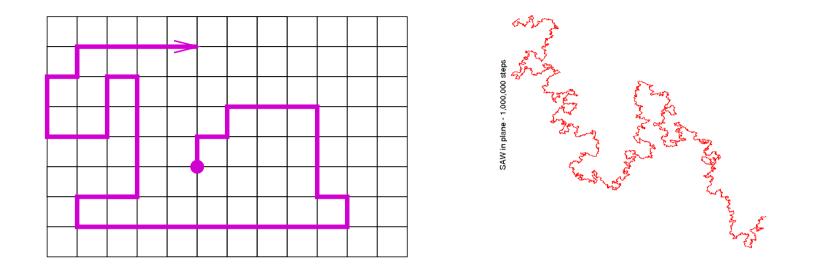
Mireille Bousquet-Mélou, CNRS, Bordeaux, France

http://www.labri.fr/~bousquet

+ ArXiv 2008

Self-avoiding walks (SAW)



Conjectures (d = 2)

- Enumeration: The number of *n*-step SAW is equivalent to $(\kappa) \mu^n n^{11/32}$ for *n* large.
- Asymptotic properties: The endpoint lies on average at distance $n^{3/4}$ from the starting point.
- Limit process: The scaling limit of SAW is $SLE_{8/3}$

(proved under an assumption of conformal invariance [Lawler et al. 02])

This is too hard!

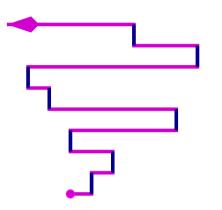
... for exact enumeration

 \Rightarrow Study of toy models, that should be as general as possible, but still tractable

- develop new techniques in exact enumeration
- solve better and better approximations of real SAW

A toy model: Partially directed walks

• Model: Self-avoiding walks with steps N, W, E



"Markovian with memory 1"

• Enumeration: generating function and asymptotics

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

• Asymptotic properties: coordinates of the endpoint

$$\mathbb{E}(|X_n|) \sim \sqrt{n}, \qquad \mathbb{E}(Y_n) \sim n$$

Definition, functional equations

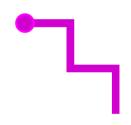
Self-directed walks [Turban-Debierre 86] Exterior walks [Préa 97] Outwardly directed SAW [Santra-Seitz-Klein 01] Prudent walks [Duchi 05], [Dethridge, Guttmann, Jensen 07], [mbm 08]

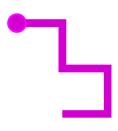


A step never points towards a vertex that has been visited before.

•



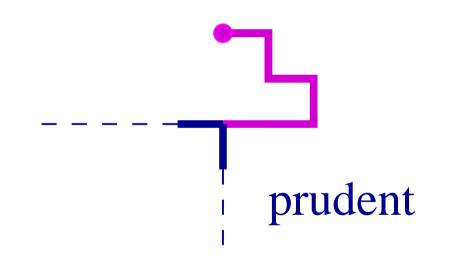


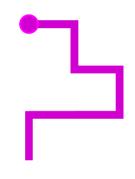


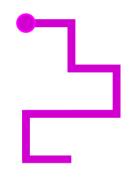


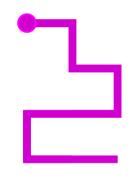
A step never points towards a vertex that has been visited before.

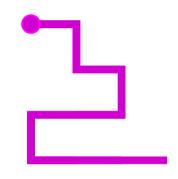
not prudent!

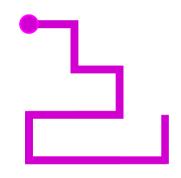


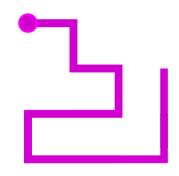


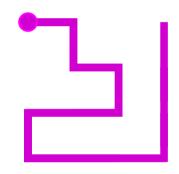


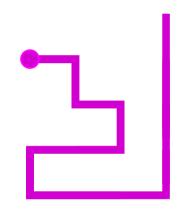


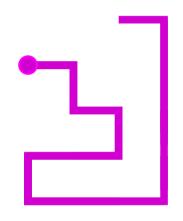


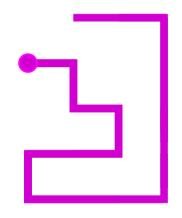


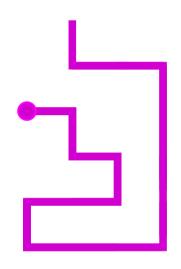


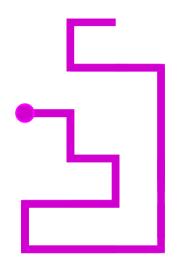


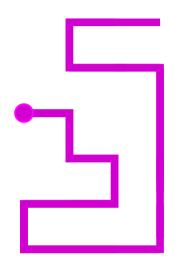


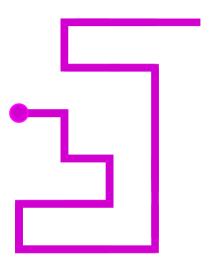


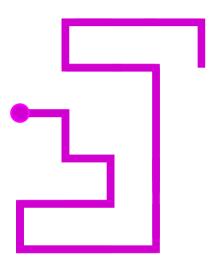


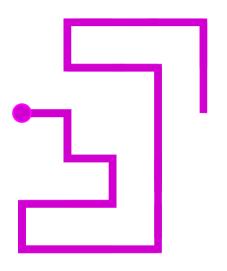


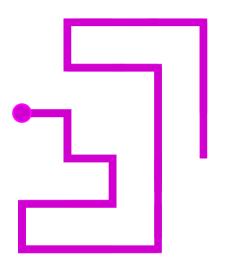


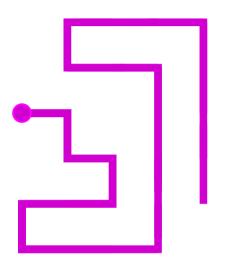


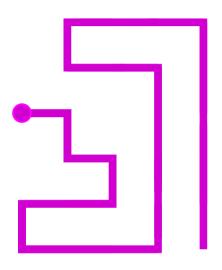


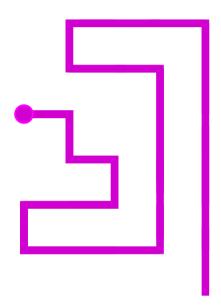


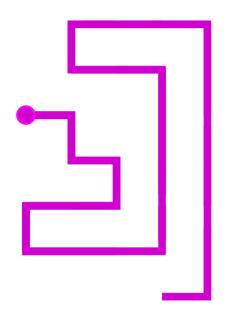


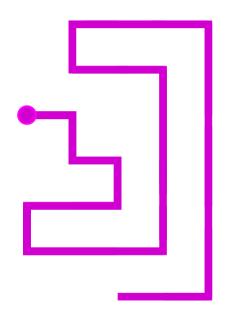


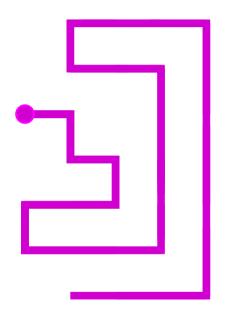


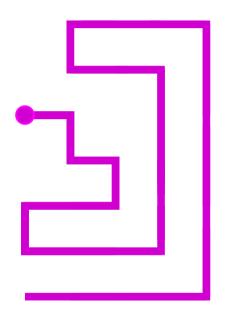


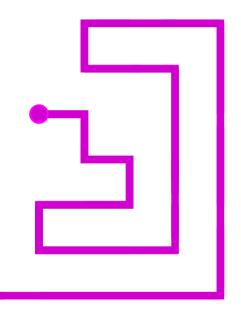


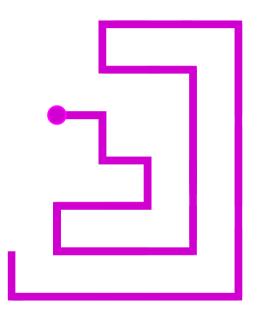


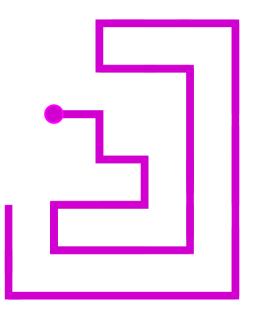


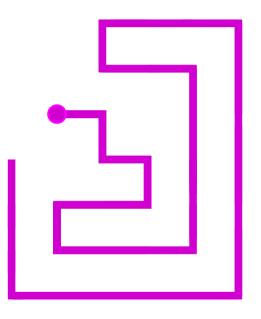


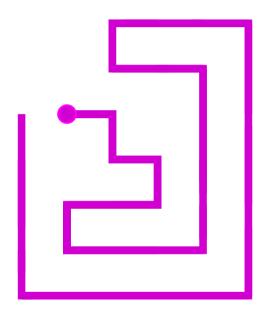


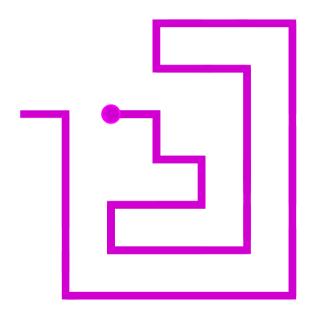


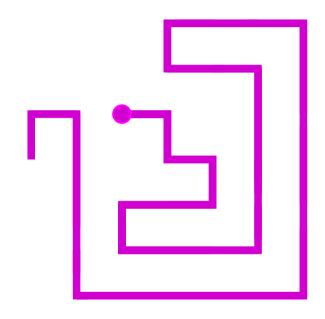


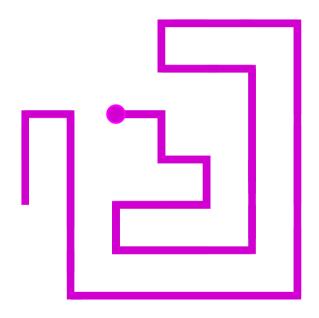


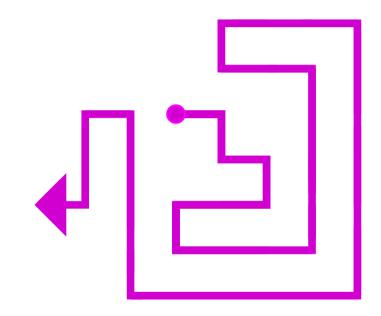




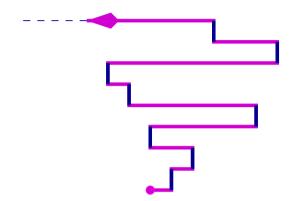








Remark: Partially directed walks are prudent

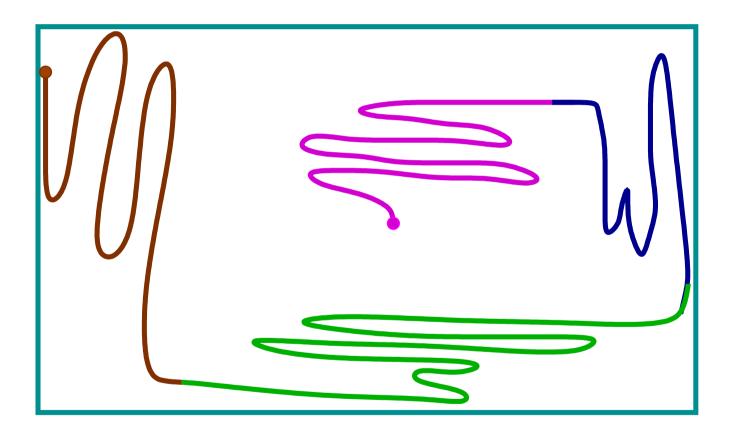


A property of prudent walks



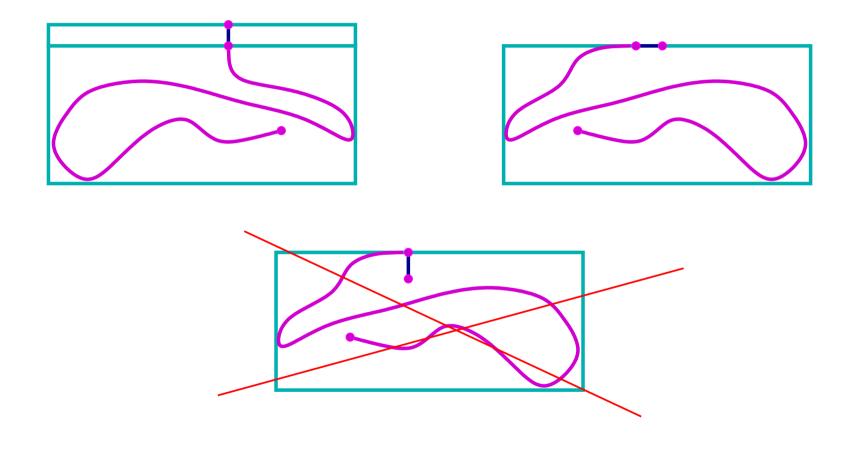
A property of prudent walks

The box of a prudent walk

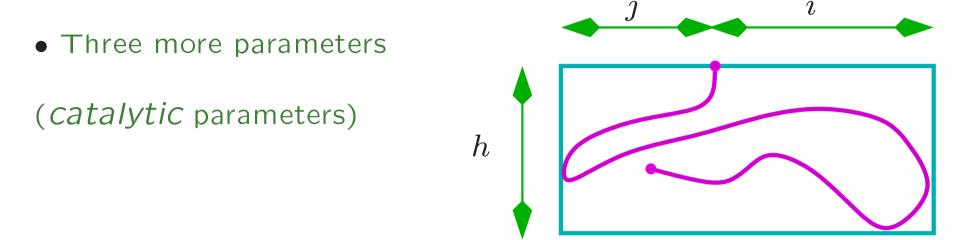


The endpoint of a prudent walk is always on the border of the box

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



Recursive construction of prudent walks: Where is the endpoint?

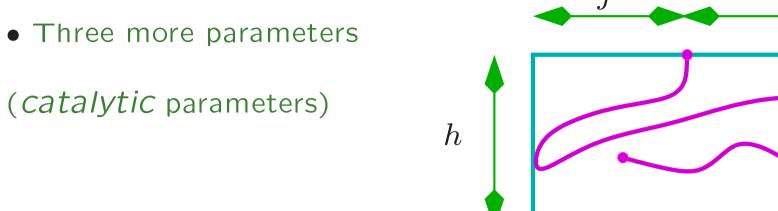


• Generating function of prudent walks ending on the top of their box:

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

Series with three catalytic variables u, v, w

Recursive construction of prudent walks: Where is the endpoint?



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

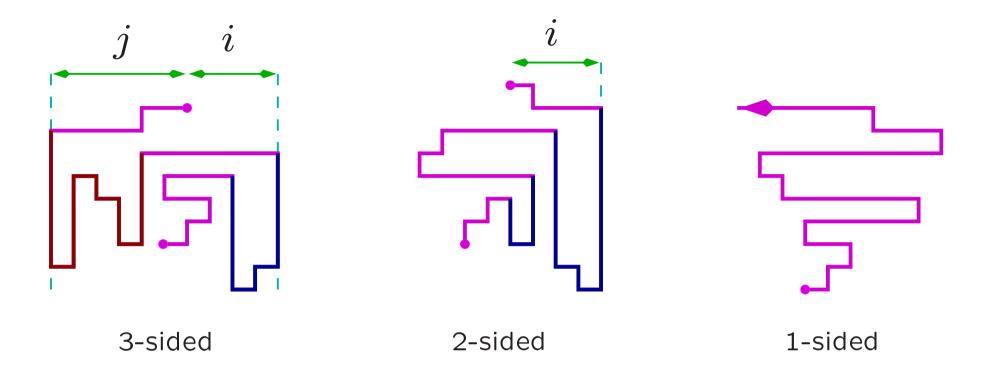
$$\left(1 - \frac{uvwt(1-t^2)}{(u-tv)(v-tu)}\right)T(t;u,v,w) = 1 + \mathcal{T}(t;w,u) + \mathcal{T}(t;w,v) - tv\frac{\mathcal{T}(t;v,w)}{u-tv} - tu\frac{\mathcal{T}(t;u,w)}{v-tu}$$
with $\mathcal{T}(t;u,w) = tvT(t;u,tu,w)$

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

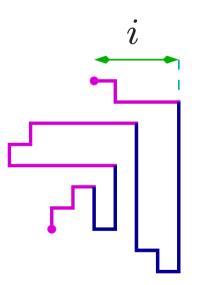
• Three-sided walks: two catalytic variables

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

• Two-sided walks: one catalytic variable

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

II. Two-sided prudent walks



Two-sided walks: exact enumeration

Proposition The length generating function of 2-sided walks is:

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

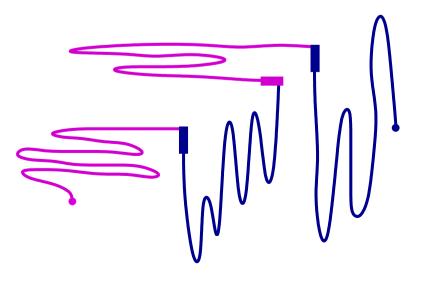
[Duchi 05]

Proofs

• Kernel method applied to

$$\begin{cases} \left((1 - tu)(u - t) - tu(1 - t^2) \right) T(t; u) = u - t + t(u - 2t)(1 - tu)T(t; t) \\ P(t) = 2T(t; 1) - T(t; 0) \end{cases}$$

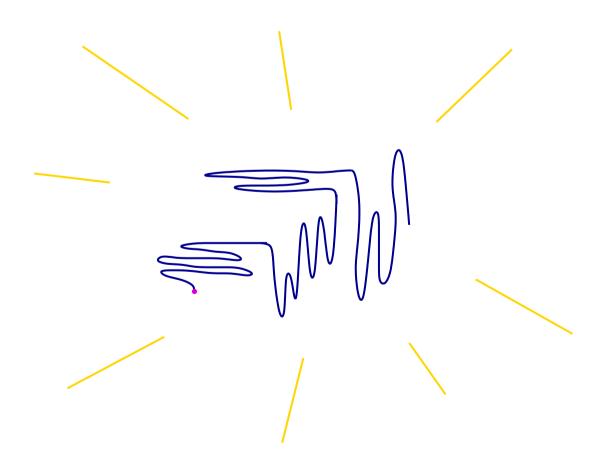
• Context-free grammar



Two-sided walks: exact enumeration

Proposition The length generating function of 2-sided walks is:

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



But there He came...

Asymptotic enumeration

Properties of large random objects

Random generation

Two-sided walks: asymptotic enumeration

• The length generating function of 2-sided walks is

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

• Dominant singularity: a simple pole for $1 - 2t - 2t^2 + 2t^3 = 0$, that is, $t_c = 0.40303...$ Asymptotically,

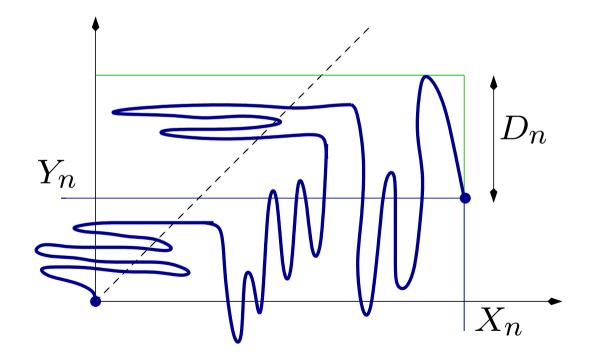
$$p(n) \sim \kappa (2.48...)^n$$

Compare with 2.41... for partially directed walks.

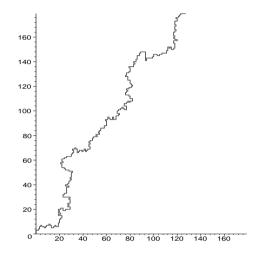
Two-sided walks: properties of large random walks (uniform distribution)

• The random variables X_n , Y_n and D_n satisfy

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



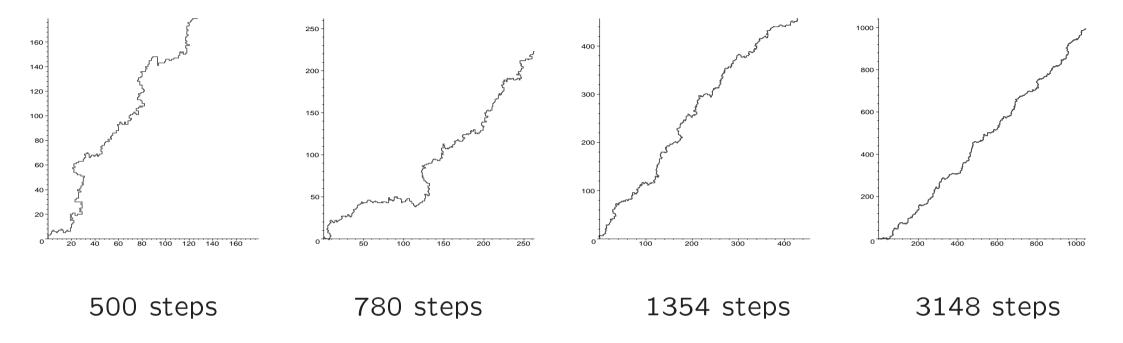
Two-sided walks: random generation (uniform distribution)



500 steps

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

Two-sided walks: random generation (uniform distribution)



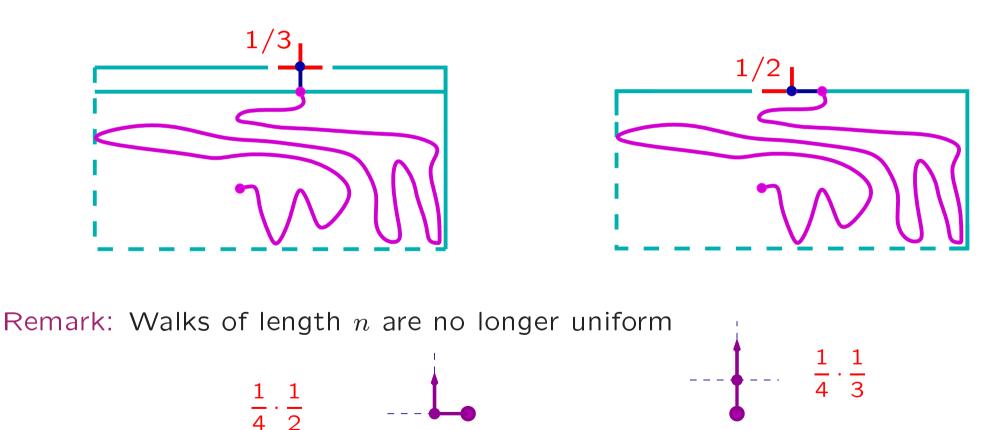
- Recursive step-by-step construction à la Wilf \Rightarrow 500 steps (precomputation of $O(n^2)$ large numbers)
- Boltzmann sampling via the context-free grammar [Duchon-Flajolet-Louchard-Schaeffer 02]

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

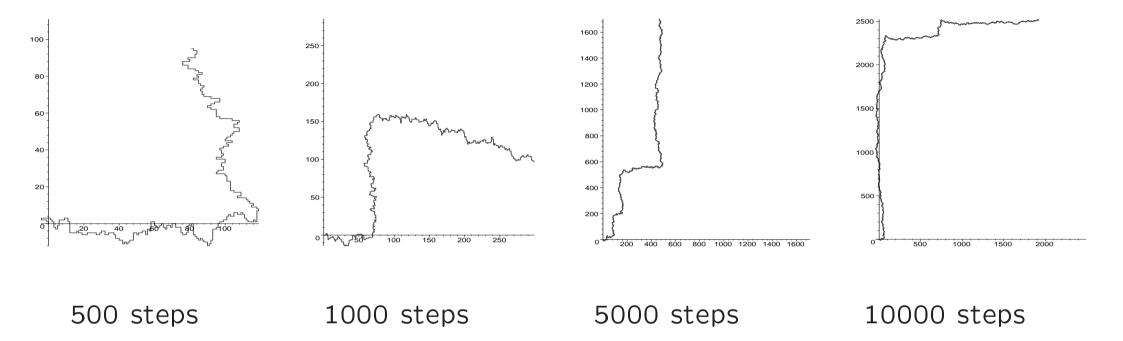
Another distribution: Kinetic two-sided walks

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

[An admissible step is one that gives a two-sided walk]



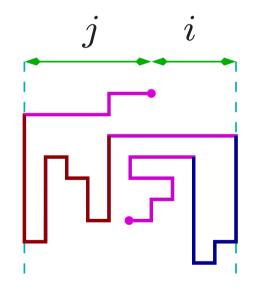
Another distribution: Kinetic two-sided walks



- Random generation: Recursive step-by-step construction à la Wilf (no precomputation)
- Asymptotic properties (from exact enumeration)

$$\mathbb{E}(X_n) = \mathbb{E}(Y_n) \sim n \qquad \mathbb{E}((X_n - Y_n)^2) \sim n^2, \qquad \mathbb{E}(D_n) \sim \sqrt{n}$$

III. Three-sided prudent walks



Three-sided walks: two catalytic variables

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

. . .

- Cancel the kernel by an appropriate choice of $v \equiv v(t; u)$
- This kernel is homogeneous in u and v

Three-sided prudent walks: exact enumeration

• The length generating function of three-sided prudent walks is:

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

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

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

Three-sided prudent walks: asymptotic enumeration and singularities

• The length generating function of three-sided prudent walks is:

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

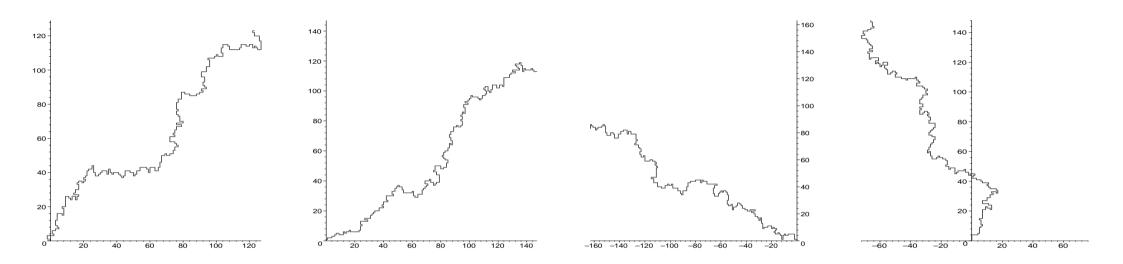
$$T(t;1,t) = \sum_{k\geq 0} (-1)^k \frac{\prod_{i=0}^{k-1} \left(\frac{t}{1-tq} - U(q^{i+1})\right)}{\prod_{i=0}^k \left(\frac{tq}{q-t} - U(q^i)\right)} \left(1 + \frac{U(q^k) - t}{t(1 - tU(q^k))} + \frac{U(q^{k+1}) - t}{t(1 - tU(q^{k+1}))}\right)$$

• Asymptotic enumeration: The dominant singularity is (again) a simple pole for $1 - 2t - 2t^2 + 2t^3 = 0$. Asymptotically,

$$p(n) \sim \kappa (2.48...)^n$$

• Singularity analysis: The series P(t) has infinitely many poles, satisfying $\frac{tq}{q-t} = U(q^i)$ for some $i \ge 0$. Hence it is neither algebraic, nor even D-finite.

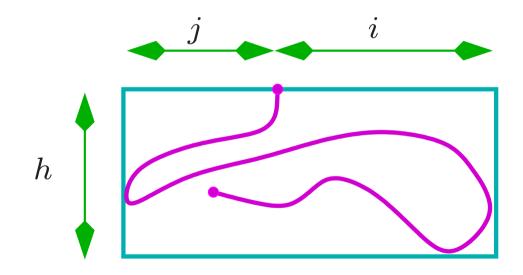
Three-sided prudent walks: random generation and asymptotic properties



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

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

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



General prudent walks: three catalytic variables

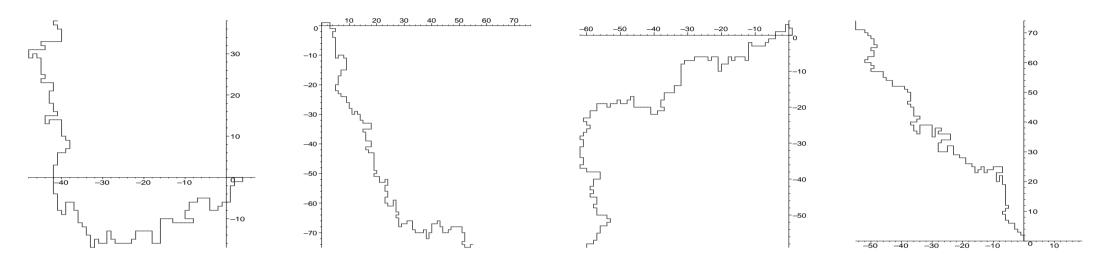
$$\left(1 - \frac{uvwt(1-t^2)}{(u-tv)(v-tu)}\right)T(u,v,w) = 1 + \mathcal{T}(w,u) + \mathcal{T}(w,v) - tv\frac{\mathcal{T}(v,w)}{u-tv} - tu\frac{\mathcal{T}(u,w)}{v-tu}$$

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

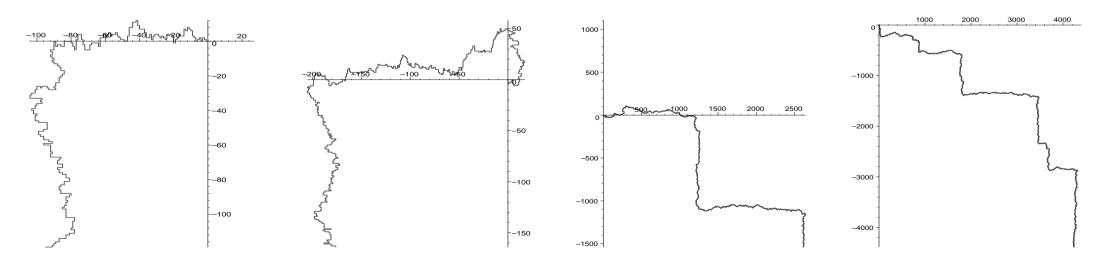
?

Random prudent walks

• Uniform model: recursive generation, 195 steps (sic! $O(n^4)$ numbers)



• Kinetic model: recursive generation with no precomputation



500 steps

1000 steps

10000 steps

20000 steps

Conjectures, and summary of the results

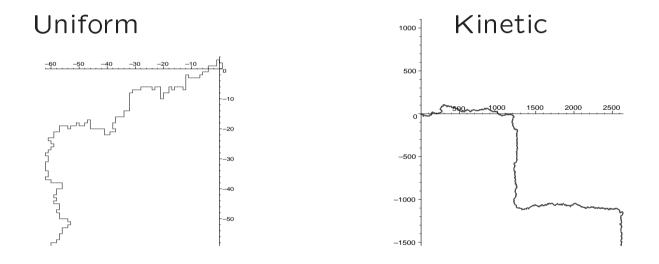
	Nature of the g.f.	Asympt. growth	End-to-end distance
1-sided (part. dir)	Rat.	$(2.41)^n$	n
2-sided	Alg. [Duchi 05]	$(2.48)^n$	n
3-sided	not D-finite	$(2.48)^n$	n
4-sided (general)	not D-finite	(2.48) ⁿ	n
square lattice SAW	?	$(2.63)^n n^{11/32}$	n ^{3/4}

Conjectures: [Dethridge, Guttmann, Jensen 07]

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...)



- Kinetic models
- Limit processes?
- More general walks (with A. Bacher), with growth constant 2.54...

Triangular prudent walks

The length generating function of triangular prudent walks is

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

with

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

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 $Yt^k(1-2t^2) = 0$)