On self-avoiding walks

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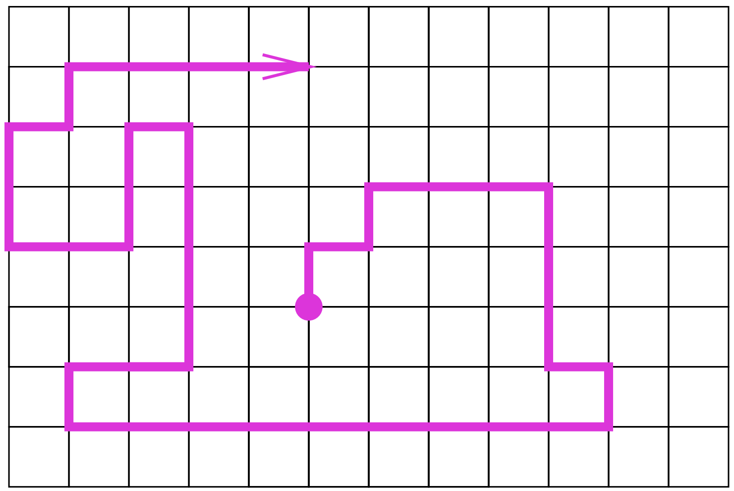
Outline

I. Self-avoiding walks (SAW): Generalities, predictions and results

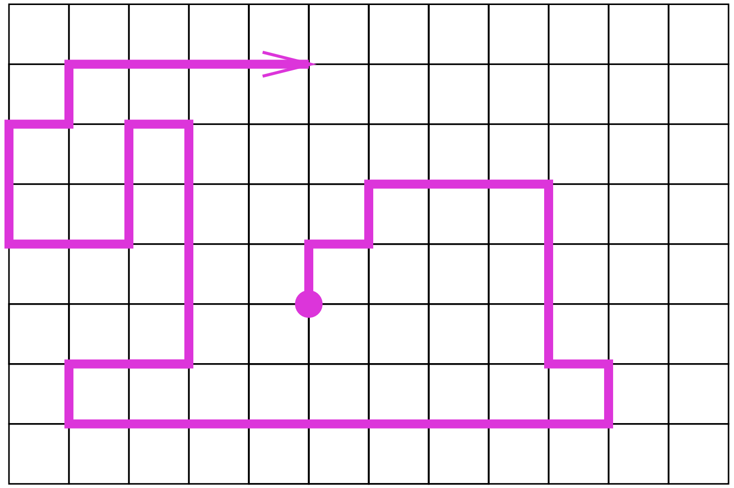
II. Some exactly solvable models of SAW

- II.0 A toy model: Partially directed walks
- II.1 Weakly directed walks
- II.2 Prudent walks
- II.3 Two related models

I. Generalities



Self-avoiding walks (SAW)



What is $c(n)$, the number of n-step SAW?

$$\begin{aligned} c(1) &= 4 \\ c(2) &= c(1) \times 3 &= 12 \\ c(3) &= c(2) \times 3 &= 36 \\ c(4) &= c(3) \times 3 - 8 &= 100 \end{aligned}$$

Not so easy! $c(n)$ is only known up to $n = 71$ [Jensen 04]

Problem: a highly non-markovian model

Some (old) conjectures/predictions

- The number of n-step SAW behaves asymptotically as follows:

$$c(n) \sim (\kappa)\,\mu^n\,n^\gamma$$

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where

- $\gamma = 11/32$ for all 2D lattices (square, triangular, honeycomb) [Nienhuis 82]

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- $\gamma = 11/32$ for all 2D lattices (square, triangular, honeycomb) [Nienhuis 82]

- $\mu = \sqrt{2+\sqrt{2}}$ on the honeycomb lattice [Nienhuis 82]
(proved this summer [Duminil-Copin & Smirnov])

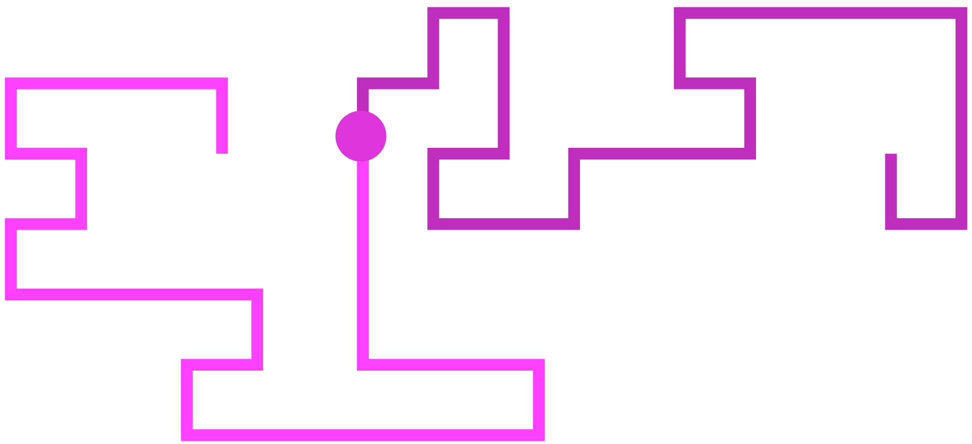
Some (old) conjectures/predictions

- The number of n-step SAW behaves asymptotically as follows:

$$c(n) \sim (\kappa)\, \mu^n\, n^\gamma$$

$\Rightarrow$ The probability that two n-step SAW starting from the same point do not intersect is

$$\frac{c(2n)}{c(n)^2} \sim n^{-\gamma}$$

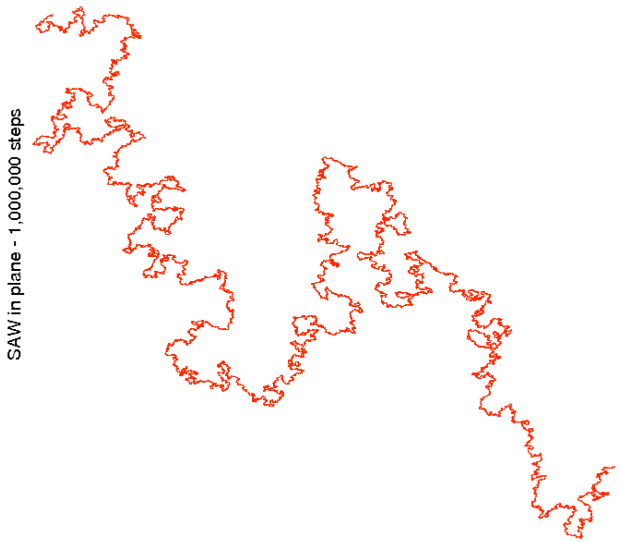


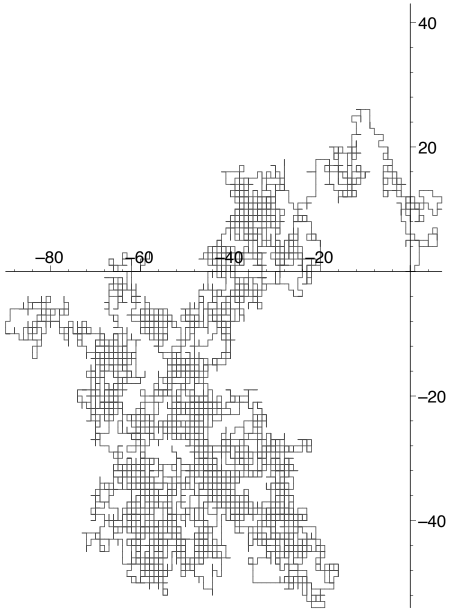
Some (old) conjectures/predictions

- The end-to-end distance is on average

$\mathbb{E}(D_n) \sim n^{3/4}$ (vs. $n^{1/2}$ for a simple random walk)

[Flory 49, Nienhuis 82]





Some (recent) conjectures/predictions

- Limit process: The scaling limit of SAW is $\mathrm{SLE}_{8/3}$.

(proved if the scaling limit of SAW exists and is conformally invariant [Lawler, Schramm, Werner 02])

This would imply

$$c(n) \sim \mu^n n^{11/32} \quad \text{and} \quad \mathbb{E}(D_n) \sim n^{3/4}$$

In 5 dimensions and above

- The critical exponents are those of the simple random walk:

$$c(n) \sim \mu^n n^{0}, \qquad \mathbb{E}(D_n) \sim n^{1/2}.$$

- The scaling limit exists and is the d-dimensional brownian motion

[Hara-Slade 92]

Proof: a mixture of combinatorics (the lace expansion) and analysis

II. Exactly solvable models

$\Rightarrow$ **Design simpler classes of SAW**, that should be natural, as general as possible... but still tractable

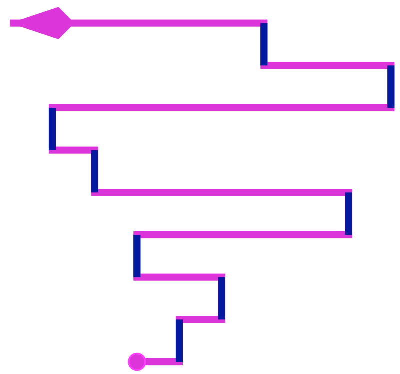
- solve better and better approximations of real SAW

- develop new techniques in exact enumeration

II.0. A toy model: Partially directed walks

Definition: A walk is partially directed if it avoids (at least) one of the 4 steps N, S, E, W.

Example: A NEW-walk is partially directed



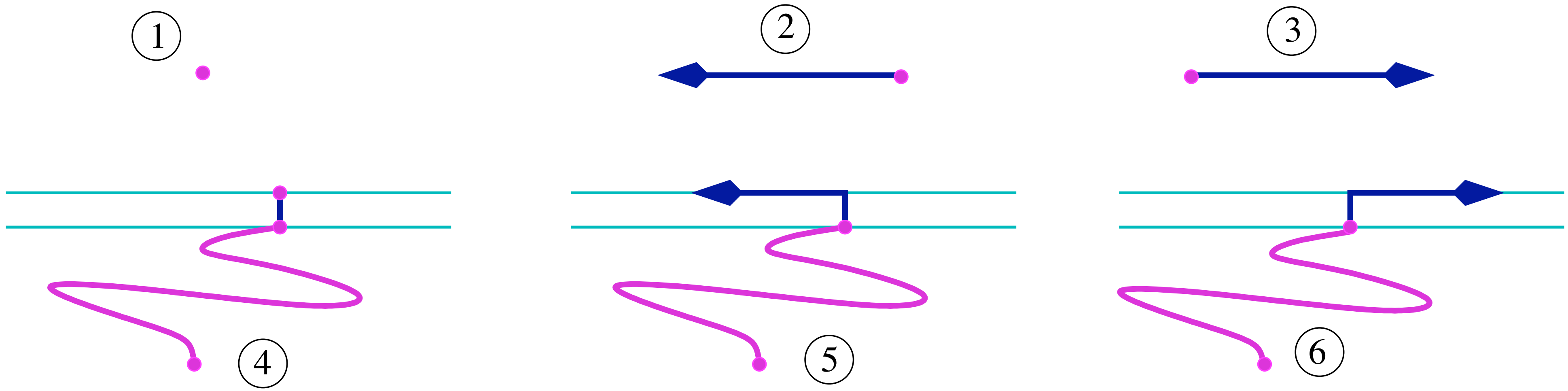
"Markovian with memory 1"

The self-avoidance condition is local.

A toy model: Partially directed walks

- Let $a(n)$ be the number of n-step NEW-walks, and $A(t) = \sum_{n\geq 0} a(n)t^n$ the associated generating function.

- Recursive description of NEW-walks:



- Generating function:

$$A(t) = 1 + 2\frac{t}{1-t} + tA(t) + 2A(t)\frac{t^2}{1-t}$$

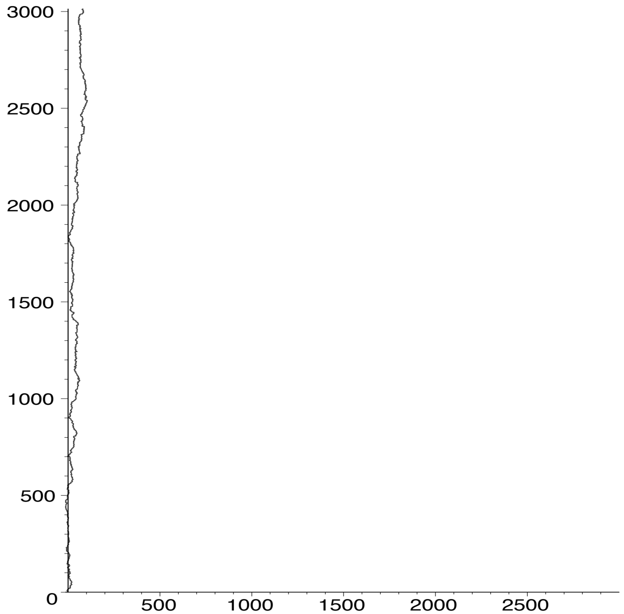
$$A(t) = \frac{1+t}{1-2t-t^2} \quad \Rightarrow \quad a(n) \sim (1+\sqrt{2})^n \sim (2.41...)^n$$

A toy model: Partially directed walks

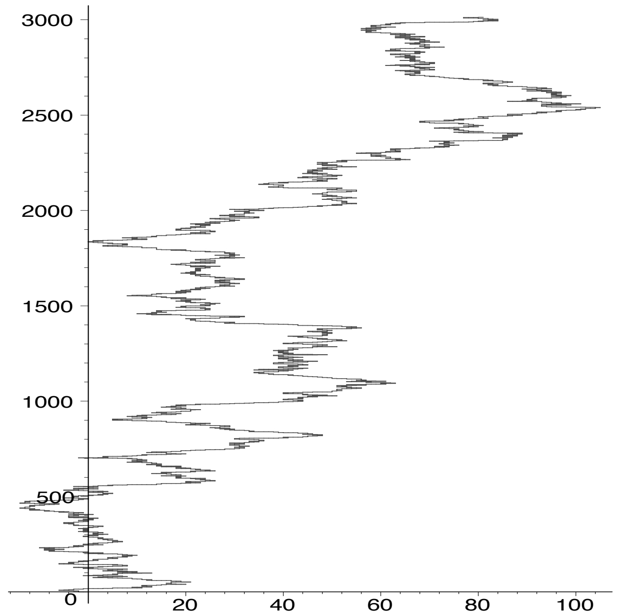
- Asymptotic properties: coordinates of the endpoint

$$\mathbb{E}(X_n) = 0, \quad \mathbb{E}(X_n^2) \sim n, \qquad \mathbb{E}(Y_n) \sim n$$

- Random NEW-walks:



Scaled by n (– and |)



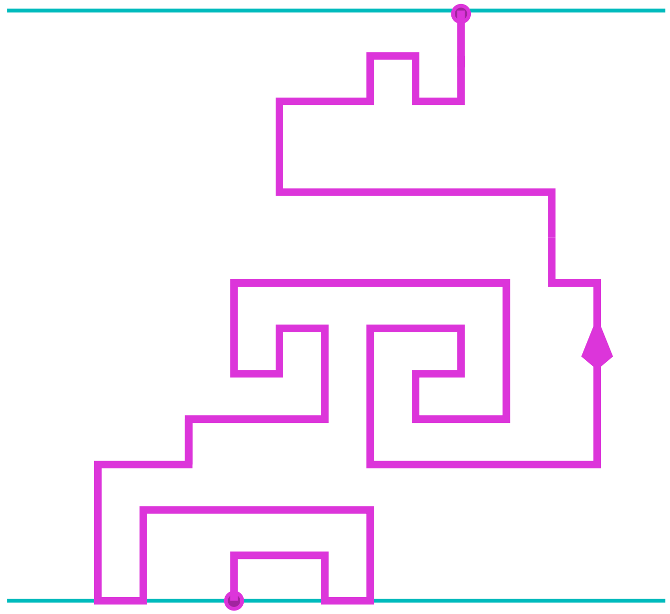
Scaled by $\sqrt{n}$ (–) and n (|)

II.1. Weakly directed walks

(joint work with Axel Bacher)

Bridges

• A walk with vertices $v_0, \ldots, v_i, \ldots, v_n$ is a bridge if the ordinates of its vertices satisfy $y_0 \leq y_i < y_n$ for $1 \leq i \leq n$.



• There are many bridges:

$$b(n) \sim \mu_{bridge}^n n^{\gamma'}$$

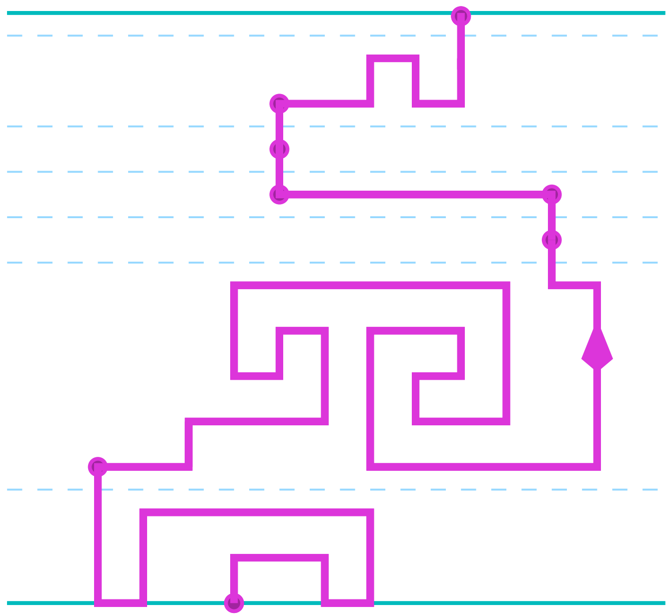
where

$$\mu_{bridge} = \mu_{SAW}$$

Irreducible bridges

Def. A bridge is irreducible if it is not the concatenation of two bridges.

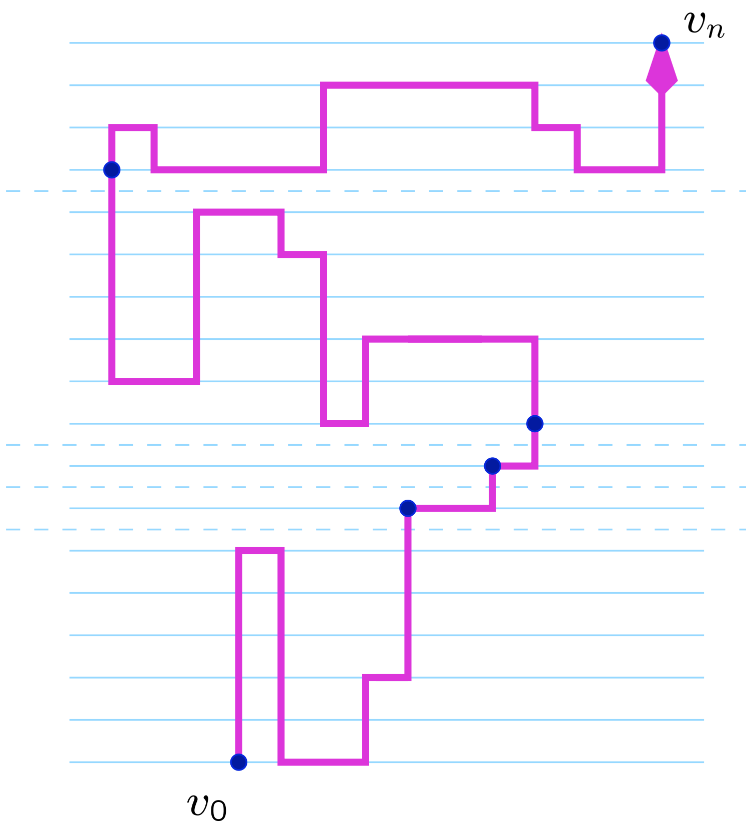
Observation: A bridge is a sequence of irreducible bridges



Weakly directed bridges

Definition: a bridge is weakly directed if each of its irreducible bridges avoids at least one of the steps N, S, E, W.

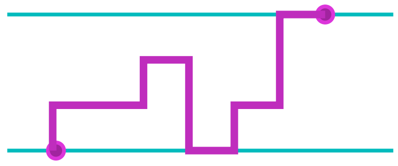
This means that each irreducible bridge is a NES- or a NWS-walk.



$\Rightarrow$ Count NES- (irreducible) bridges

Enumeration of NES-bridges

Proposition



- The generating function of NES-bridges of height $k+1$ is

$$B^{(k+1)}(t) = \sum_n b_n^{(k+1)} t^n = \frac{t^{k+1}}{G_k(t)},$$

where $G_{-1} = 1$, $G_0 = 1 - t$, and for $k \geq 0$,

$$G_{k+1} = (1 - t + t^2 + t^3) G_k - t^2 G_{k-1}.$$

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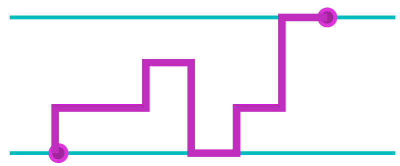

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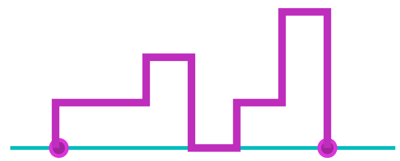
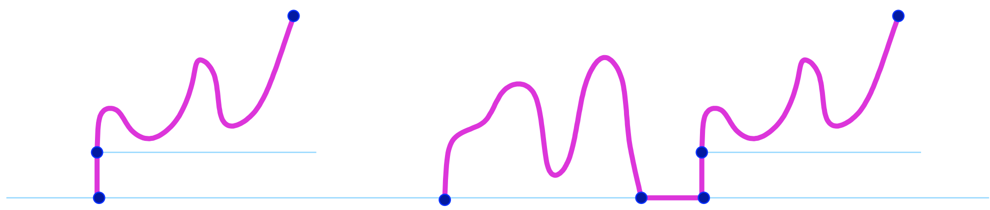
- The generating function of NES-excursions of height at most k is

$$E^{(k)}(t) = \frac{1}{t} \left(\frac{G_{k-1}}{G_k} - 1 \right).$$

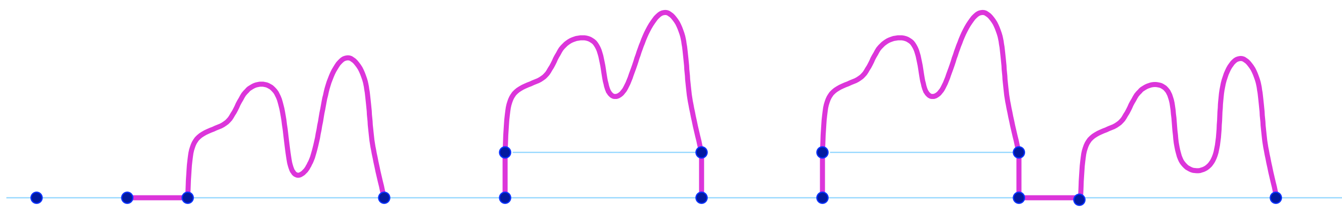


Excursion: $y_0 = 0 = y_n$ and $y_i \geq 0$ for $1 \leq i \leq n$.

Enumeration of NES-bridges



Last return to height 0



First return to height 0

- Bridges of height $k+1$:

$$B^{(k+1)} = tB^{(k)} + E^{(k)}t^2B^{(k)}$$

- Excursions of height at most k

$$E^{(k)} = 1 + tE^{(k)} + t^2\left(E^{(k-1)} - 1\right) + t^3\left(E^{(k-1)} - 1\right)E^{(k)}$$

- Initial conditions: $E^{(-1)} = 1$, $B^{(1)} = t/(1-t)$.

Enumeration of NES-bridges

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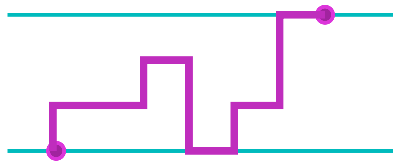

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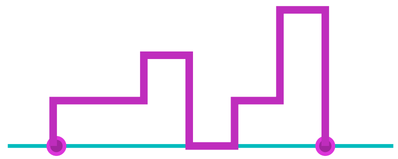

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Enumeration of weakly directed bridges

- GF of NES-bridges:

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- GF of weakly directed bridges (sequences of irreducible NES- or NWS-bridges):

$$W(t) = \frac{1}{1 - (2I(t) - t)} = \frac{1}{1 - \left(\frac{2B(t)}{1+B(t)} - t\right)}$$

with $G_{-1} = 1$, $G_0 = 1 - t$, and for $k \geq 0$,

$$G_{k+1} = (1 - t + t^2 + t^3)G_k - t^2 G_{k-1}.$$

[Bacher-mbm 10]

Asymptotic results and nature of the generating functions

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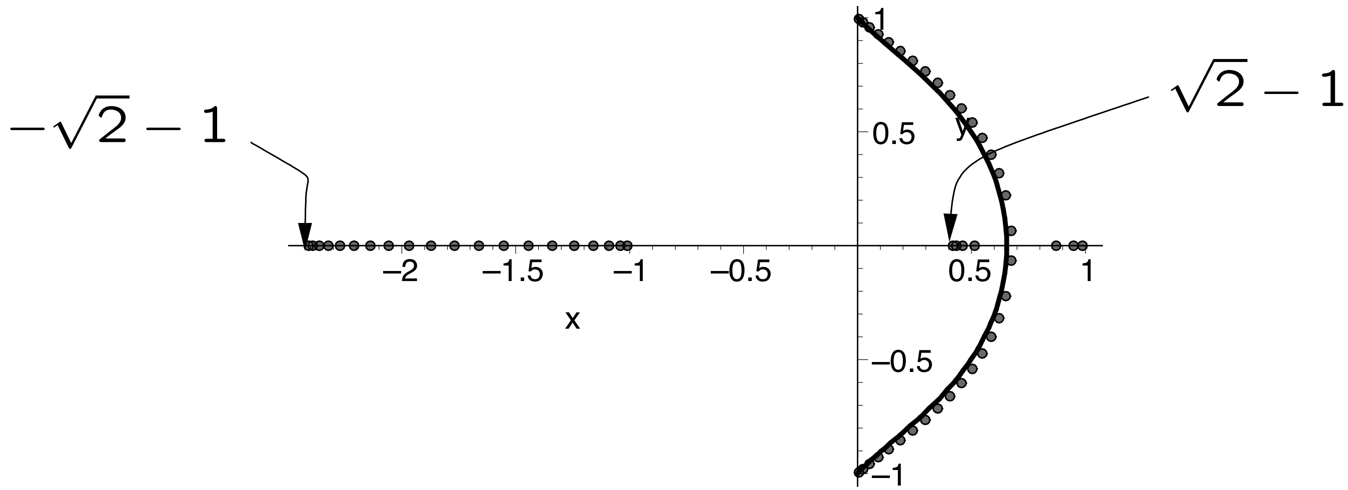
The zeroes of G_k (here, $k = 20$):



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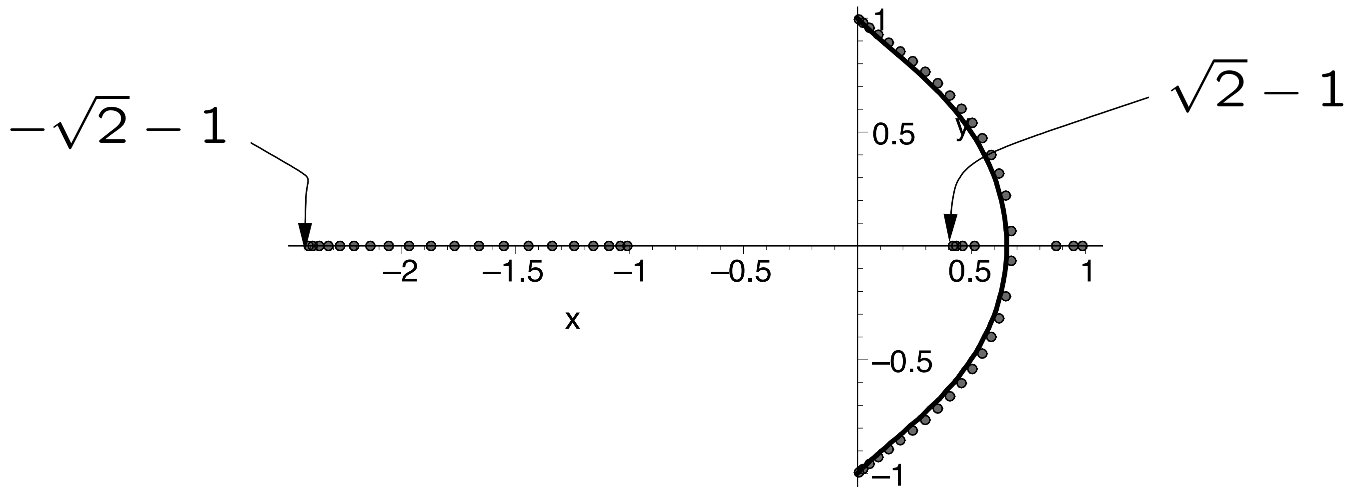
• The series $B(t)$ and $W(t)$ are meromorphic in $\mathbb{C} \setminus \mathcal{E}$, where $\mathcal{E}$ consists of the two real intervals $[-\sqrt{2}-1, -1]$ and $[\sqrt{2}-1, 1]$, and of the curve

$$\mathcal{E}_0 = \left\{ x + iy : x \geq 0,\ y^2 = \frac{1 - x^2 - 2x^3}{1 + 2x} \right\}.$$

This curve is a natural boundary of B and W. These series thus have infinitely many singularities.



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• The series $B(t)$ has radius $\sqrt{2}-1$, while $W(t)$ has a simple pole ρ of smaller modulus (for which $1 = \frac{2B(\rho)}{1+B(\rho)} - \rho$).

• The number $w(n)$ of weakly directed bridges of length n satisfies

$$w(n) \sim \mu^n,$$

with $\mu \simeq 2.54$ (the current record).

The number of irreducible bridges

• The generating function of weakly directed bridges, counted by the length and the number of irreducible bridges, is

$$W(t,x) = \frac{1}{1 - x\left(\frac{2B(t)}{1+B(t)} - t\right)}$$

• Let N_n denote the number N_n of irreducible bridges in a random weakly directed bridge of length n. Then

$$\mathbb{E}(N_n) \sim \mathfrak{m}\, n, \qquad \mathbb{V}(N_n) \sim \mathfrak{s}^2\, n,$$

where

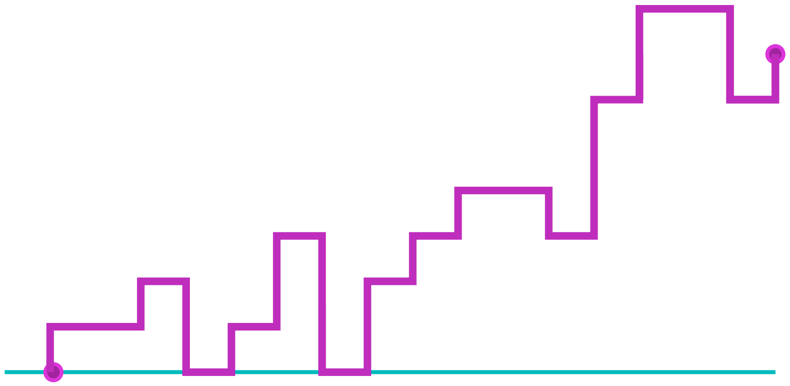
$$\mathfrak{m} \simeq 0.318 \quad \text{and} \quad \mathfrak{s}^2 \simeq 0.7,$$

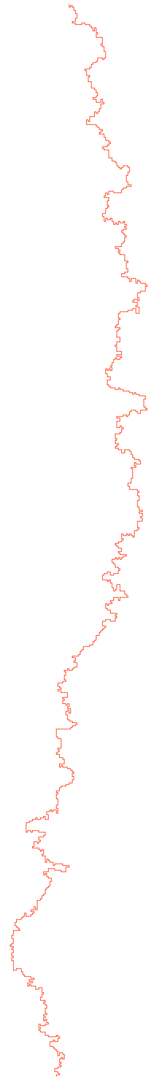
and the random variable $\frac{N_n - \mathfrak{m}\, n}{\mathfrak{s}\sqrt{n}}$ converges in law to a standard normal distribution. In particular, the average end-to-end distance, being bounded from below by $\mathbb{E}(N_n)$, grows linearly with n.

Random weakly directed bridges

Random weakly directed bridges

- Use a recursive Boltzmann sampler to sample non-negative NES-walks:





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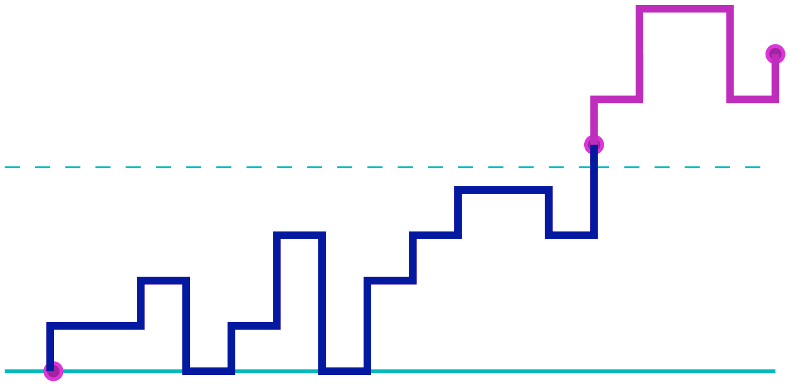
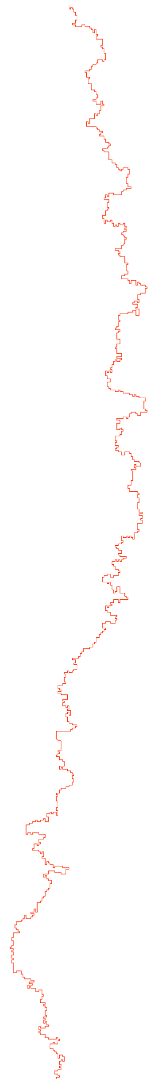


• If the first irreducible factor is a bridge, keep it, otherwise, discard the whole walk.

• Form a sequence of irreducible NES- or NWS-bridges.

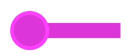


II. 2. Prudent self-avoiding walks

Self-directed walks [Turban-Debierre 86]
Exterior walks **[Préa 97]**
Outwardly directed SAW [Santra-Seitz-Klein 01]
Prudent walks **[Duchi 05], [Dethridge, Guttmann, Jensen 07], [mbm 08]**

Prudent self-avoiding walks

A step never points towards a vertex that has been visited before.



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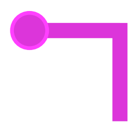

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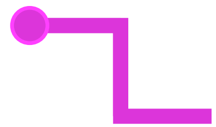

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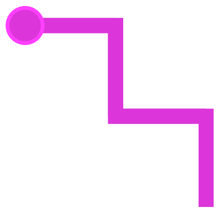

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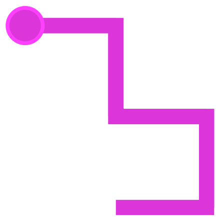

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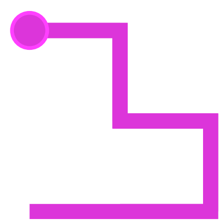

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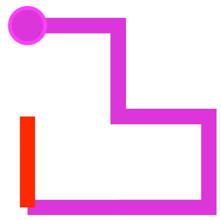

not prudent!

Prudent self-avoiding walks

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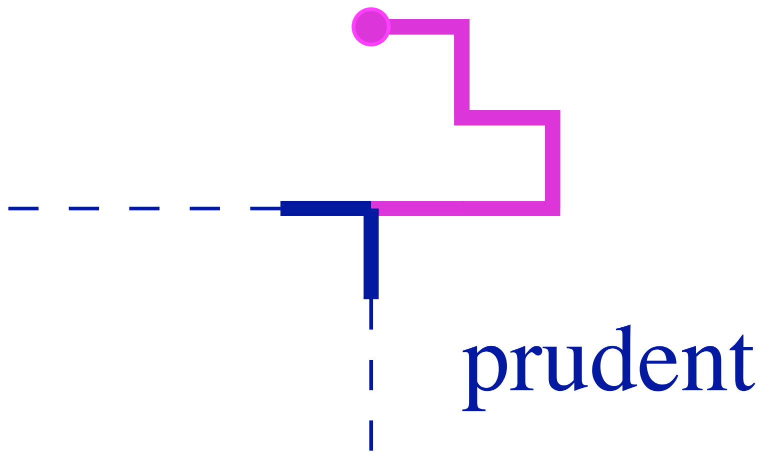

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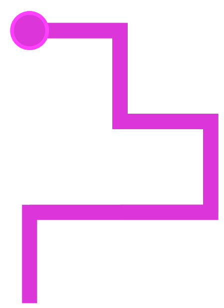

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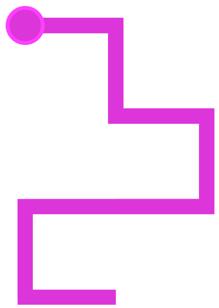

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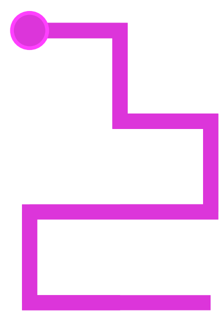

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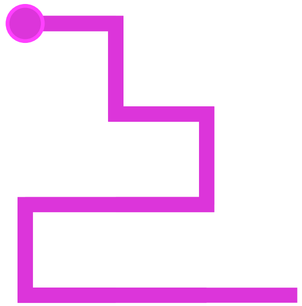

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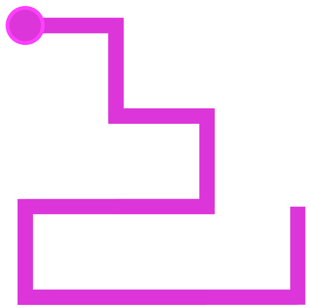

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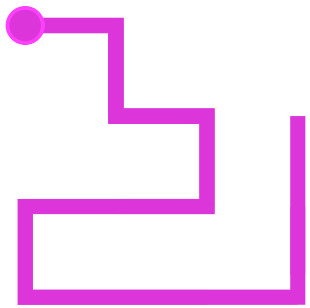

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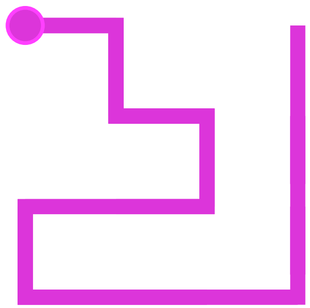

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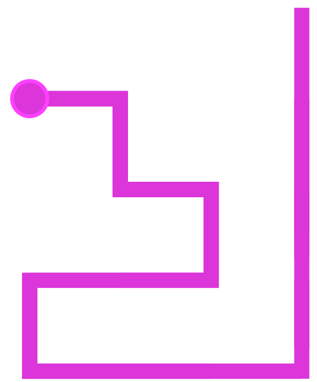

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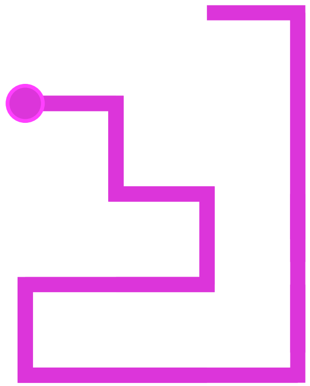

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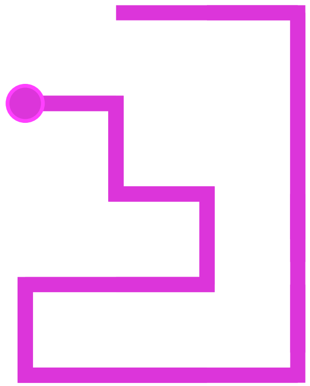

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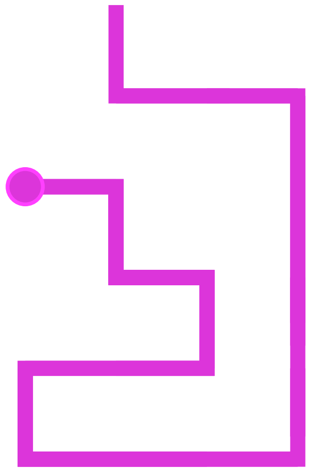

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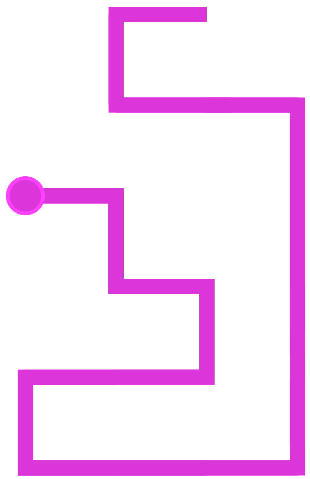

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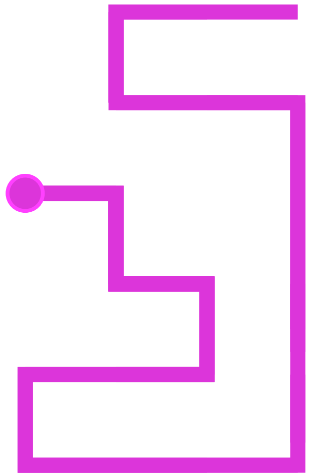

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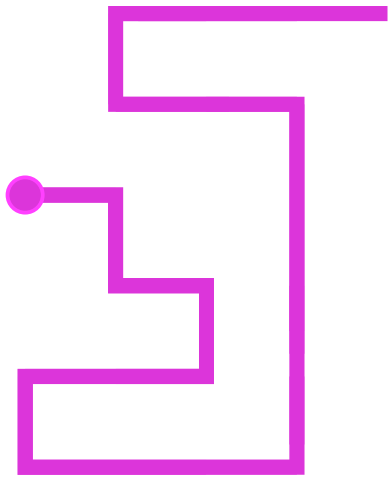

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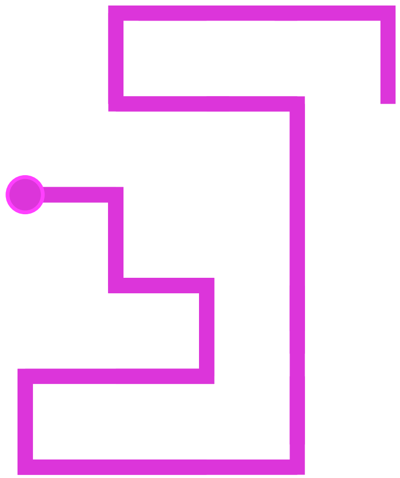

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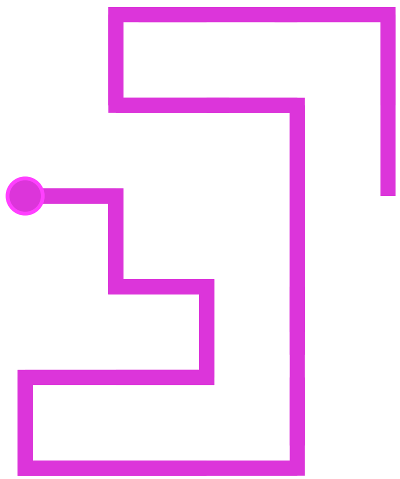

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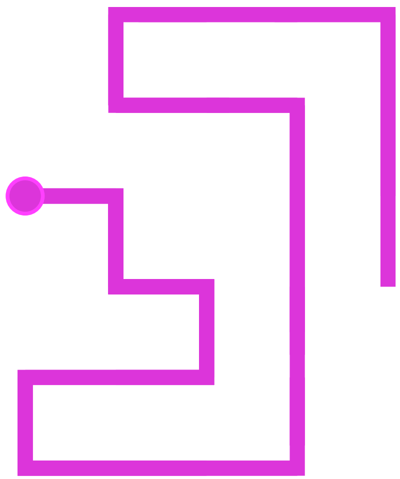

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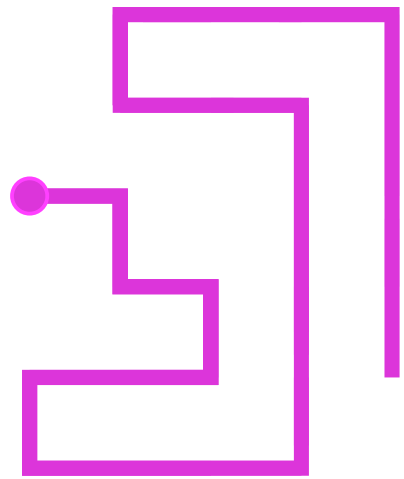

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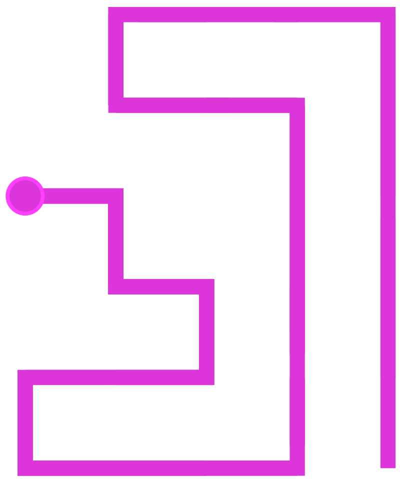

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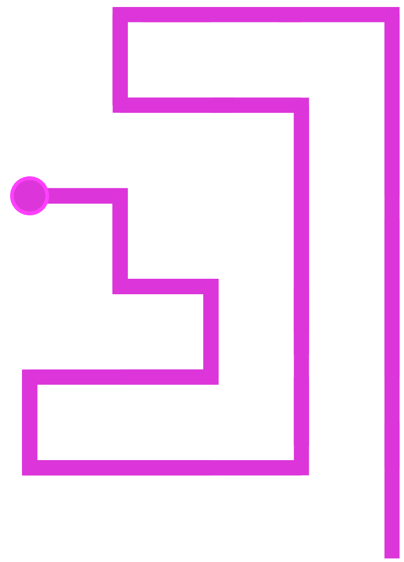

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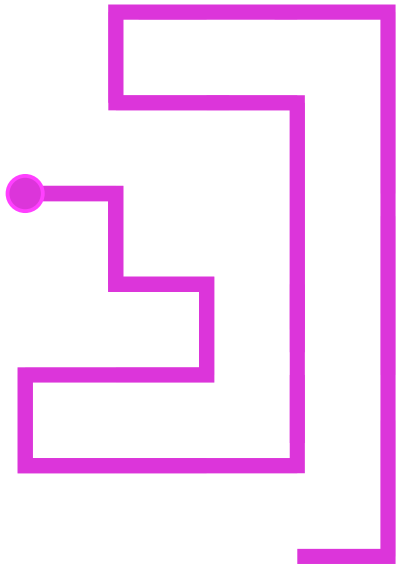

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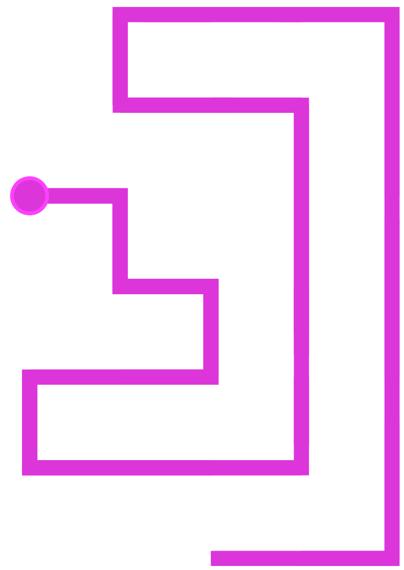

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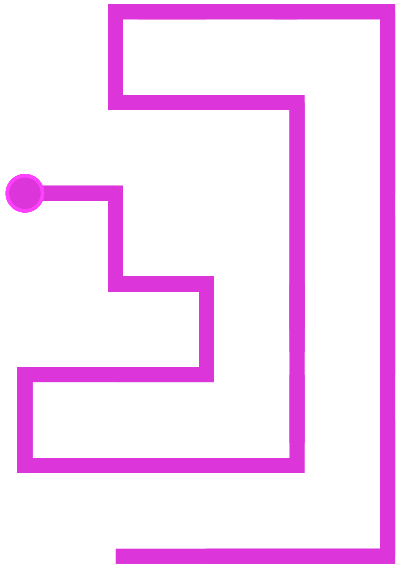

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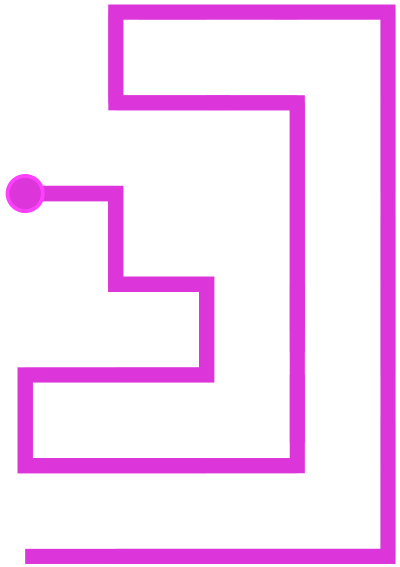

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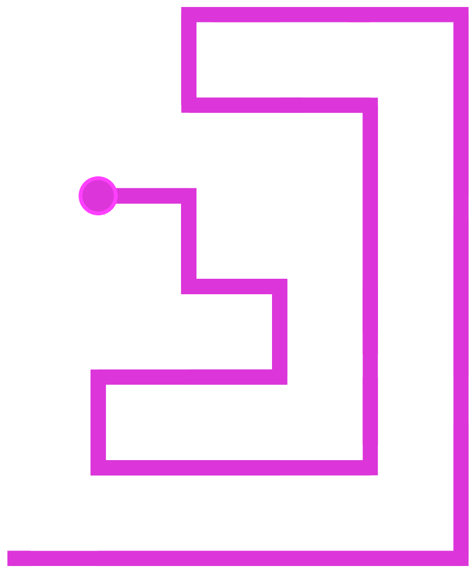

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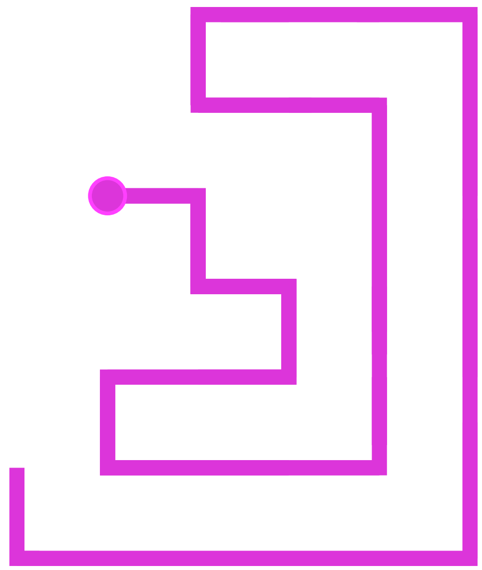

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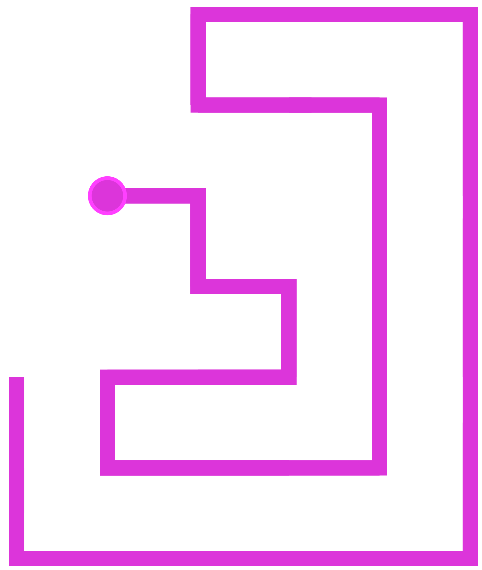

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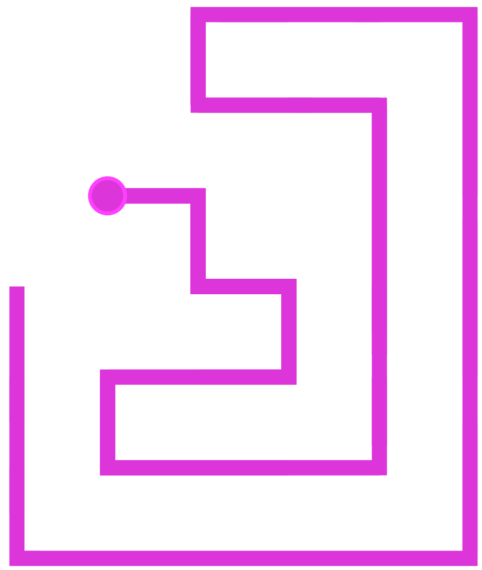

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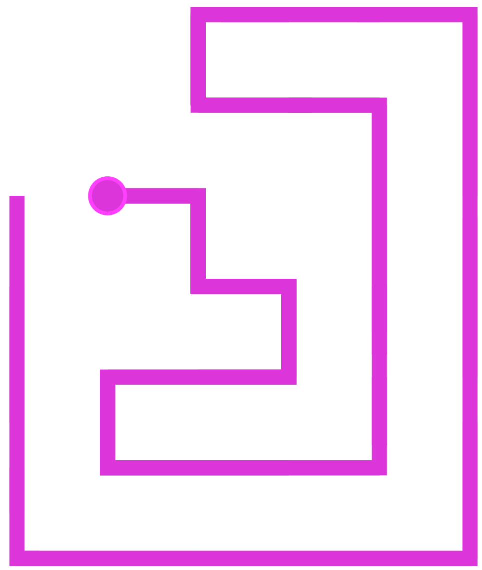

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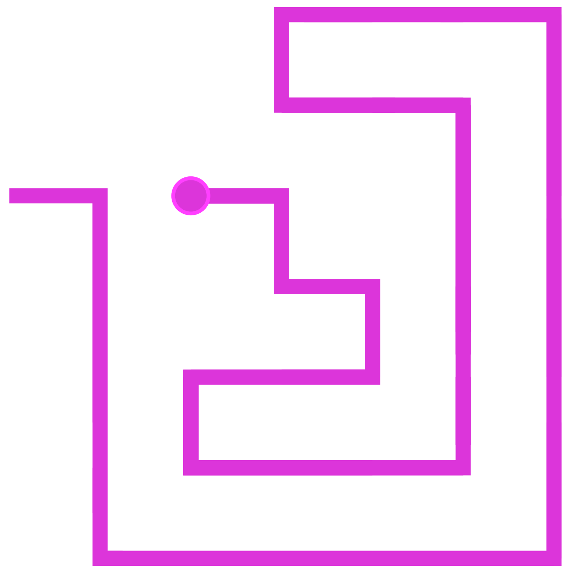

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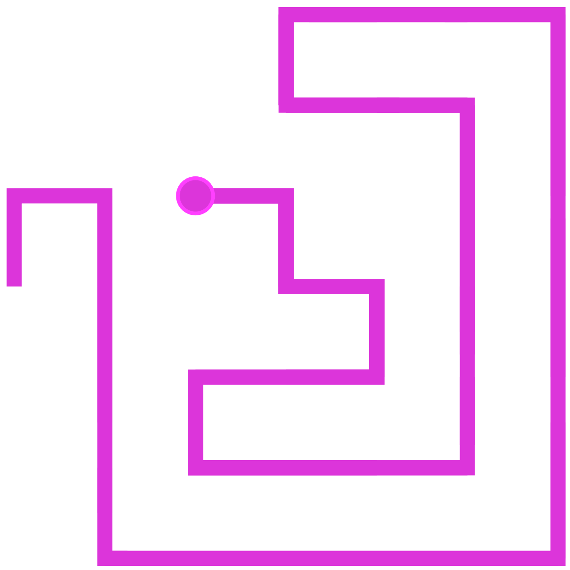

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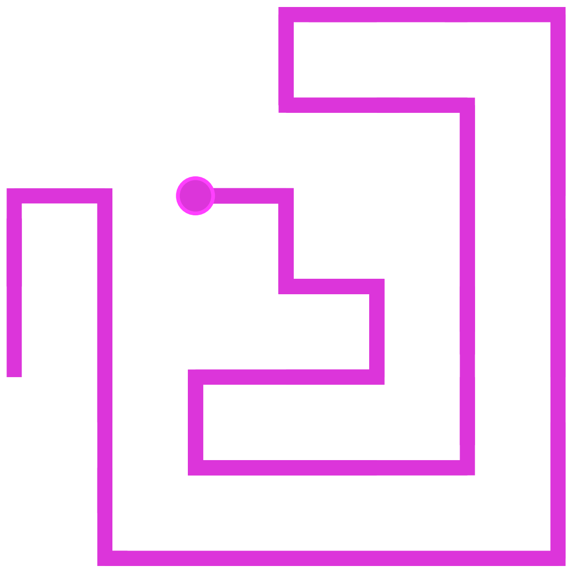

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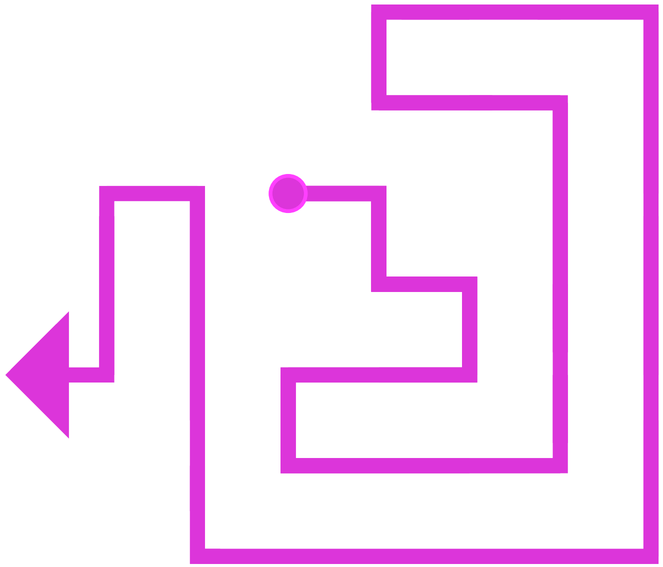
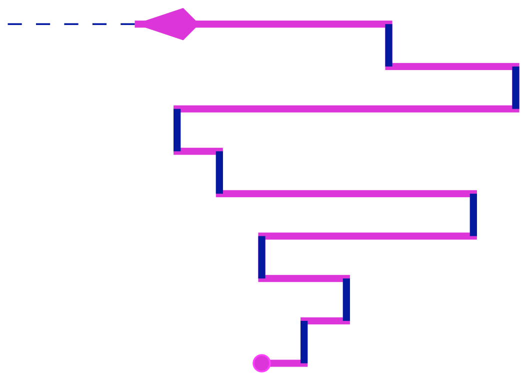


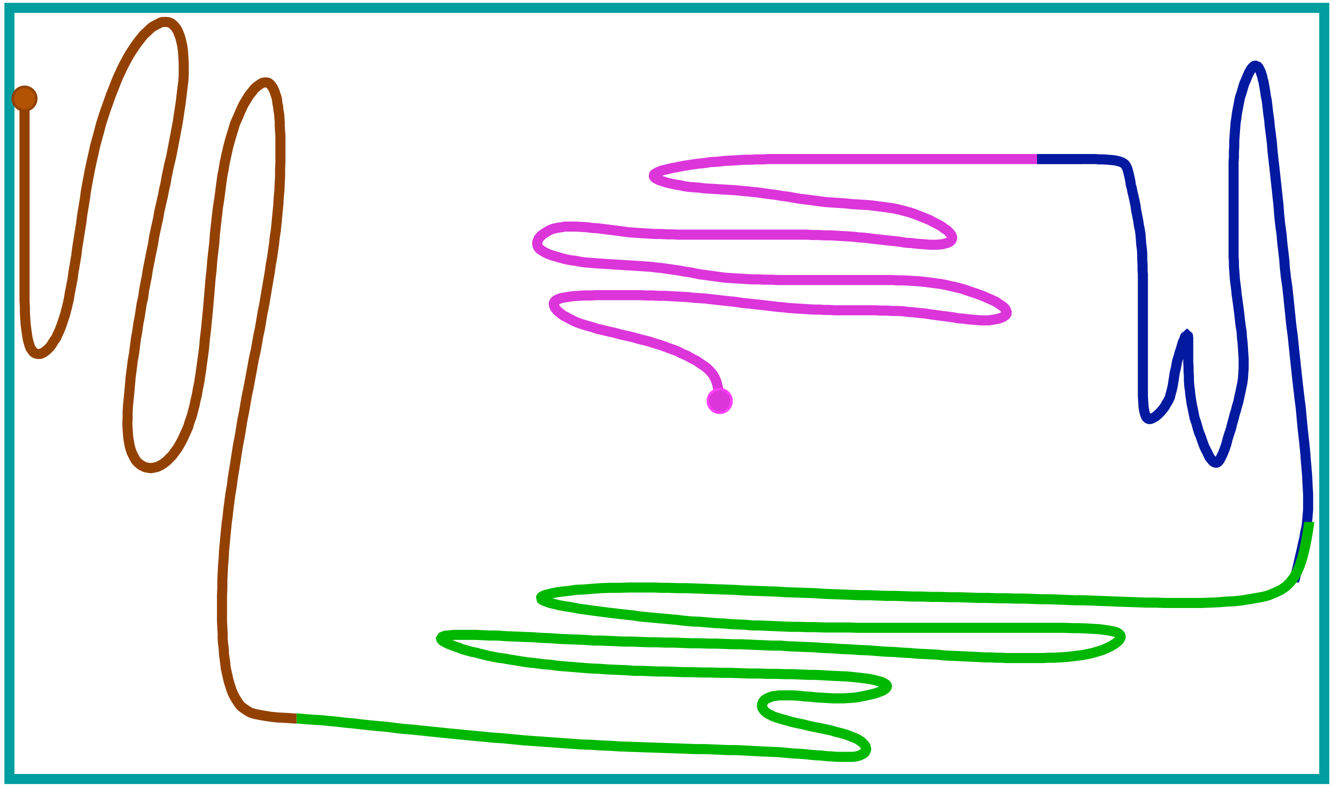
Remark: Partially directed walks are prudent



A property of prudent walks

A property of prudent walks

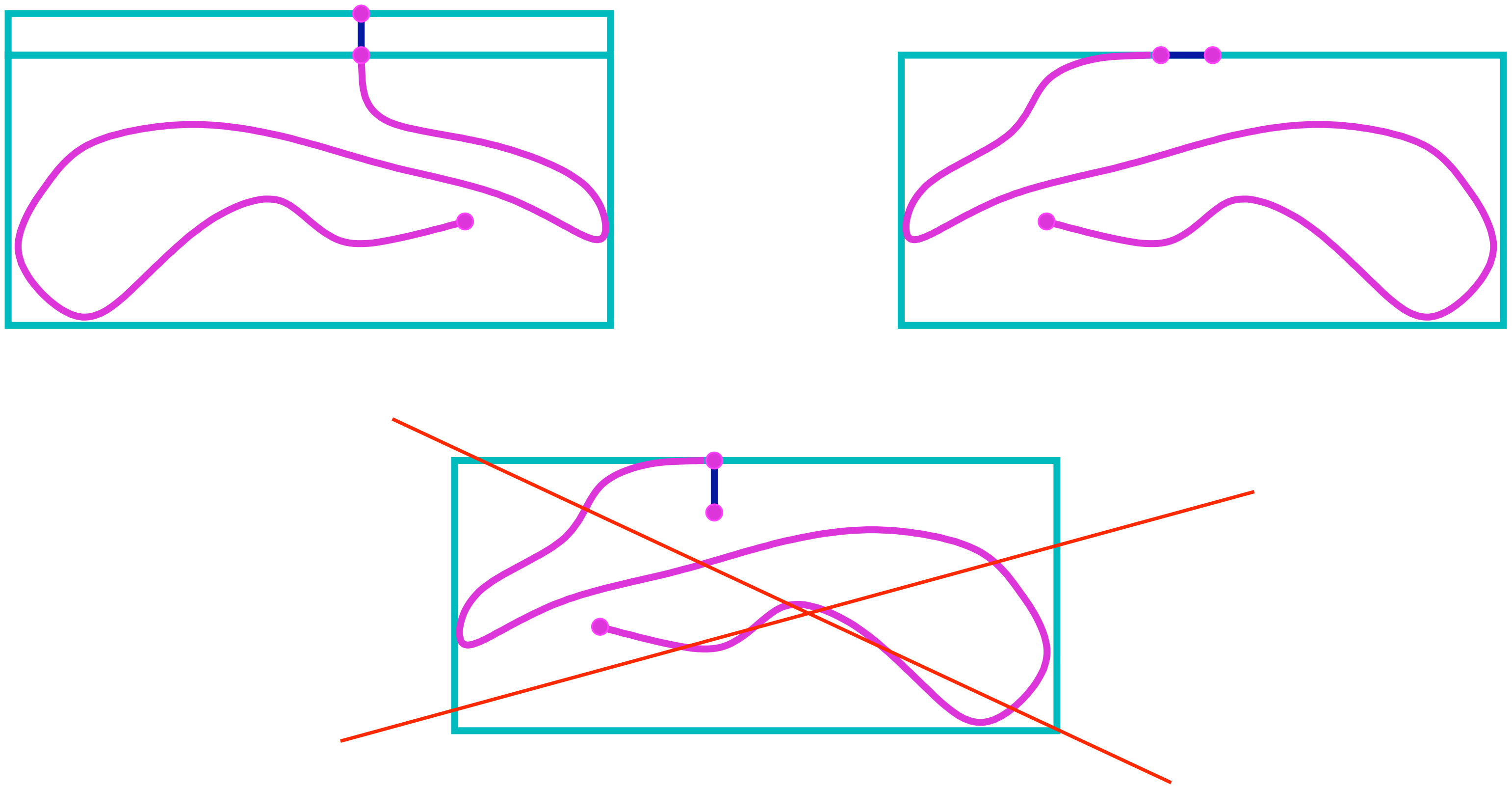
The box of a prudent walk



The endpoint of a prudent walk is always on the border of the box

Recursive construction of prudent walks

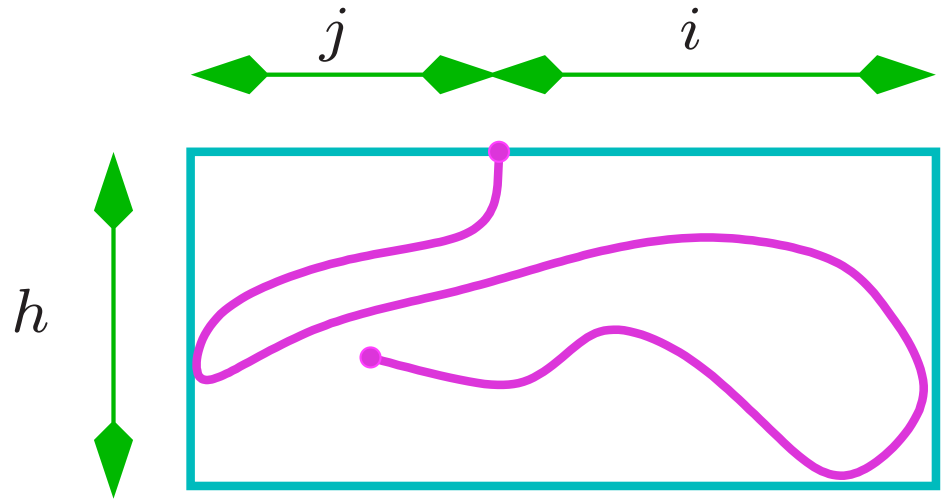
Each new step either inflates the box or walks (prudently) along the border.



Recursive construction of prudent walks

- Three more parameters

(*catalytic* parameters)



- Generating function of prudent walks ending on the top of their box:

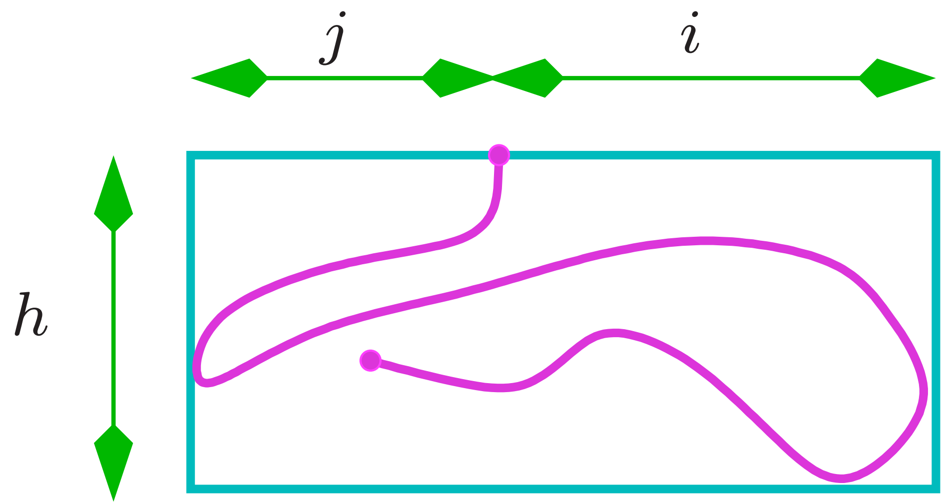
$$T(t; u, v, w) = \sum_{\omega} t^{|\omega|} u^{i(\omega)} v^{j(\omega)} w^{h(\omega)}$$

Series with three catalytic variables u, v, w

Recursive construction of prudent walks

• Three more parameters

(*catalytic* parameters)



• Generating function of prudent walks ending on the top of their box:

$$\left(1-\frac{uvwt(1-t^2)}{(u-tv)(v-tu)}\right)T(t;u,v,w)=$$

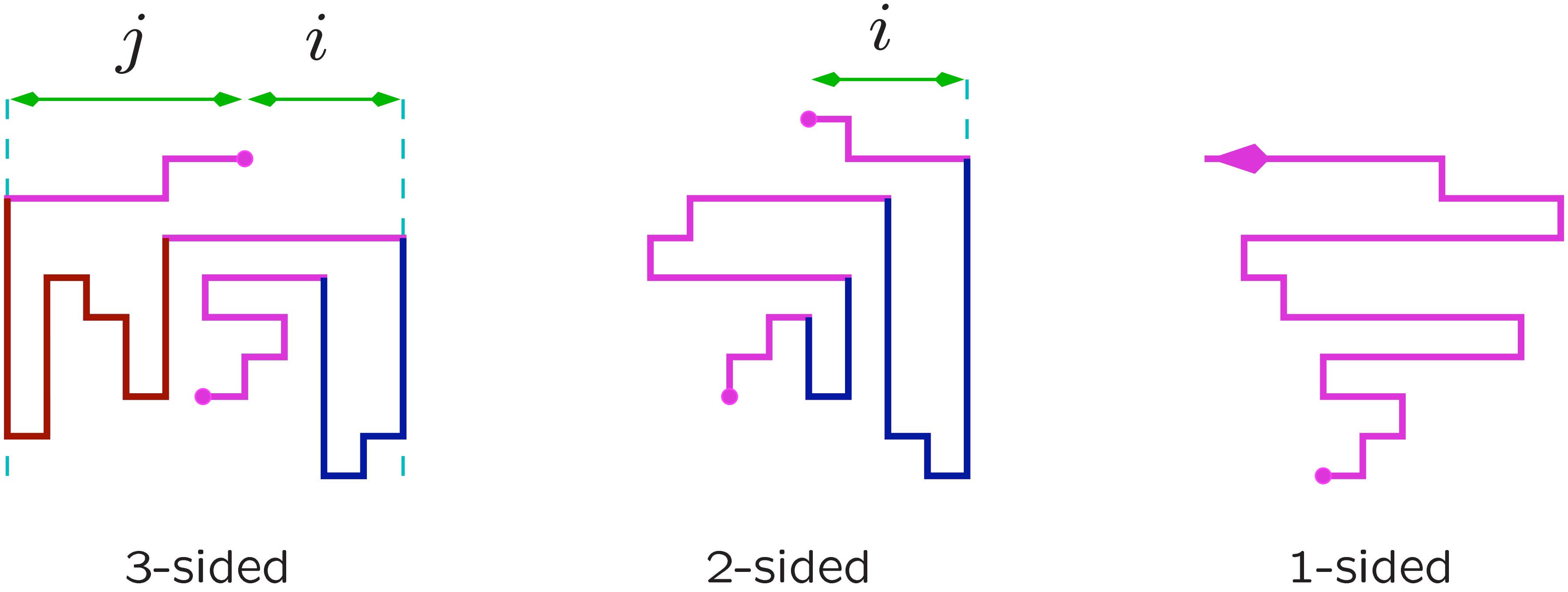
$$1+\mathcal{T}(t;w,u)+\mathcal{T}(t;w,v)-tv\frac{\mathcal{T}(t;v,w)}{u-tv}-tu\frac{\mathcal{T}(t;u,w)}{v-tu}$$

with $\mathcal{T}(t;u,v)=tvT(t;u,tu,v)$.

• Generating function of all prudent walks, counted by the length and the half-perimeter of the box:

$$P(t;u)=1+4T(t;u,u,u)-4T(t;0,u,u)$$

Simpler families of prudent walks [Préa 97]



• The endpoint of a 3-sided walk lies always on the top, right or left side of the box

• The endpoint of a 2-sided walk lies always on the top or right side of the box

• The endpoint of a 1-sided walk lies always on the top side of the box (= partially directed!)

Functional equations for prudent walks: The more general the class, the more additional variables

(Walks ending on the top of the box)

- General prudent walks: three catalytic variables

$$\left(1-\frac{uvwt(1-t^2)}{(u-tv)(v-tu)}\right)T(t;u,v,w)=1+\mathcal{T}(w,u)+\mathcal{T}(w,v)-tv\frac{\mathcal{T}(v,w)}{u-tv}-tu\frac{\mathcal{T}(u,w)}{v-tu}$$

with $\mathcal{T}(u,v)=tvT(t;u,tu,v)$.

- Three-sided walks: two catalytic variables

$$\left(1-\frac{uvt(1-t^2)}{(u-tv)(v-tu)}\right)T(t;u,v)=1+\cdots-\frac{t^2v}{u-tv}T(t;tv,v)-\frac{t^2u}{v-tu}T(t;u,tu)$$

- Two-sided walks: one catalytic variable

$$\left(1-\frac{tu(1-t^2)}{(1-tu)(u-t)}\right)T(t;u)=\frac{1}{1-tu}+t\,\frac{u-2t}{u-t}\,T(t;t)$$

Two- and three-sided walks: exact enumeration

Proposition

1. The generating function of 2-sided walks is algebraic:

$$P_2(t) = \frac{1}{1-2t-2t^2+2t^3}\left(1+t-t^3+t(1-t)\sqrt{\frac{1-t^4}{1-2t-t^2}}\right)$$

[Duchi 05]

2. The generating function of 3-sided prudent walks is...

Two- and three-sided walks: exact enumeration

2. The generating function of 3-sided prudent walks is:

$$P_3(t) = \frac{1}{1-2t-t^2}\left(\frac{1+3t+tq(1-3t-2t^2)}{1-tq} + 2t^2q\ T(t;1,t)\right)$$

where

$$T(t;1,t) = \sum_{k\geq 0} (-1)^k \frac{\prod_{i=0}^{k-1}\left(\frac{t}{1-tq} - U(q^{i+1})\right)}{\prod_{i=0}^{k}\left(\frac{tq}{q-t} - U(q^i)\right)} \left(1 + \frac{U(q^k)-t}{t(1-tU(q^k))} + \frac{U(q^{k+1})-t}{t(1-tU(q^{k+1}))}\right)$$

with

$$U(w) = \frac{1-tw+t^2+t^3w-\sqrt{(1-t^2)(1+t-tw+t^2w)(1-t-tw-t^2w)}}{2t},$$

and

$$q = U(1) = \frac{1-t+t^2+t^3-\sqrt{(1-t^4)(1-2t-t^2)}}{2t}.$$

A series with infinitely many poles.

[mbm 08]

Two- and three-sided walks: asymptotic enumeration

- The numbers of 2-sided and 3-sided n-step prudent walks satisfy

$$p_2(n) \sim \kappa_2 \, \mu^n, \quad p_3(n) \sim \kappa_3 \, \mu^n$$

where $\mu \simeq 2.48...$ is such that

$$\mu^3 - 2\mu^2 - 2\mu + 2 = 0.$$

Compare with 2.41... for partially directed walks, 2.54... for weakly directed bridges, but 2.64... for general SAW.

- Conjecture: for general prudent walks

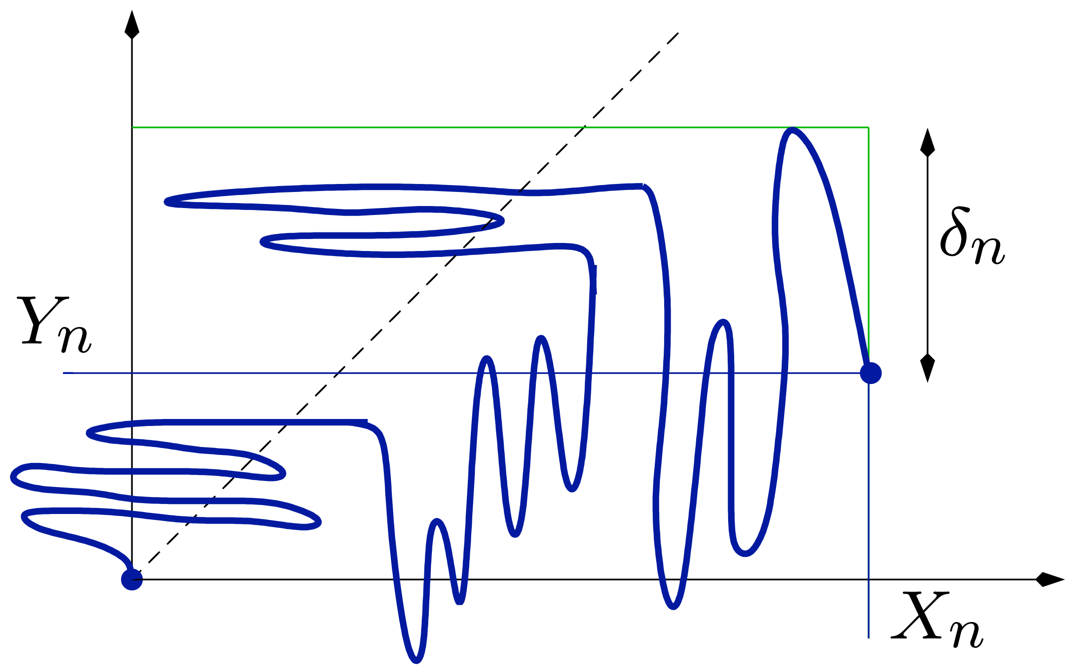
$$p_4(n) \sim \kappa_4 \, \mu^n$$

with the same value of μ as above [Dethridge, Guttmann, Jensen 07].

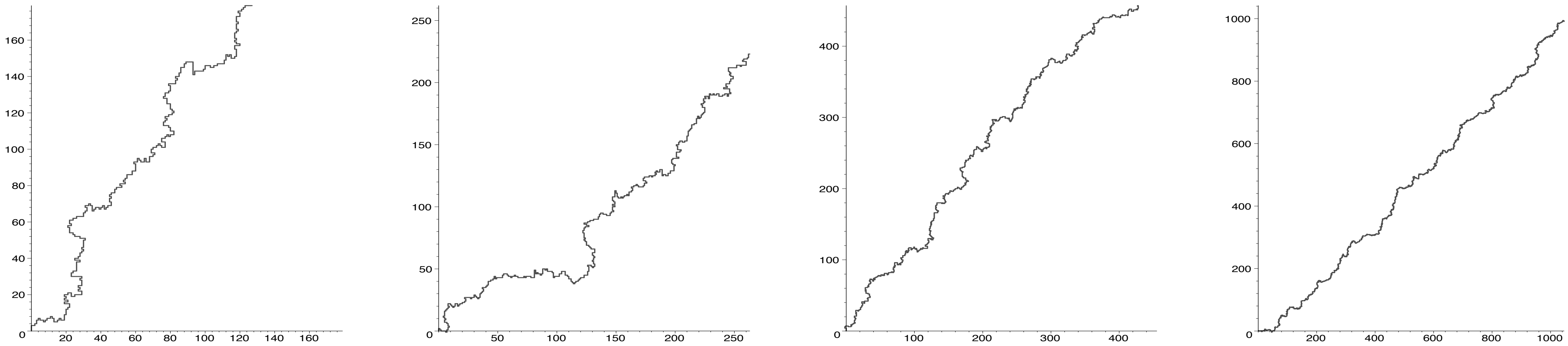
Two-sided walks: properties of large random walks (uniform distribution)

- The random variables X_n, Y_n and δ_n satisfy

$$\mathbb{E}(X_n) = \mathbb{E}(Y_n) \sim n \qquad \mathbb{E}((X_n - Y_n)^2) \sim n, \qquad \mathbb{E}(\delta_n) \sim 4.15\ldots$$



Two-sided walks: random generation (uniform distribution)



500 steps | 780 steps | 1354 steps | 3148 steps

• Recursive step-by-step construction à la Wilf $\Rightarrow$ 500 steps (precomputation of $O(n^2)$ large numbers)

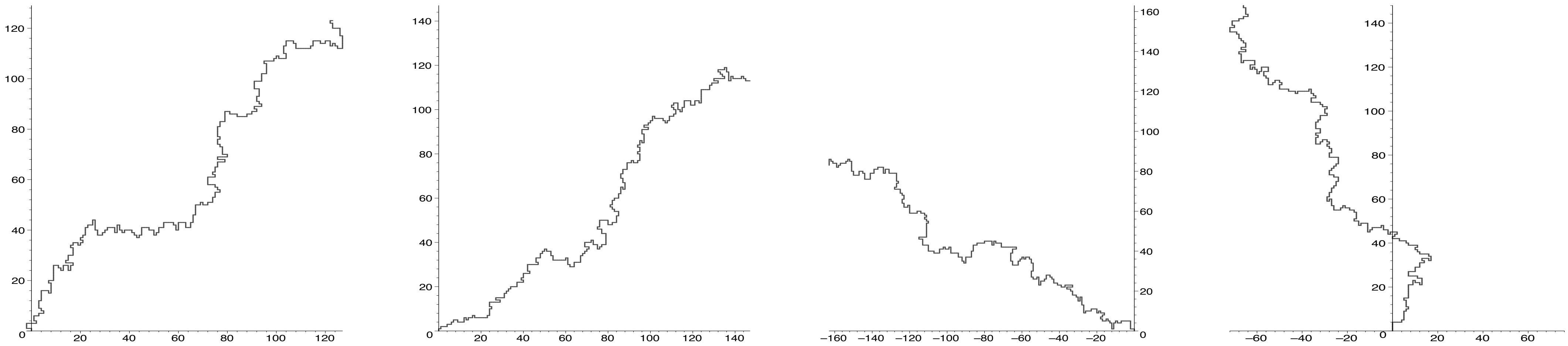
• Boltzmann sampling via a context-free grammar [Duchon-Flajolet-Louchard-Schaeffer 02]

$$\mathbb{E}(X_n) = \mathbb{E}(Y_n) \sim n \qquad \mathbb{E}((X_n - Y_n)^2) \sim n, \qquad \mathbb{E}(\delta_n) \sim 4.15\ldots$$

Three-sided prudent walks:
random generation and asymptotic properties

- Asymptotic properties: The average width of the box is $\sim \kappa n$

- Random generation: Recursive method à la Wilf $\Rightarrow$ 400 steps
(pre-computation of $O(n^3)$ numbers)



Four-sided (i.e. general) prudent walks

- An equation with 3 catalytic variables:

$$\left(1-\frac{uvwt(1-t^2)}{(u-tv)(v-tu)}\right)T(u,v,w)=1+\mathcal{T}(w,u)+\mathcal{T}(w,v)-tv\frac{\mathcal{T}(v,w)}{u-tv}-tu\frac{\mathcal{T}(u,w)}{v-tu}$$

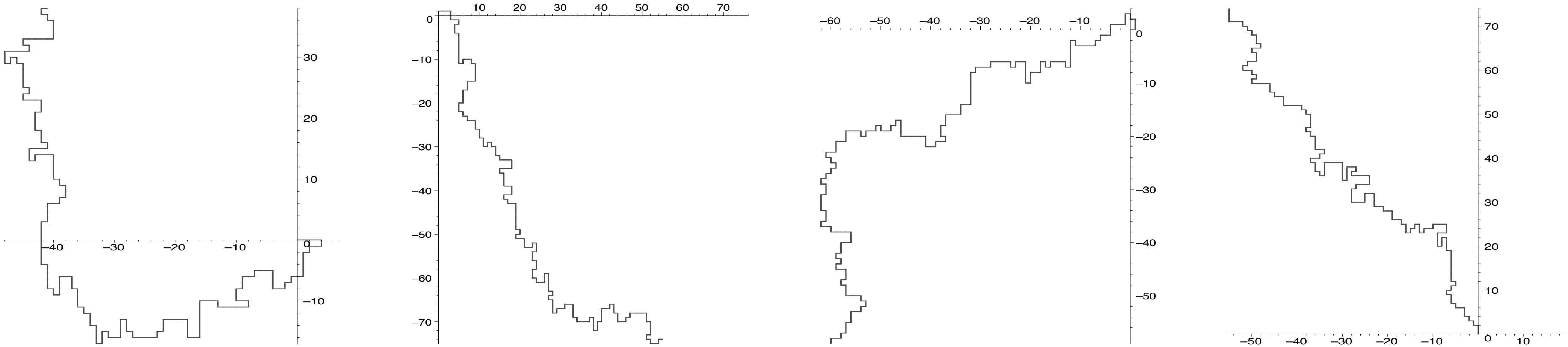
with $\mathcal{T}(u,v)=tvT(u,tu,v)$.

- Conjecture:

$$p_4(n)\sim\kappa_4\,\mu^n$$

where $\mu\simeq 2.48$ satisfies $\mu^3-2\mu^2-2\mu+2=0$.

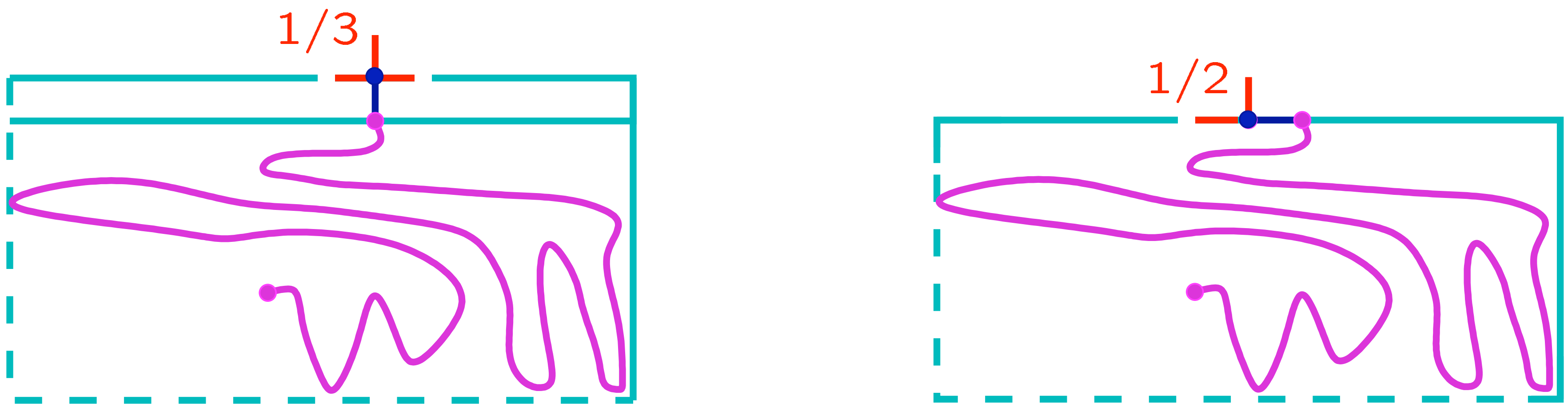
- Random prudent walks: recursive generation, 195 steps (sic! $O(n^4)$ numbers)



II.3. Another distribution: Kinetic prudent walks

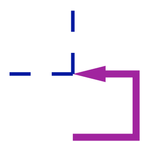
At time n, the walk chooses one of the admissible steps with uniform probability.

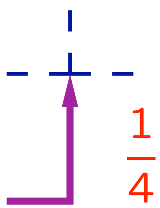
[An admissible step is one that gives a prudent walk]



Remark: Walks of length n are no longer uniform

$\frac{1}{4}\cdot\frac{1}{3}\cdot\frac{1}{3}\cdot\frac{1}{2}$

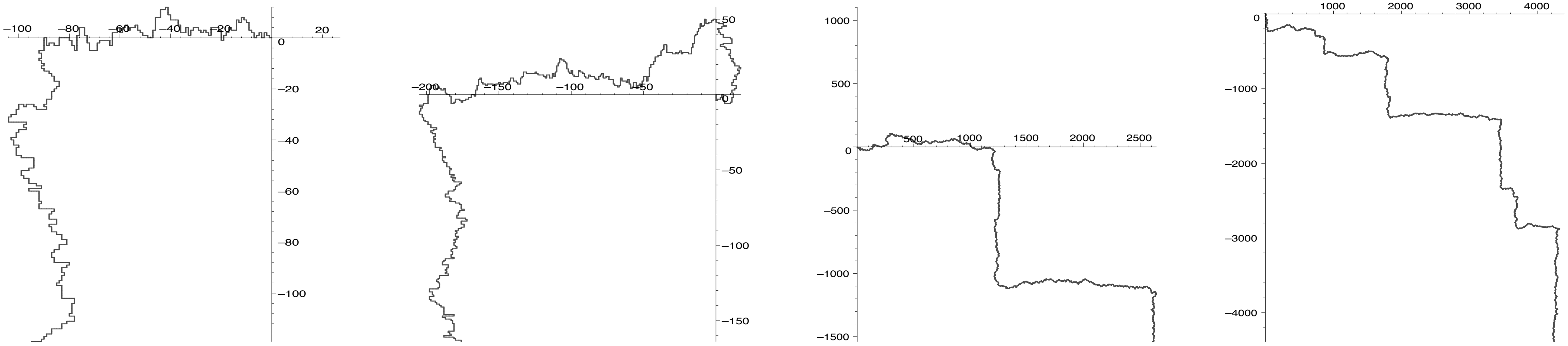




$\frac{1}{4}\cdot\frac{1}{3}\cdot\frac{1}{3}\cdot\frac{1}{3}$

Another distribution: Kinetic prudent walks

- Kinetic model: recursive generation with no precomputation



500 steps 1000 steps 10000 steps 20000 steps

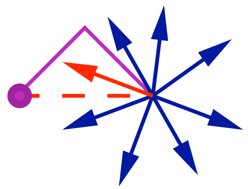
- Theorem: The walk chooses uniformly one quadrant, say the NE one, and then its scaling limit is given by

$$Z(u) = \int_0^{3u/7} \left(1_{W(s)\geq 0}\; e_1 + 1_{W(s)<0}\; e_2 \right) ds$$

where e_1, e_2 form the canonical basis of $\mathbb{R}^2$ and $W(s)$ is a brownian motion. [Beffara, Friedli, Velenik 10]

A kinetic, continuous space version: The rancher's walk

At time n, the walk takes a uniform unit step in $\mathbb{R}^2$, conditioned so that the new step does not intersect the convex hull of the walk.



Theorem: the end-to-end distance is linear. More precisely, there exists a constant $a > 0$ such that

$$\liminf \frac{||\omega_n||}{n} \geq a.$$

[Angel, Benjamini, Virág 03], [Zerner 05]

Conjectures

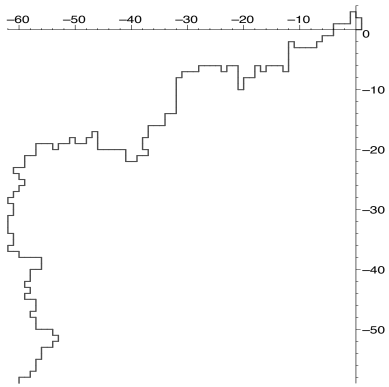
- Linear speed: There exists $a > 0$ such that $\frac{||\omega_n||}{n} \to a$ a.s.

- Angular convergence: $\frac{\omega_n}{||\omega_n||}$ converges a.s.

What's next?

• Exact enumeration: General prudent walks on the square lattice – Growth constant?

• Uniform random generation: better algorithms (maximal length 200 for general prudent walks...)



• A mixture of both models: walks formed of a sequence of prudent irreducible bridges?

Triangular prudent walks

The length generating function of triangular prudent walks is

$$P(t;1) = \frac{6t(1+t)}{1-3t-2t^2}\Big(1 + t\,(1+2t)\,R(t;1,t)\Big)$$

with

$$R(t;1,t) = (1+Y)(1+tY) \sum_{k\geq 0} \frac{t^{\binom{k+1}{2}} \left(Y(1-2t^2)\right)^k}{(Y(1-2t^2);t)_{k+1}} \left(\frac{Yt^2}{1-2t^2};t\right)_k$$

and

$$Y = \frac{1-2t-t^2-\sqrt{(1-t)(1-3t-t^2-t^3)}}{2t^2}$$

Notation:

$$(a;q)_n = (1-a)(1-aq)\cdots(1-aq^{n-1}).$$

• The series $P(t;1)$ is neither algebraic, nor even D-finite (infinitely many poles at $Yt^k(1-2t^2)=0$)