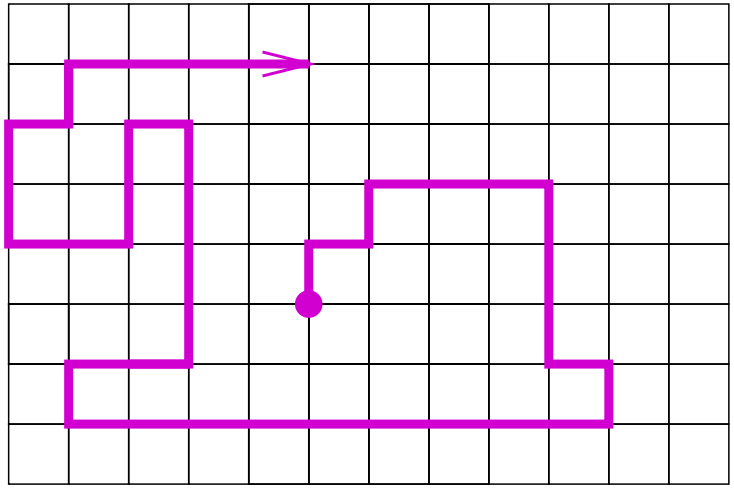
Exactly solvable models of self-avoiding walks

Mireille Bousquet-Mélou

CNRS, LaBRI, Bordeaux, France

http://www.labri.fr/∼bousquet

Self-avoiding walks (SAW): Some predictions



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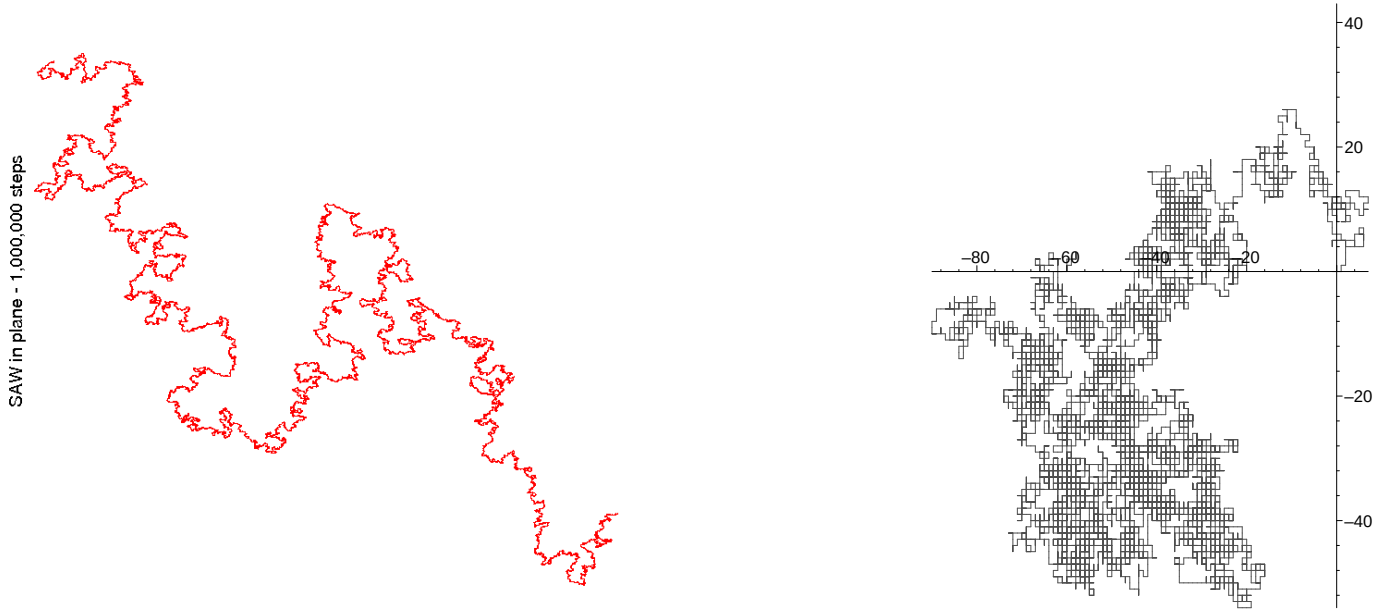


- The number of n-step SAW behaves asymptotically as follows:

$$c(n) \sim (\kappa)\, 2.64^n\, n^{11/32}$$

- The end-to-end distance is on average

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

[Flory 49, Nienhuis 82]

Exactly solvable models

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

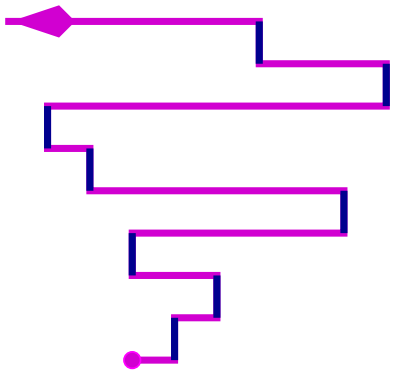
- solve better and better approximations of real SAW

- develop new techniques in exact enumeration

1. 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

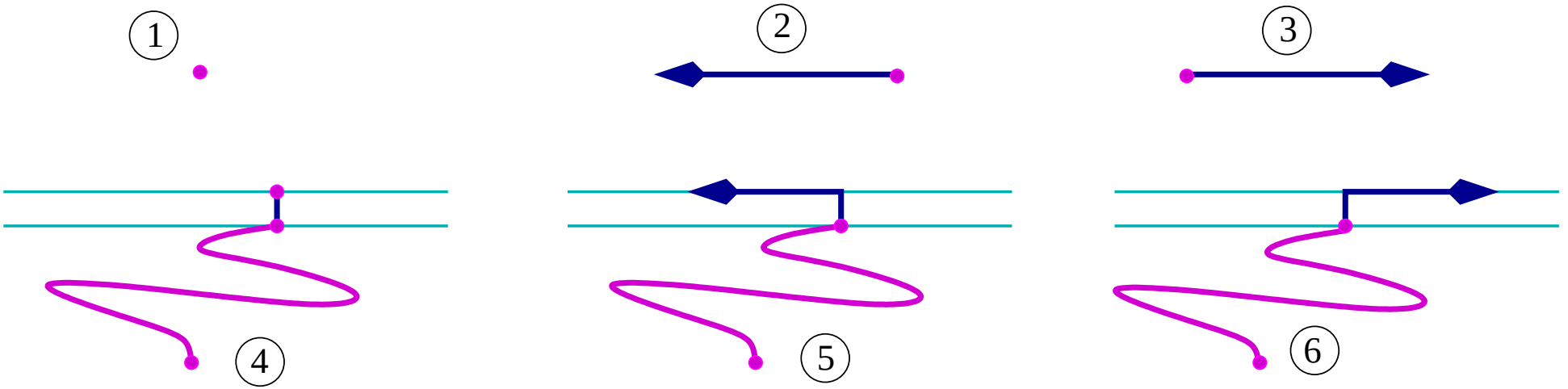


The self-avoidance condition is local.

Let $a(n)$ be the number of n-step NEW-walks.

A toy model: Partially directed walks

- Recursive description of NEW-walks:



$$
\begin{aligned}
a(0) &= 1 \\
a(n) &= 2 + a(n-1) + 2\sum_{k=0}^{n-2} a(k) \quad \text{for } n \geq 1
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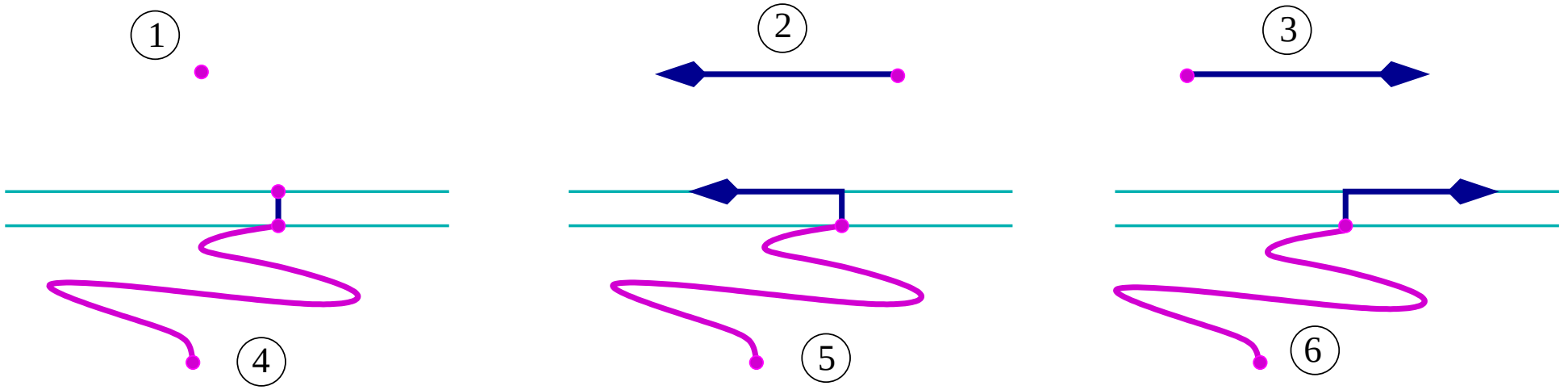

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- Generating function:

$$A(t) := \sum_{n\geq 0} a(n)t^n = 1 + 2\frac{t}{1-t} + tA(t) + 2A(t)\frac{t^2}{1-t}$$

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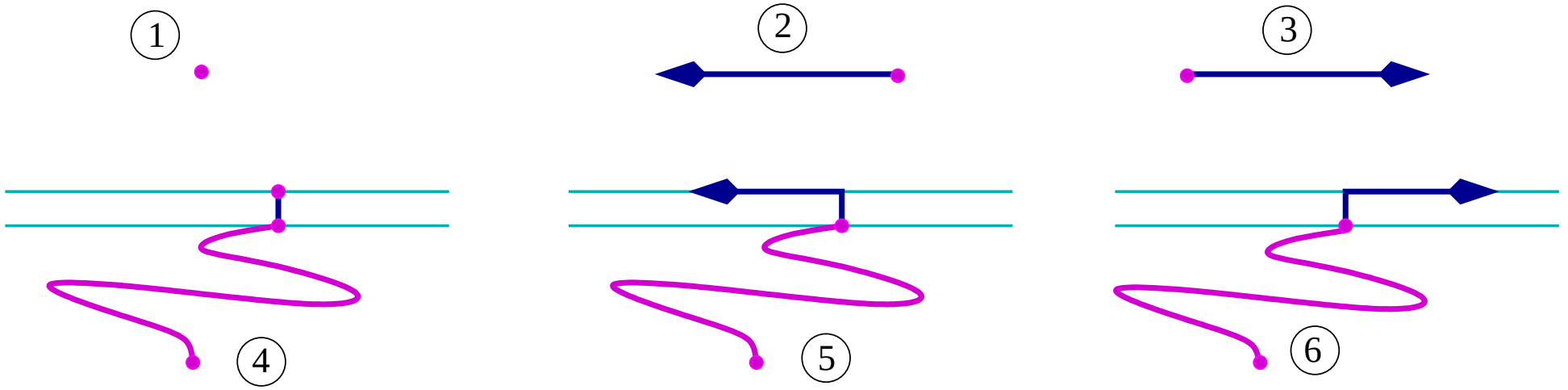

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$$A(t) = \frac{1+t}{1-2t-t^2} \quad \Rightarrow \quad a(n) \sim (1+\sqrt{2})^n \sim (2.41\ldots)^n$$

Generating functions

Let $\mathcal{A}$ be a set of discrete objects equipped with a size:

$$\begin{array}{rccc} size : \mathcal{A} & \to & \mathbb{N} \\ a & \mapsto & |a| \end{array}$$

Assume that there is a finite number of objects of size n, for all n. Denote this number by $a(n)$.

The generating function of the objects of $\mathcal{A}$, counted by their size, is

$$\begin{aligned} A(t) &:= \sum_{n \geq 0} a(n) t^n \\ &= \sum_{a \in \mathcal{A}} t^{|a|}. \end{aligned}$$

Notation: $[t^n]A(t) := a(n)$

Combinatorial constructions and operations on series: A dictionary

Construction	Numbers	Generating function
Union $\mathcal{A} = \mathcal{B} \cup \mathcal{C}$	$a(n) = b(n) + c(n)$	$A(t) = B(t) + C(t)$
Product $\mathcal{A} = \mathcal{B} \times \mathcal{C}$ $\lvert(\beta, \gamma)\rvert = \lvert\beta\rvert + \lvert\gamma\rvert$	$a(n) =$ $b(0)c(n) + \cdots + b(n)c(0)$	$A(t) = B(t) \cdot C(t)$
Sequence $\mathcal{A} = \mathrm{Seq}(\mathcal{B})$ $\mathcal{A} = \{\epsilon\} \cup \mathcal{B} \cup (\mathcal{B} \times \mathcal{B}) \cup \cdots$		$A(t) = \frac{1}{1-B(t)}$

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Transfer theorems: under certain hypotheses, if $A(t)$ has a unique dominant singularity at $1/\mu$,

$$A(t) \sim \frac{1}{(1-\mu t)^{1+\alpha}} \Longrightarrow a(n) \sim \frac{1}{\Gamma(\alpha+1)} \mu^n n^\alpha$$

Analytic combinatorics [Flajolet-Sedgewick 09]

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Analytic combinatorics [Flajolet-Sedgewick 09]

Example: $A(t) = \frac{1+t}{1-2t-t^2}$ has a simple pole ($\alpha = 0$) at $t_c = \sqrt{2}-1$
$\Longrightarrow a(n) \sim \kappa(\sqrt{2}+1)^n n^0$

Multivariate generating functions

- Enumeration according to the size (main parameter) and another parameter:

$$A(t,x) = \sum_{a\in\mathcal{A}} t^{|a|} x^{p(a)}$$

- Then

$$[t^n]\,\frac{\partial A}{\partial x}(t,x)\Big|_{x=1} = \sum_{a:|a|=n} p(a),$$

so that

$$\Rightarrow \quad \frac{[t^n]\frac{\partial A}{\partial x}A(t,1)}{[t^n]A(t,1)} = \mathbb{E}(p(a_n))$$

is the average value of $p(a_n)$, when a_n is taken uniformly at random among objects of size n.

Example: the number of North steps in a partially directed walk

- The bivariate generating function is

$$A(t,x) = \sum_{\omega} t^{|\omega|} x^{\mathsf{N}(\omega)} = \frac{1+t}{1-t-tx(1+t)}$$

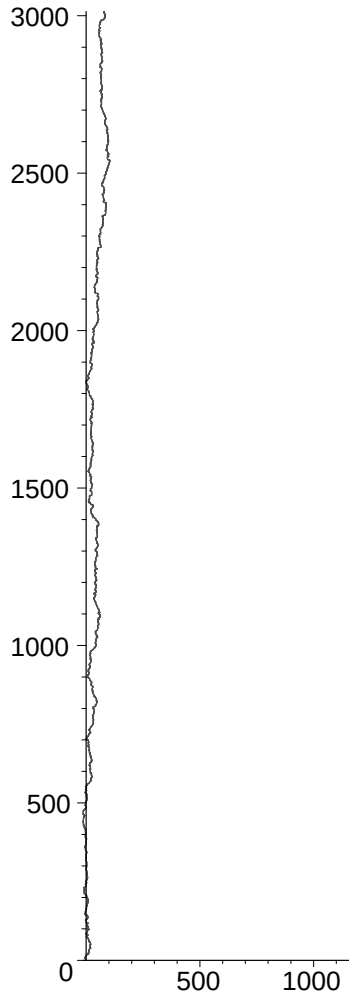
- The derivative, taken at $x = 1$, is

$$\left.\frac{\partial A}{\partial x}(t,x)\right|_{x=1} = \frac{t(1+t)^2}{(1-t-t(1+t))^2}.$$

- The number N_n of North steps satisfies

$$\mathbb{E}(N_n) \sim \kappa\, n,$$

for some $\kappa > 0$.
In particular, the end-to-end distance grows linearly with n.

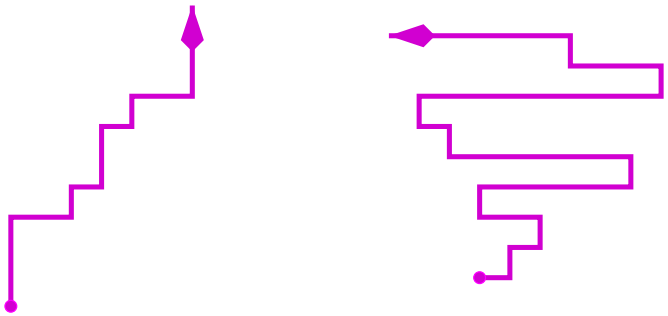


More solvable models

directed → partially directed

2^n

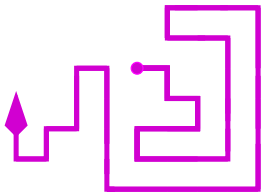
2.41^n



prudent

2.48^n (conj.)

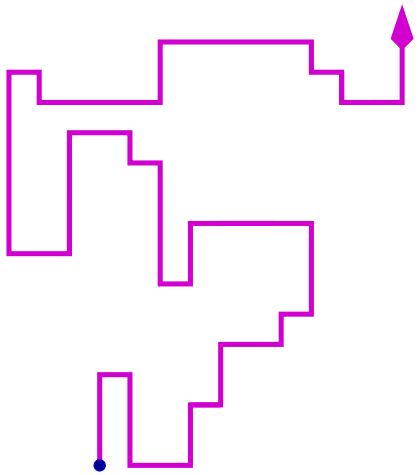
[Turban-Debierre 86]
[Préa 97]
[Santra-Seitz-Klein 01]
[Duchi 05]
[Dethridge-Guttmann-Jensen 07]
[mbm 08]
[Schwerdtfeger 10]
[Beaton-Flajolet-Guttmann 11]



weakly directed

2.54^n

[Bacher-mbm 11]



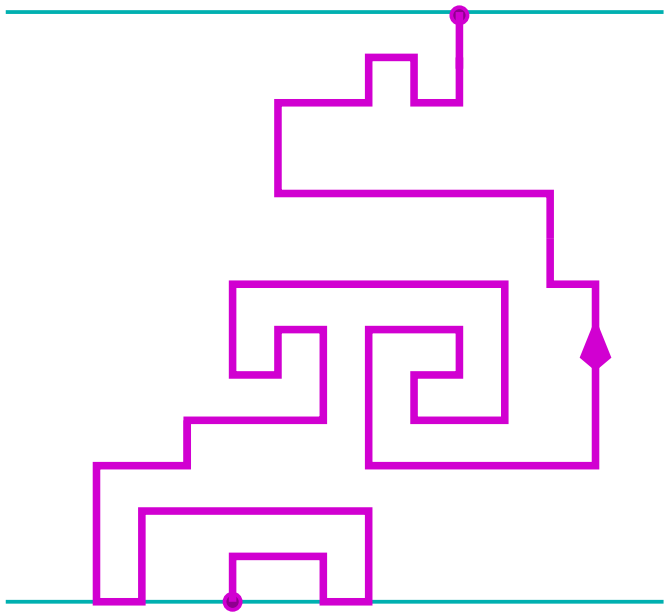
...

2. 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:

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

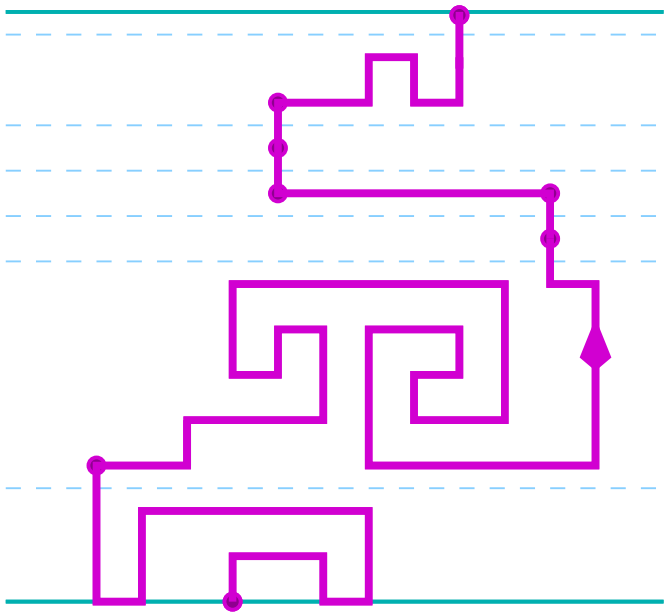
where

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

Irreducible bridges

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

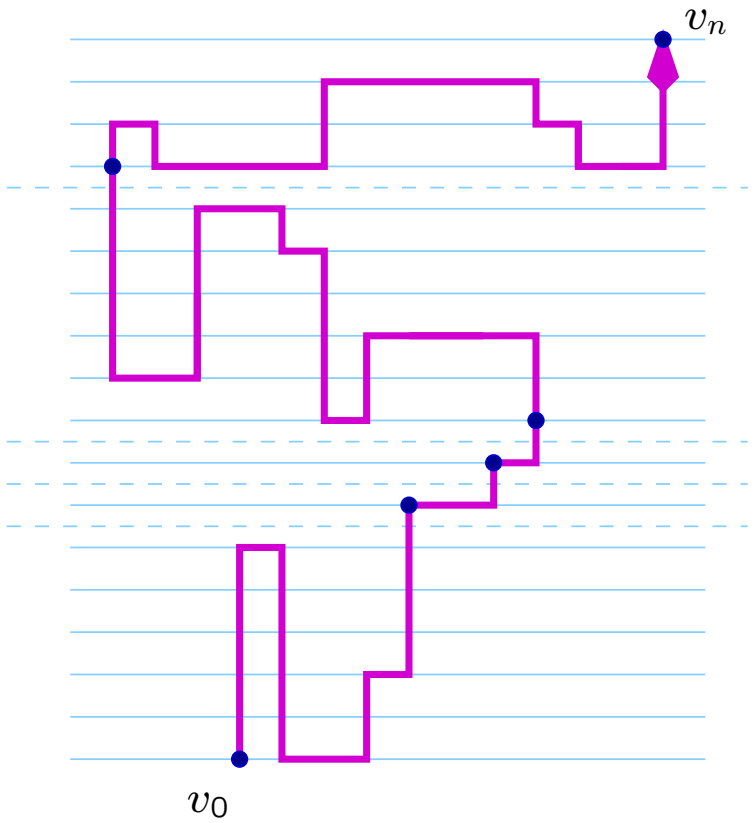
Observation: A bridge is a sequence of irreducible bridges



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.

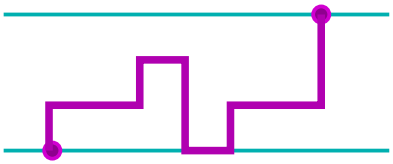
This means that each irreducible bridge is a NES- or a NWS-walk.



$\Rightarrow$ 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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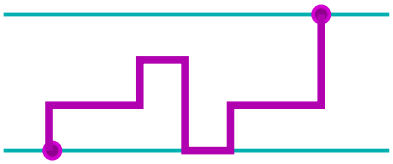

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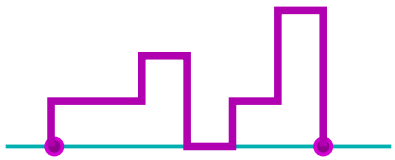
- The generating function of NES-excursions of height at most k is

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

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



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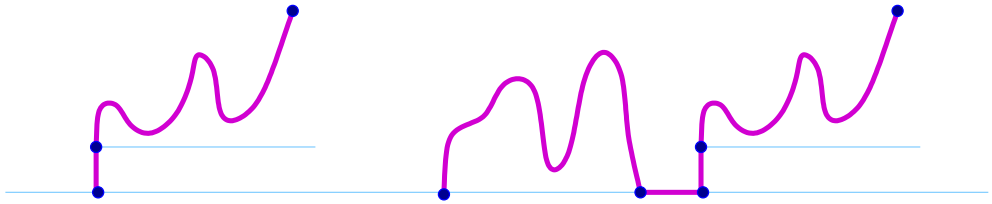
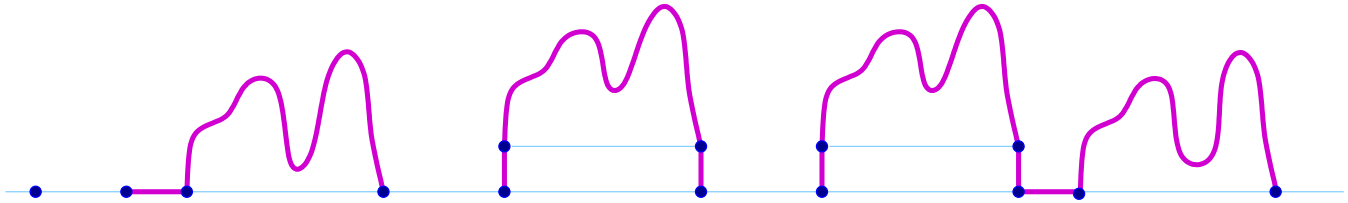


Last return to height 0



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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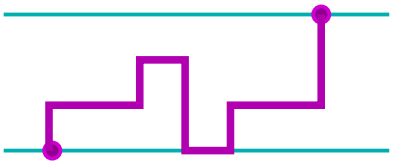

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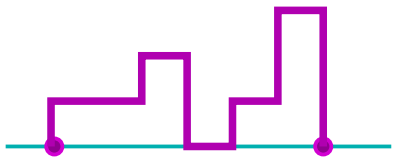

Enumeration of weakly directed bridges

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$$B(t) = \frac{I(t)}{1 - I(t)} \Rightarrow I(t) = \frac{B(t)}{1 + B(t)}$$

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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]

Nature of the generating function

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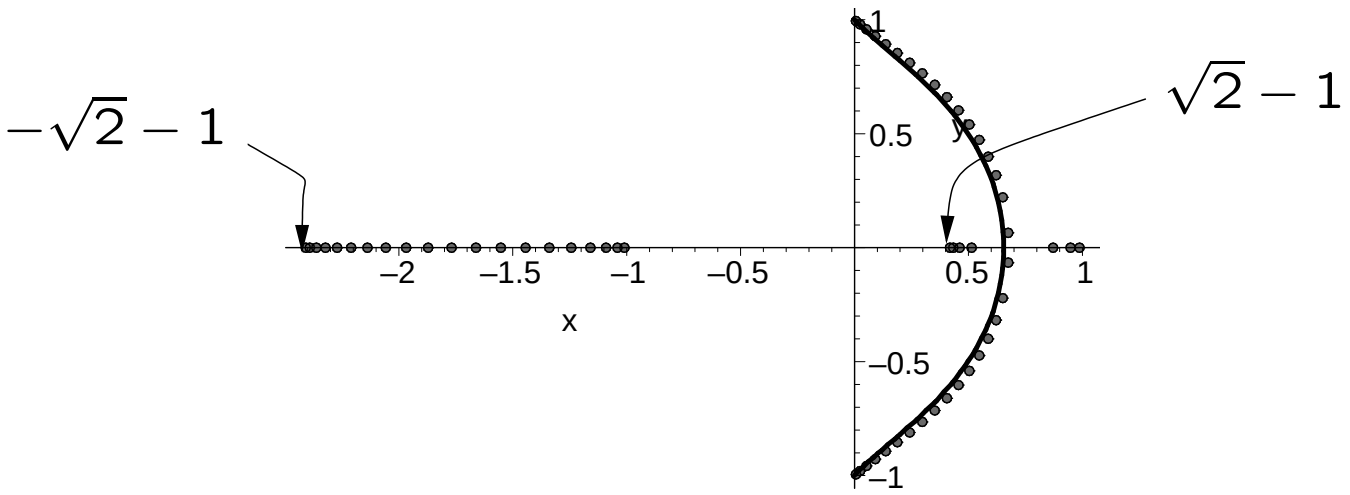
The zeroes of G_k (here, $k = 20$):



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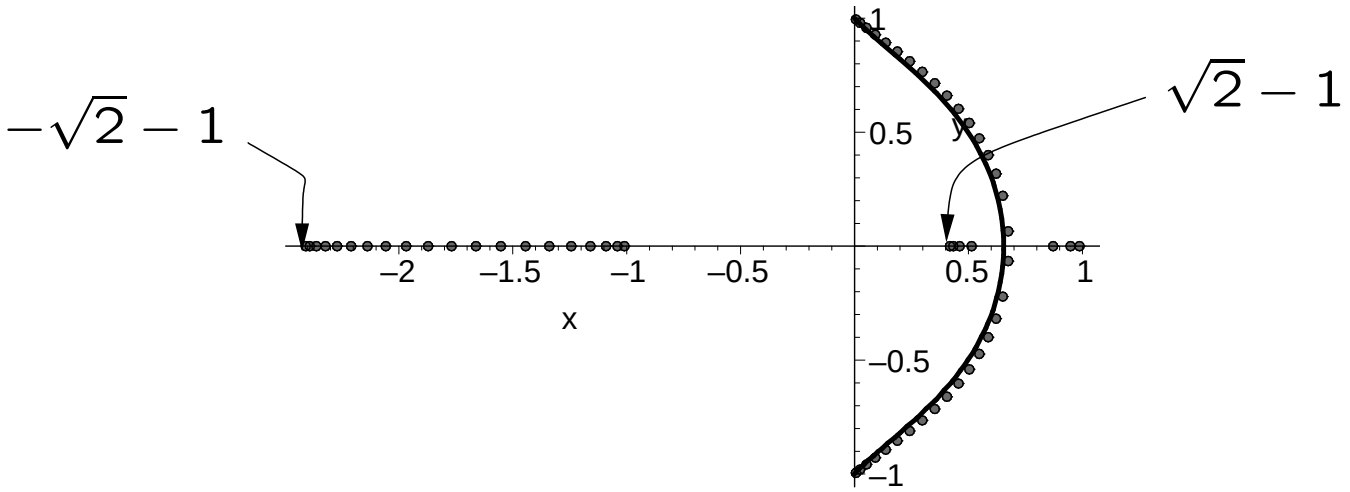
• The series $B(t)$ and $W(t)$ are meromorphic in $\mathbb{C} \setminus \mathcal{E}$, where $\mathcal{E}$ consists of the two real intervals $[-\sqrt{2}-1, -1]$ and $[\sqrt{2}-1, 1]$, and of the curve

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

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



The number of irreducible bridges

• In the disk $\{|z| < \sqrt{2}-1\}$, the series $W(t)$ has a unique pole at $\rho \simeq 0.39$, which is simple.

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

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

with $\mu \simeq 2.5447$ (the current record).

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

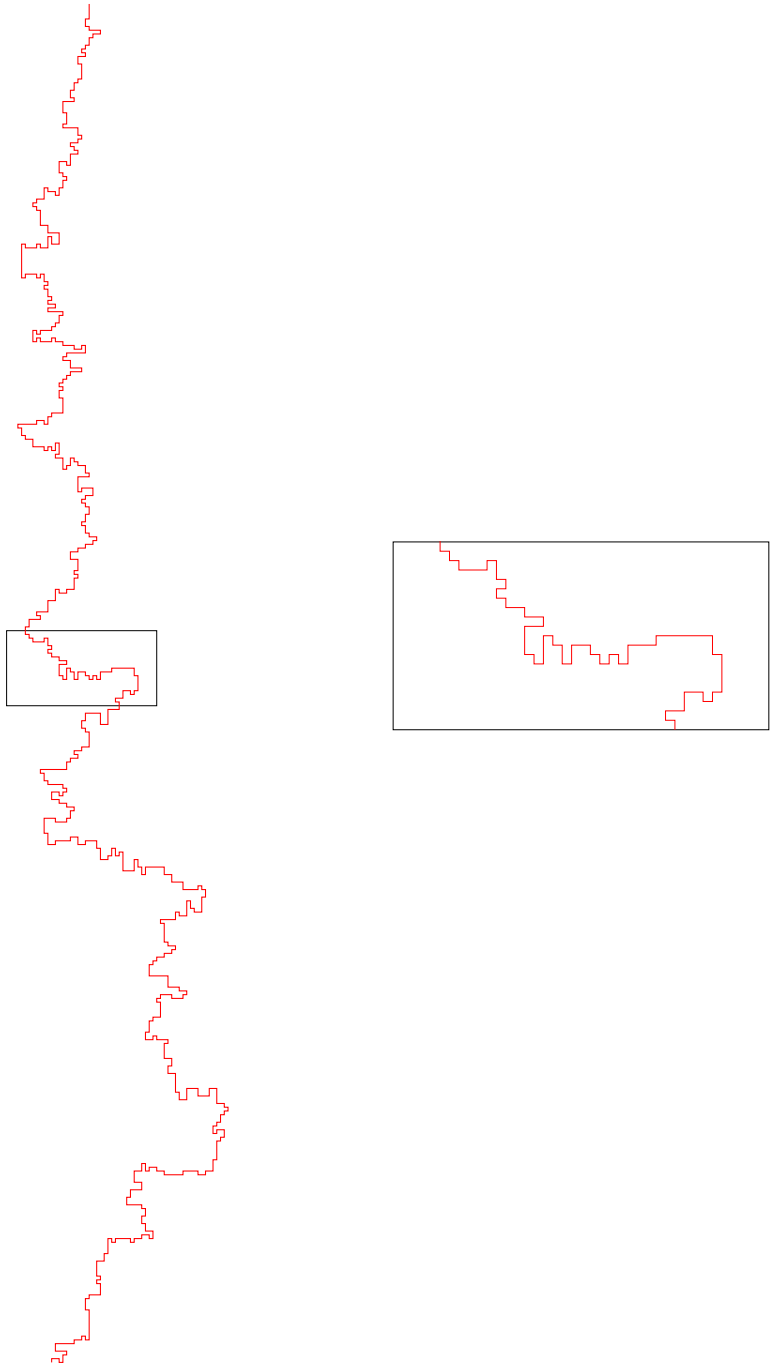
$$W(t,x) = \frac{1}{1 - x\left(\frac{2B(t)}{1+B(t)} - t\right)}$$

• The number N_n of irreducible bridges in a random weakly directed bridge of length n satisfies

$$\mathbb{E}(N_n) \sim \kappa\, n,$$

where $\kappa \simeq 0.318$. In particular, the average end-to-end distance, being bounded from below by $\mathbb{E}(N_n)$, grows linearly with n.

A random weakly directed bridge of size 1009



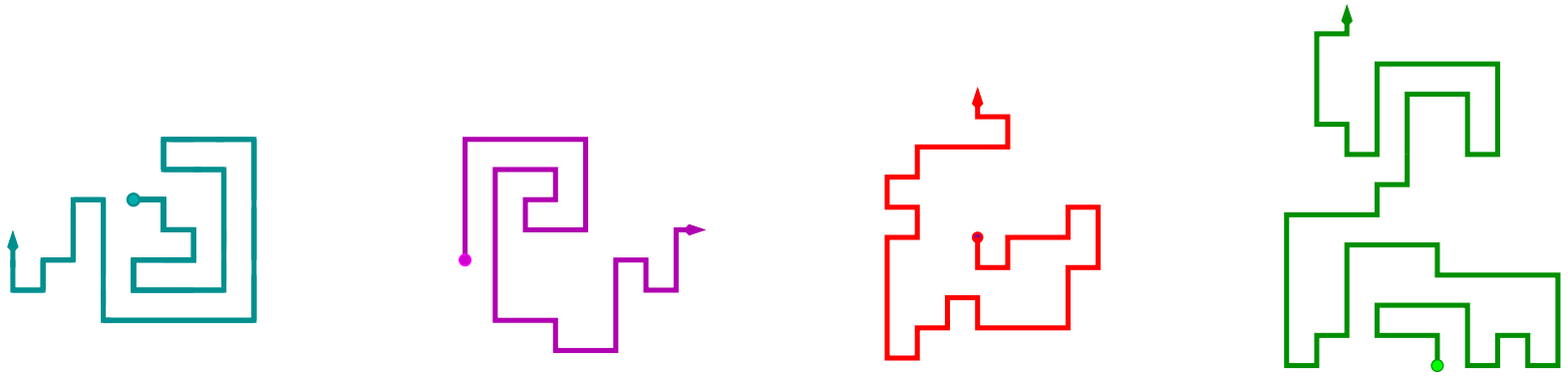
What's next?

• Prudent walks: A functional equation, and a conjecture for the growth constant (~ 2.48)

• Axel Bacher's walks: A very strange functional equation — The growth constant seems a bit above that of weakly directed walk (2.549)

• Pascal Préa's k-fractal walks: hope for a sub-linear end-to-end distance

• A mixture of prudent and weakly directed walks: walks formed of a sequence of prudent irreducible bridges



3. 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

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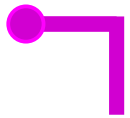

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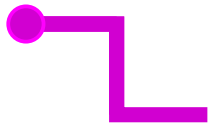

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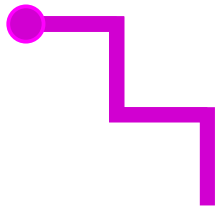

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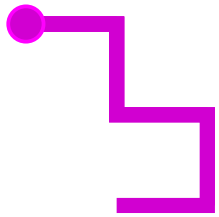

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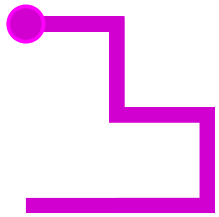

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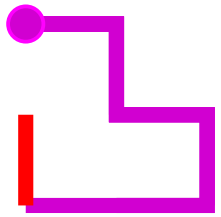

not prudent!

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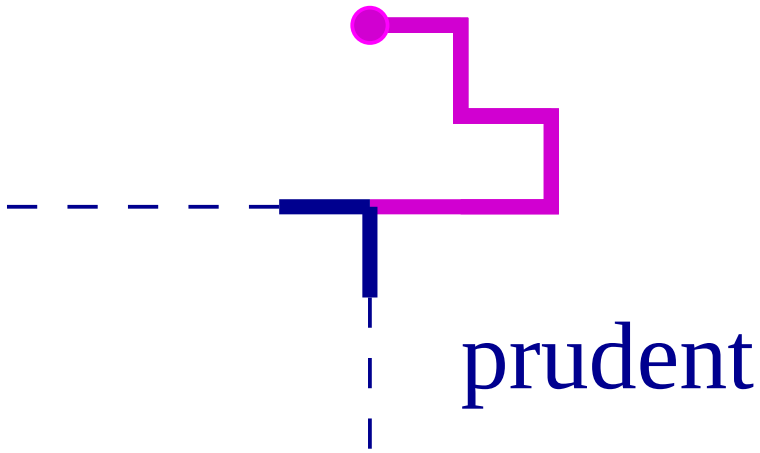

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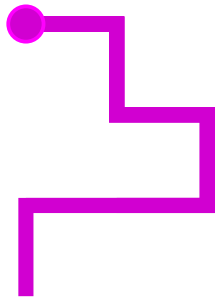

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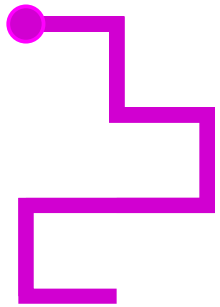

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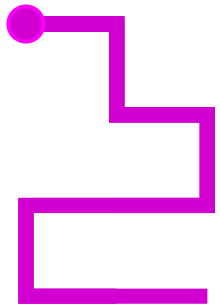

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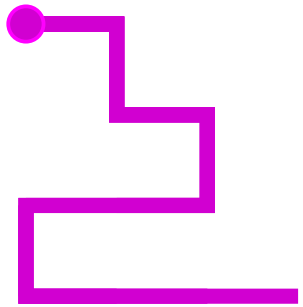

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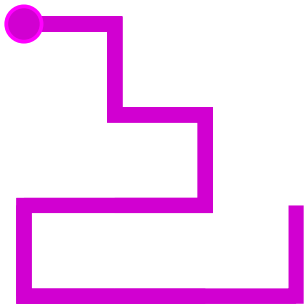

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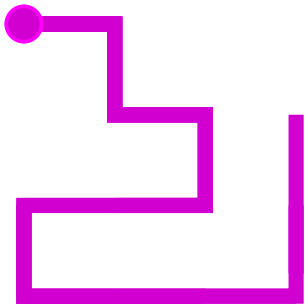

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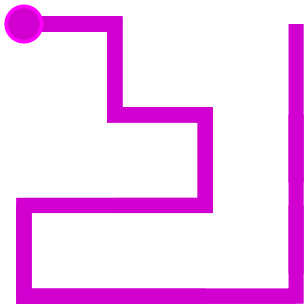

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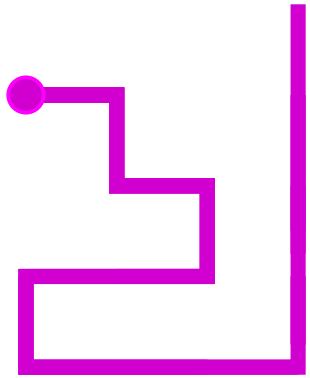

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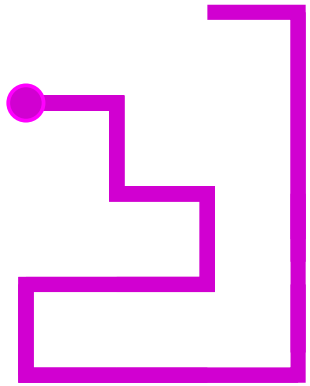

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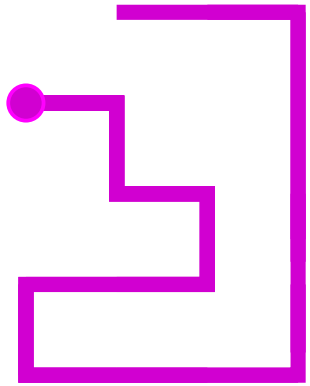

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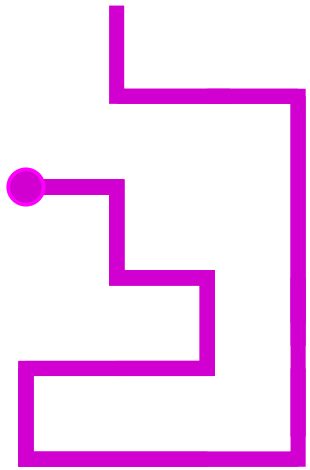

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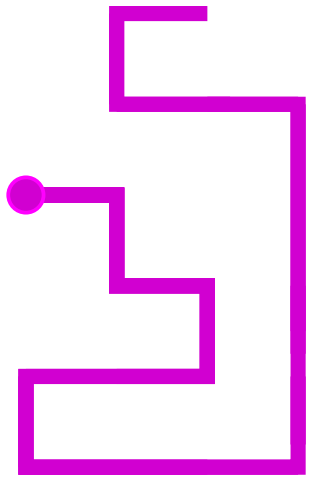

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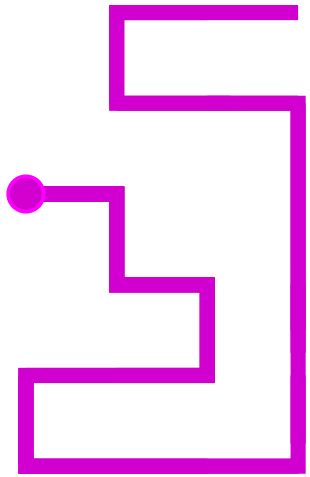

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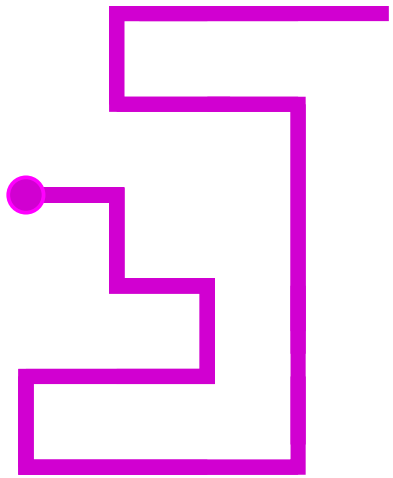

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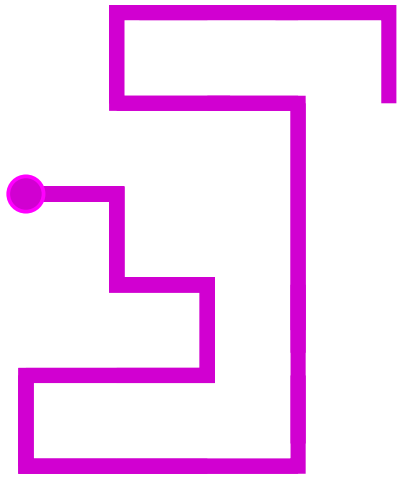

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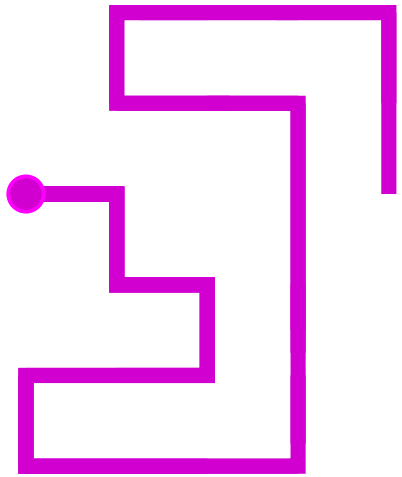

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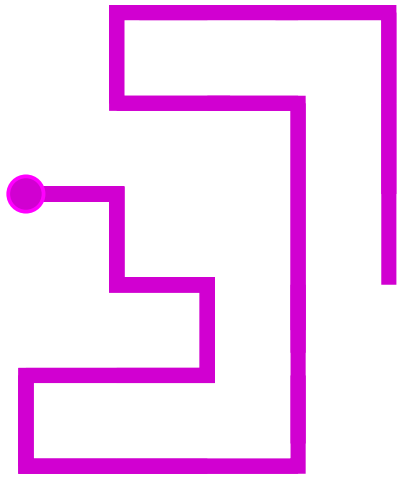

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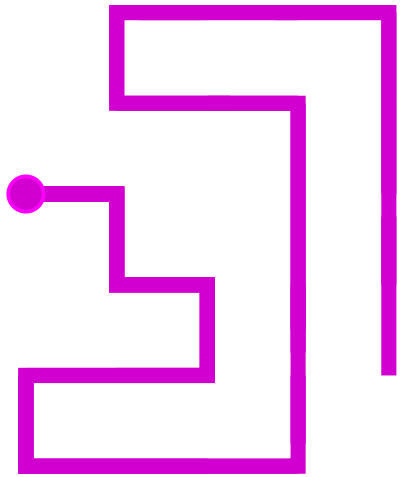

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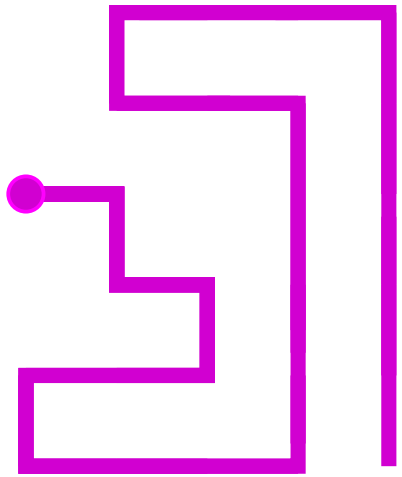

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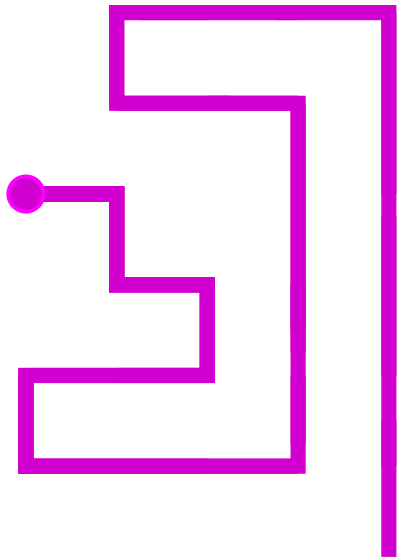

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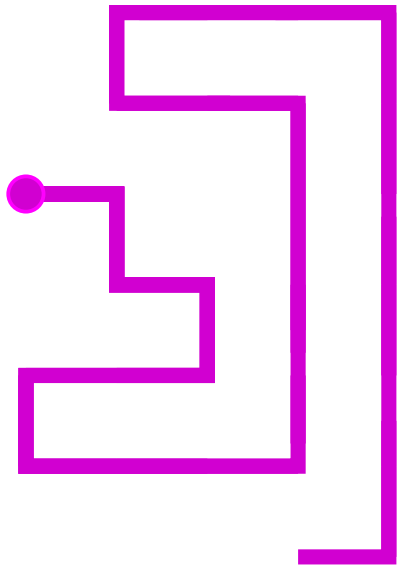

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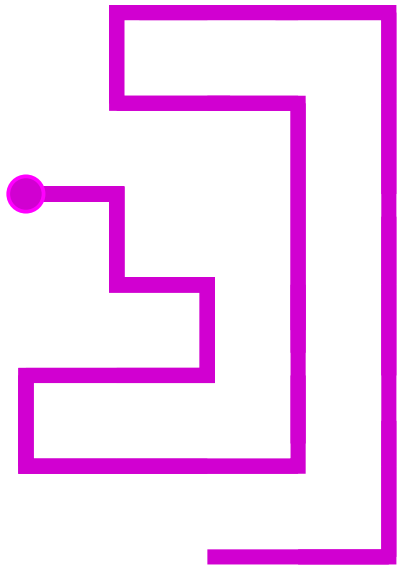

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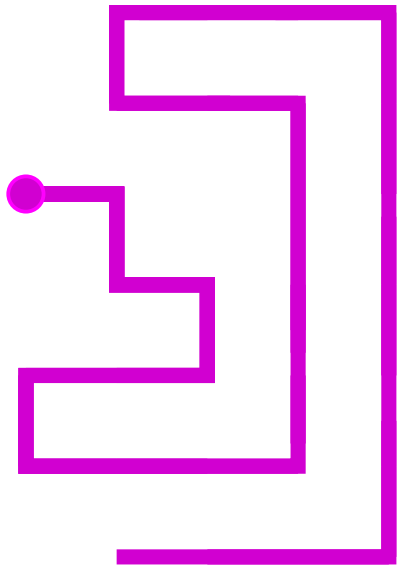

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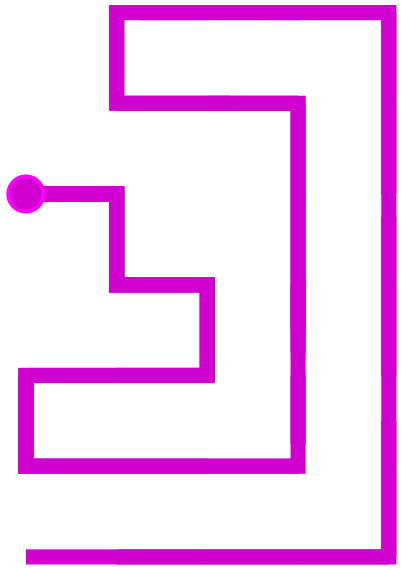

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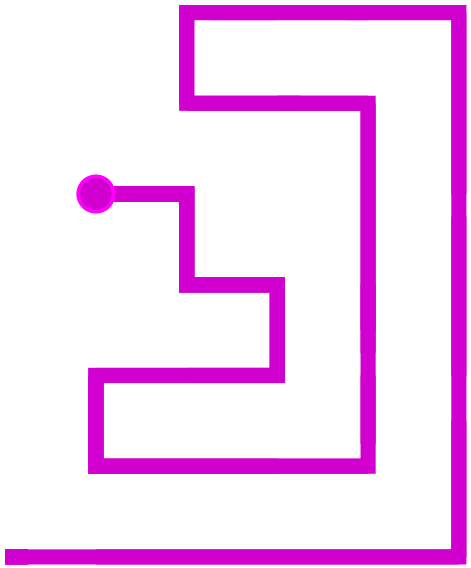

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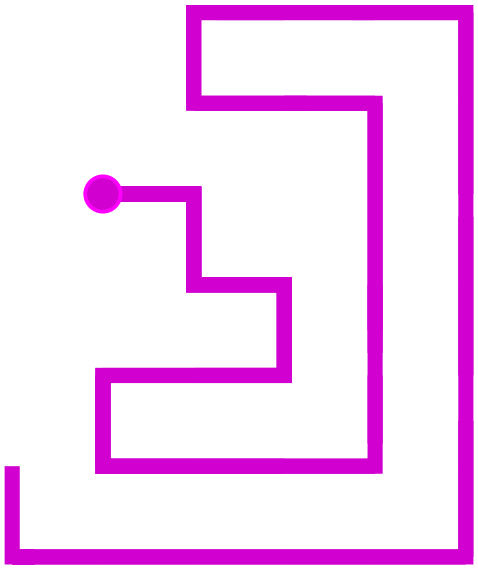

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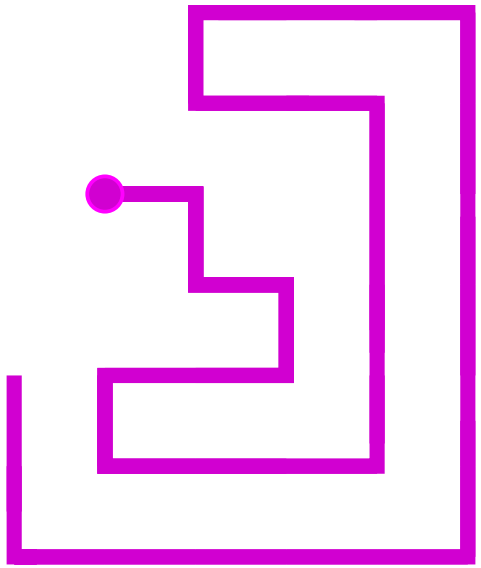

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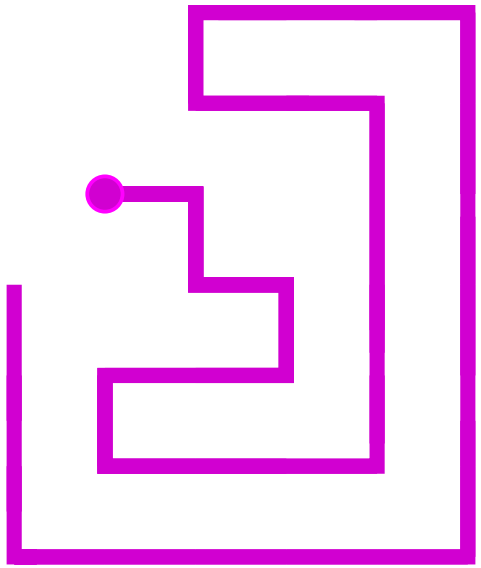

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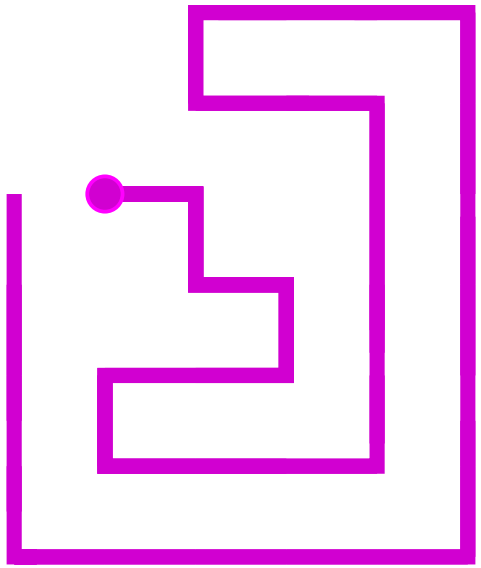

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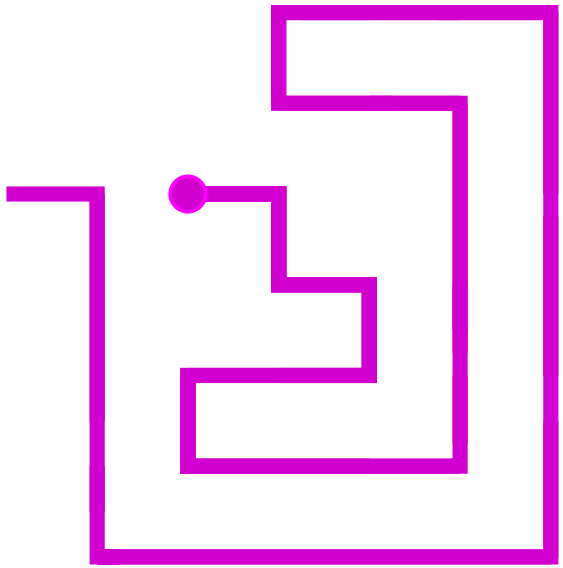

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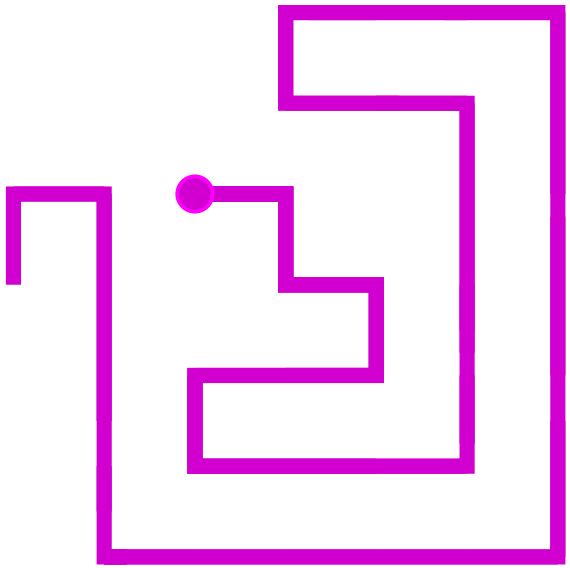

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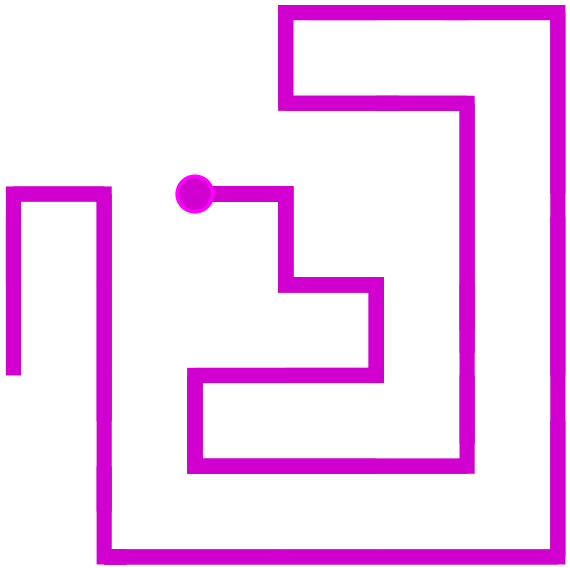

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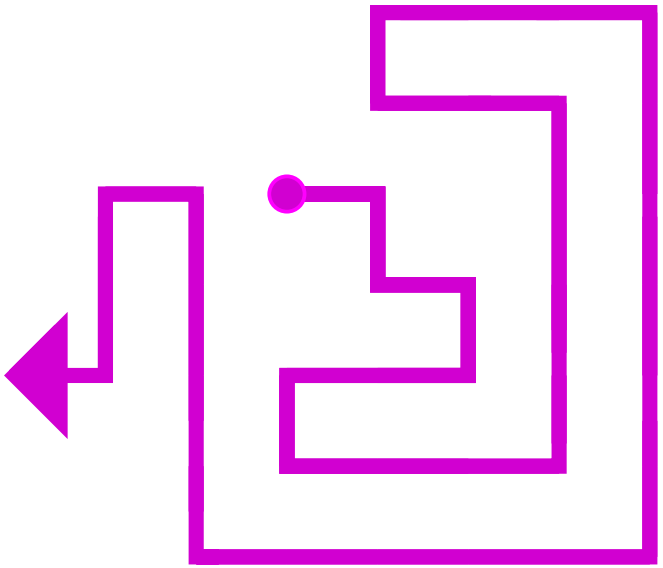

Enumeration of prudent walks

- 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)