almost the same as 2-sided prudent ramps, but now we have surface interactions.
Construct two generating functions:

$$R(u, v) \equiv R(z; u, v; y) = \sum_{n,i,j,\alpha} R_{n,i,j,\alpha} z^n u^i v^j y^\alpha$$

$$T(u, v) \equiv T(z; u, v; y) = \sum_{n,i,j,\alpha} T_{n,i,j,\alpha} z^n u^i v^j y^\alpha$$

where $R_{n,i,j,\alpha}$ (resp. $T_{n,i,j,\alpha}$) is the number of n-step 2-sided prudent walks ending on the right (resp. top) side of their bounding rectangle at a distance i from the NE corner of the rectangle and a distance j from the surface, with α steps along the surface.
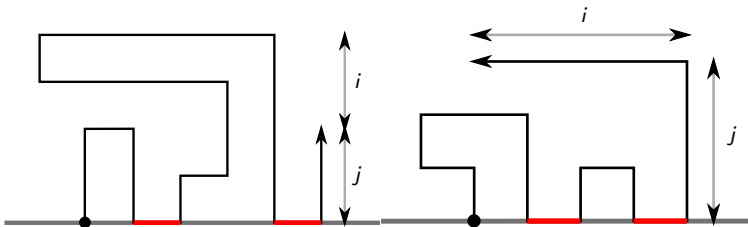
Construct walks in the same way as before – look at last inflating step.

Lemma

The gfs $T(u, v)$ and $R(u, v)$ satisfy

$$L(u, v)T(u, v) = \frac{1}{1 - zuy} - \frac{z^2 v}{u - z}T(z, v) + zR(zv, v) - z(1 - y)R(zv, 0)$$

$$M(u, v)R(u, v) = 1 + zvT(z, v) - \frac{z^2 v}{u - zv}R(zv, v) - \frac{z^2 u}{v - zu}R(u, zu)$$
$$- \frac{zu(1 - y)}{u - zv}R(u, 0) + \frac{z^2 v(1 - y)}{u - zv}R(zv, 0)$$

where

$$L(u, v) \equiv L(z; u, v) = 1 - \frac{zuv(1 - z^2)}{(u - z)(1 - zu)}$$

$$M(u, v) \equiv M(z; u, v) = 1 - \frac{zuv(1 - z^2)}{(v - zu)(u - zv)}$$

Similar equations hold for the gfs of 1- and 2-sided triangular prudent walks.

Solutions obtained in the same way, via the iterated kernel method.
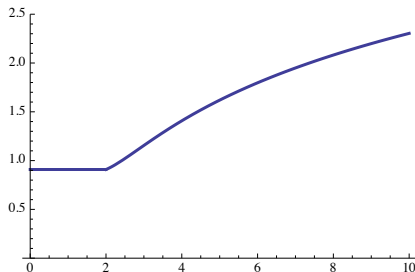
Free energy

> **Theorem**
>
> The dominant singularity of $R(z; 1, 1; y)$ and $T(z; 1, 1; y)$ is
>
> $$z_c(y) = \begin{cases} \theta \approx 0.403032 & y \leq 2 \\ h(y) & y > 2, \end{cases}$$
>
> where θ is a root of $1 - 2\theta - 2\theta^2 + 2\theta^3 = 0$, and $h(y)$ is a root of
>
> $$1 - y - y(1 - y)h(y) + yh(y)^2 + y(1 - y)h(y)^3 = 0.$$

So the free energy is $\kappa(y) = -\log z_c(y)$:

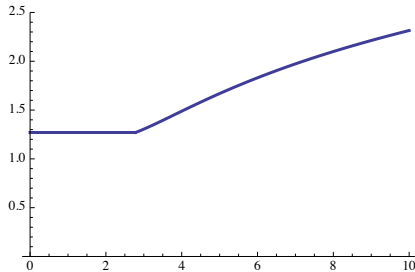The phase transition is first-order, as $\kappa'(y)$ is not continuous.

Theorem

For both 1-sided and 2-sided triangular prudent walks, dominant singularity is

$$z_c(y) = \begin{cases} \frac{\sqrt{17}-3}{4} \approx 0.281, & 0 \le y \le y_c \\ \frac{y^2 - \sqrt{y(-4+8y-4y^2+y^3)}}{2y(y-1)}, & y > y_c \end{cases}$$

where $y_c = \frac{7+\sqrt{17}}{4} \approx 2.78$.

So the free energy is $\kappa(y) = -\log z_c(y)$:

Again, a first-order phase transition. But why the same for both?

Every inflating step raises the top of the bounding triangle ⇒ as walks get longer and longer, it gets harder to "turn the corner" and move between LHS and RHS. So as walks get longer, they tend to get "stuck" as either 1-sided walks or reflections thereof.

Not the case for 2-sided square walks, where an inflating E step does not move the top of the bounding box. Not so hard to turn the corner ⇒ different free energy to PDWs.

Order of phase transitions

However, there is another question. All the directed models (Dyck paths, Motzkin paths, PDWs) have second-order phase transitions. And general SAWs are expected (from simulations etc) to also have a second-order transition.

⇒ Adsorption occurs smoothly.

So why do our models have first-order transitions?

For all the directed models, the endpoint of an n-step walk in the desorbed phase has mean height $O(n^{1/2})$ above the surface. So walks "drift" away from the surface slowly.

For general SAWs, expect this to be $O(n^{\nu}) = O(n^{3/4})$.

But for our models, the mean height of the endoint is $O(n)$. So walks quickly move away from the surface ⇒ adsorption is harder and non-smooth.

What happens if we force the walks to end on the surface?

Adsorbing loops

A loop (aka arch, excursion) is a SAW which starts and ends on the surface.

If our prudent walks have a first-order transition because they move away from the surface quickly, then we might expect prudent loops to have second-order transitions.

Already have the generating functions $\Rightarrow$ just need to set $v = 0$ in the existing functions.

Triangular loops (1- and 2-sided) do have a second-order transition. But 2-sided square loops still have a first-order transition!

Introduction I: SAWs   Previously solved models   Weakly prudent bridges   Introduction II: Polymer adsorption   **Adsorbing prudent walks**   Conclusion

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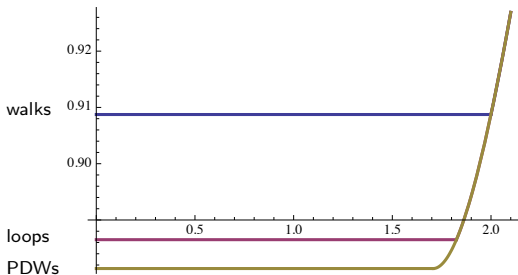
Even if the endpoints are tied to the surface, a large part of the walk may be far away, so adsorption could still be difficult.
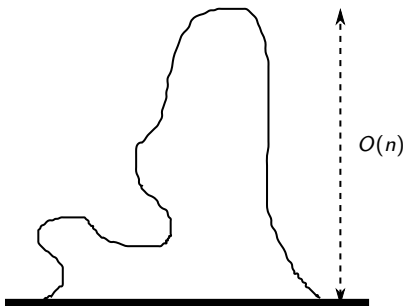
Should look at the mean maximum height of loops. For square loops, already have the catalytic variable u which tracks height. For triangular loops, need to include another variable to track height. (Not the height of the bounding triangle!) Still solve the same way.

We observe that triangular loops (1- and 2-sided) have mean maximum height $O(n^{1/2})$, while square loops have mean maximum height $O(n)$. So the adsorption for square loops should be non-smooth!

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Moreover, once they adsorb, 2-sided square walks and loops have the same free energy as PDWs:

In the desorbed phase, still relatively easy to "turn the corner" and become a non-PDW, hence the free energies are different there. But after adsorption, turning the corner incurs too great an energy loss, so prudent walks become "stuck" as PDWs.

Conclusion and further work

- Weakly prudent walks are solvable, with an exponential growth rate closer to that of SAWs than previously solved models.

- We have new solvable models of polymer adsorption, including models which are non-directed. They undergo a first-order adsorption transition, unlike most other exactly solved models. Square loops also have a first-order transition, while triangular loops have second-order.

- Can use vertex weights instead of edge weights. The solution follows similarly but the dominant singularity is harder to determine.

- Square lattice: unable to solve the full case, as it requires 3 catalytic variables. Some sub-cases solvable.

- Can add another fugacity corresponding to stiffness – the tendency of the walk to continue in straight lines.

- Inhomogeneous polymers/surfaces (eg. striped, random patterns).