Sequences Arising From Prudent Self-Avoiding Walks

Shanzhen Gao, Heinrich Niederhausen
Florida Atlantic University, Boca Raton, Florida 33431

Abstract

A self-avoiding walk (SAW) is a sequence of moves on a lattice not visiting the same point more than once. A SAW on the square lattice is prudent if it never takes a step towards a vertex it has already visited. Prudent walks differ from most sub-classes of SAWs that have been counted so far in that they can wind around their starting point. Some problems and some sequences arising from prudent walks are discussed in this paper.

Keywords: Self-avoiding walk, prudent self-avoiding walk, generating function, kernel method

1 Introduction

A well-known long standing problem in combinatorics and statistical mechanics is to find the generating function for self-avoiding walks (SAW) on a two-dimensional lattice, enumerated by perimeter. A SAW is a sequence of moves on a square lattice which does not visit the same point more than once. It has been considered by more than one hundred researchers in the pass one hundred years, including George Polya, Tony Guttmann, Laszlo Lovasz, Donald Knuth, Richard Stanley, Doron Zeilberger, Mireille Bousquet-Mélou, Thomas Prellberg, Neal Madras, Gordon Slade, Agnes Dittel, E.J. Janse van Rensburg, Harry Kesten, Stuart G. Whittington, Lincoln Chayes, Iwan Jensen, Arthur T. Benjamin, and others. More than three hundred papers and a few volumes of books were published in this area. A SAW is interesting for simulations because its properties cannot be calculated analytically. Calculating the number of self-avoiding walks is a common computational problem [12], [8], [9]. In the past few decades, many mathematicians have studied the following two problems:

Problem 1

What is the number of SAWs from $(0,0)$ to $(n-1,n-1)$ in an $n\times n$ grid, taking steps from $\{\uparrow,\downarrow,\leftarrow,\rightarrow\}$?

Donald Knuth claimed that the number is between 1.3×10^{24} and 1.6×10^{24} for $n=11$ and he did not believe that he would ever in his lifetime know the exact answer to this problem in 1975. However, after a few years, Richard Schroeppel pointed out that the exact value is $1,568,758,030,464,750,013,214,100 = 2^2 3^2 5^2 31\times 115\,422\,379\times 487\,148\,912\,401$ [1], [10], [5]. It is still an unsolved problem for $n>25$.

Problem 2

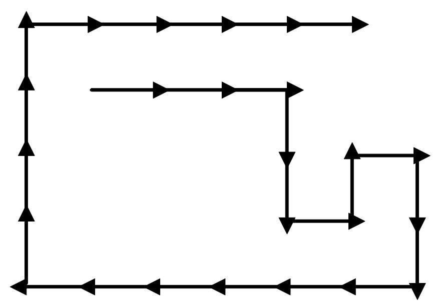
What is the number $f(n)$ of n-step SAWs, on the square lattice, taking steps from $\{\uparrow,\downarrow,\leftarrow,\rightarrow\}$?

The number $f(n)$ is known for $n\le 71$ [10], [11], [3], [1].

A recently proposed model called prudent self-avoiding walks (PSAW) was first introduced to the mathematics community in an unpublished manuscript of Préa, who called them *exterior walks*. A prudent walk is a connected path on square lattice such that, at each step, the extension of that step along its current trajectory will never intersect any previously occupied vertex. Such walks are clearly self-avoiding [6], [13], [4], [7], [2]. We will talk about some sequences arising from PSAWs in the following.

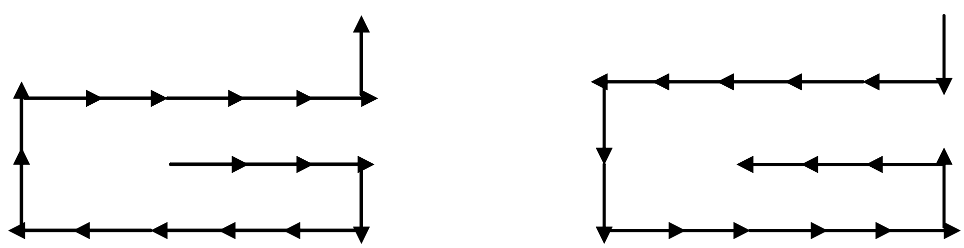
2 Prudent Self-Avoiding Walks: Definitions and Examples

A PSAW is a proper subset of SAWs on the square lattice. The walk starts at $(0, 0)$, and the empty walk is a PSAW. A PSAW grows by adding a step to the end point of a PSAW such that the extension of this step - by any distance - never intersects the walk. Hence the name prudent. The walk is so careful to be self-avoiding that it refuses to take a single step in any direction where it can see - no matter how far away - an occupied vertex. The following walk is a PSAW.



2.1 Properties of a PSAW

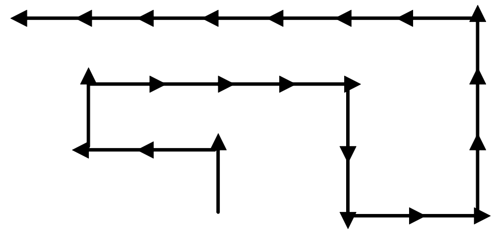
Unlike SAW, PSAW are usually not reversible. There is such an example in the following figure.



Each PSAW possesses a minimum bounding rectangle, which we call *box*. Less obviously, the endpoint of a prudent walk is always a point on the boundary of the box. Each new step either inflates the box or walks (prudently) along the border. After an inflating step, there are 3 possibilities for a walk to go on. Otherwise, only 2.

In a *one-sided* PSAW, the endpoint lies always on the top side of the box. The walk is *partially directed*.

A prudent walk is *two-sided* if its endpoint lies always on the top side, or on the right side of the box. The walk in the following figure is a two-sided PSAW.



3 Some Sequences Arising from One-sided PSAWs

Sequence 1

What is the number (say $f(n)$) of one-sided n-step prudent walks, taking steps from $\{\uparrow, \leftarrow, \rightarrow\}$?

The generating function equals

$$\sum_{n\geq 0} f(n)\, t^n = \frac{1+t}{1-2t-t^2} = 1+3t+7t^2+17t^3+41t^4+99t^5+239t^6+...$$

Also,

$$\begin{aligned} f(n) &= 2f(n-1)+f(n-2) \\ &= \frac{(1-\sqrt{2})^n+(1+\sqrt{2})^n}{2} \\ &= \begin{bmatrix} 1 & 0 \end{bmatrix} \left(\sum_{k=0}^{n+1} \binom{n+1}{k} \begin{bmatrix} 0 & 1 \\ 2 & 0 \end{bmatrix}^k \right) \begin{bmatrix} 1 \\ 0 \end{bmatrix}. \end{aligned}$$

We obtain sequence $A001333$ of the On-Line Encyclopedia of Integer Sequences.

Sequence 2

The number of one-sided n-step prudent walks, starting from $(0,0)$ and ending on y-axis, taking steps from $\{\uparrow, \leftarrow, \rightarrow\}$ is

$$1+\sum_{k=1}^{\lfloor (n-1)/2 \rfloor} \sum_{i=1}^{\min\{n-2k,k\}} \binom{n-2k+1}{i} \binom{k-1}{k-i} \binom{n-k-i}{k}.$$

We obtain sequence $A136029$.

Sequence 3

Consider the number of one-sided prudent walks starting from $(0,0)$ to (x,y), taking steps from $\{\uparrow, \leftarrow, \rightarrow\}$. The number of such walks with $k+x$ right $\rightarrow$ steps, k left $\leftarrow$ steps and y up $\uparrow$ steps, is

$$\sum_{i=1}^{\min\{y,k+x\}} \binom{y+1}{i} \binom{k+x-1}{k+x-i} \binom{y+k-i}{k}.$$

If $k=2$ and $x=y=n$, we obtain sequence $A119578$.

Sequence 4

The number of one-sided n-step prudent walks, from $(0,0)$ to (x,y), ($n-x-y$ is even) taking steps from $\{\uparrow, \leftarrow, \rightarrow\}$ is

$$\sum_{i=0}^{\min\{y, \frac{n+x-y}{2}\}} \binom{y+1}{i} \binom{\frac{n+x-y}{2}-1}{\frac{n+x-y}{2}-i} \binom{\frac{n-x+y}{2}-i}{\frac{n-x-y}{2}}.$$

If $x=y=3$, we obtain sequence $A163761$.

Sequence 5

What is the number of the one-sided n-step prudent walks, avoiding k or more consecutive east steps, $\rightarrow^{\geq k}$?

The generating function equals

$$\frac{1+t-t^k}{1-2t-t^2+t^{k+1}}$$

If $k=2$, we obtain sequence $A006356$, counting the number of paths for a ray of light that enters two layers of glass and then is reflected exactly n times before leaving the layers of glass.

If $k=3$, we obtain sequence $A033303$ (see also page 244 in [14]).

Sequence 6

The number of one-sided n-step prudent walks, taking steps from $\{\uparrow, \leftarrow, \rightarrow, \nearrow\}$ equals

$$\frac{5+\sqrt{17}}{2\sqrt{17}}\left(\frac{3+\sqrt{17}}{2}\right)^n - \frac{5-\sqrt{17}}{2\sqrt{17}}\left(\frac{3-\sqrt{17}}{2}\right)^n.$$

We obtain sequence $A055099$.

Sequence 7

What is the number of one-sided n-step prudent walks, taking steps from $\{\rightarrow, \leftarrow, \uparrow, \nearrow, \searrow\}$?

The generating function is

$$\frac{1+t}{1-4t-3t^2}.$$

We obtain sequence $A126473$.

Sequence 8

What is the number of one-sided n-step prudent walks in the first quadrant, starting from $(0,0)$ and ending on the y-axis, taking steps from $\{\uparrow, \leftarrow, \rightarrow\}$?

The generating function is

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

Sequence 9

What is the number of one-sided n-step prudent walks *exactly* avoiding $\leftarrow^{=k}$, taking steps from $\{\uparrow, \leftarrow, \rightarrow\}$?

The generating function equals

$$\frac{1+t-t^k+t^{k+1}}{1-2t-t^2+t^{k+1}-t^{k+2}}.$$

If $k=1$, we obtain sequence $A078061$.

Sequence 10

What is the number of one-sided n-step prudent walks exactly avoiding $\leftarrow^{=k}$ and $\uparrow^{=k}$ (both at the same time)?

The generating function is

$$\frac{1+t-2t^k+2t^{k+1}}{1-2t-t^2+2t^{k+1}-2t^{k+2}}.$$

For $k=1$,

$$f(n)=\left(2^{n+2}-(-1)^{\lfloor n/2\rfloor}+2(-1)^{\lfloor (n+1)/2\rfloor}\right)/5,$$

also,

$$f(n)=2f(n-1)-f(n-2)+2f(n-3)$$
$$\text{with } f(1)=1, f(2)=3, f(3)=7.$$

This is sequence $A007909$.

4 Some Sequences Arising from Two-sided PSAWs

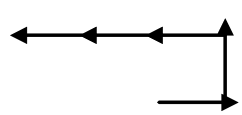
What is the number of two-sided, n-step prudent walks ending on the top side of their box avoiding both patterns $\leftarrow^{\geq 2}$, $\downarrow^{\geq 2}$ (both at the same time), taking steps from $\{\uparrow,\downarrow,\leftarrow,\rightarrow\}$?

Theorem 1 *The generating function (say $T(t,u)$) of the above two-sided prudent walks ending on the top side of their box satisfies*

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

where u counts the distance between the endpoint and the north-east (NE) corner of the box.

For instance, in the following figure, a walk takes 5 steps, and the distance between the endpoint and the north-east corner is 3. So we can use t^5u^3 to count this walk.



Outline of the proof of the theorem:

Case 1: Neither the top nor the right side has ever moved; the walk is only a west step. This case contributes 1 to the generating function.

Case 2: The last inflating step goes east. This implies that the endpoint of the walk was on the right side of the box before that step. After that east step, the walk has made a sequence of north steps to reach the top side of the box. Observe that, by symmetry, the series $T(t,u)$ also counts walks ending on the right side of the box by the length and the distance between the endpoint and the north-east corner. These two observations give the generating function for this class as $T(t,t)$.

Case 3: The last inflating step goes north. After this step, there is either a west step or a bounded sequence of East steps. This gives the generation function for this class as

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

Putting the three cases together, we get the generating function (1) for $T(t,u)$.

Solve this generating function for $T\left(t,u\right)$ using the Kernel Method:

From

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

we can get

$$\begin{aligned}&(1-tu)\left(u - tu - t - t^2u^2 + t^3u\right)T(t,u)\\&= (u-t)(1-tu)(1+tu) - T(t,t)\left(1-tu\right)t\left(2t-u\right)\end{aligned}$$

Set $(1-tu)\left(u - tu - t - t^2u^2 + t^3u\right) = 0$, then there is only one *power series* solution for u

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

Let U be this solution,

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

Set

$$(1+tu)(u-t)(1-tu) + T(t,t)\left(1-tu\right)t\left(u-2t\right) = 0,$$

and replace u by U:

$$T(t,t) = (1+tU)\,\frac{t-U}{t\left(U-2t\right)}. \tag{3}$$

From

$$\begin{aligned}&(1-tu)\left(u - t - tu - t^2u^2 + t^3u\right)T(t,u)\\&= (u-t)(1-tu)(1+tu) - T(t,t)\left(1-tu\right)t\left(2t-u\right)\end{aligned}$$

get

$$T(t,u) = \frac{(t-u)(1-tu)(1+tu) + T(t,t)\left(1-tu\right)t\left(2t-u\right)}{\left(1-tu\right)\left(u - t - tu - t^2u^2 + t^3u\right)}.$$

Replace $T(t,t)$ by (3). Now

$$T(t,u) = \frac{(1+tu)(u-t)}{u-t-tu-t^2u^2+t^3u} - \frac{(1+tU)(U-t)(1-tu)(u-2t)}{(U-2t)(1-tu)(u-t-tu-t^2u^2+t^3u)}$$

where $U(t)$ has been defined in (2).

Sequence 11

Notice that $T(t,1)$ is the generating function of the number of two-sided n-step prudent walks ending on the top side of their box avoiding both patterns $\leftarrow^{\geq 2}$, $\downarrow^{\geq 2}$, taking steps from $\{\uparrow,\downarrow,\leftarrow,\rightarrow\}$, thus $T(t,1) =$

$$\frac{(1-2t)(1-t)\sqrt{(1-t-t^3)^2-4t^4}-(1+t)(1-7t+14t^2-11t^3+10t^4-4t^5)}{2t(1-2t-t^2+t^3)(1-2t-2t^3)}$$
$$= 1+3t+6t^2+15t^3+35t^4+83t^5+195t^6+460t^7+1085t^8+...$$

Sequence 12

Note that $T(t,0)$ is the generating function of the number of two-sided n-step prudent walks ending at the north-east corner of their box avoiding both patterns $\leftarrow^{\geq 2}$, $\downarrow^{\geq 2}$, taking steps from $\{\uparrow,\downarrow,\leftarrow,\rightarrow\}$, so $T(t,0) =$

$$\frac{(1-t)\sqrt{(1-t-t^3)^2-4t^4}-1+3t-t^2+t^3+t^4}{(1-2t-2t^3)\,t}$$
$$= 1+2t+4t^2+10t^3+24t^4+56t^5+130t^6+304t^7+714t^8+1678t^9+...$$

Sequence 13

Furthermore, $2T(t,1)-T(t,0)$ is the generating function of the number of two-sided n-step prudent walks ending on the top side or right side of their box avoiding both patterns $\leftarrow^{\geq 2}$, $\downarrow^{\geq 2}$, taking steps from $\{\uparrow,\downarrow,\leftarrow,\rightarrow\}$, thus $2T(t,1)-T(t,0) =$

$$\frac{t(1-t)^2\sqrt{(1-t-t^3)^2-4t^4}+1-t-2t^2-2t^3-2t^4+4t^5-t^6}{(1-2t-t^2+t^3)(1-2t-2t^3)}$$
$$= 1+4t+8t^2+20t^3+46t^4+110t^5+260t^6+616t^7+1456t^8+3442t^9+...$$

Open Problem 1

What is the number of two-sided n-step prudent walks, ending on the top side of their box, avoiding both $\leftarrow^{\geq k}$, and $\downarrow^{\geq k}$ ($k>2$) taking steps from $\{\uparrow,\downarrow,\leftarrow,\rightarrow\}$?

The generating function satisfies:

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

where u counts the distance between the endpoint and the north-east corner of the box. For $k=3$,

$$\frac{u-t-t^2u^2+t^3u-t^3u^3+t^4u^2-t^4u^4+t^5u^3-tu}{u-t}T(t,u)$$
$$=1+tu+t^2u^2+t^3u^3+\frac{u-2t}{u-t}tT(t,t)$$

i.e.,

$$(-t+\left(1+t^3-t\right)u+\left(t^4-t^2\right)u^2+\left(t^5-t^3\right)u^3+-t^4u^4)T(t,u)$$
$$=(1+tu+t^2u^2+t^3u^3)(u-t)+t\,(u-2t)\,T(t,t).$$

Set $-t+(1+t^3-t)\,u+(t^4-t^2)\,u^2+(t^5-t^3)\,u^3-t^4u^4=0$, and solve for u, as a power series of t. We obtained the first one hundred terms for u, beginning with

$$u=t+t^2+t^3+t^4+2t^5+4t^6+8t^7+16t^8+33t^9+69t^{10}+...$$

Using this u, we can get many examples for the sequence.

Open Problem 2

What is the number of two-sided n-step prudent walks, ending on the top side of their box, exactly avoiding both $\leftarrow^{=2}$, $\downarrow^{=2}$, taking steps from $\{\uparrow,\downarrow,\leftarrow,\rightarrow\}$?

The generating function is

$$(1-\frac{t^2u}{1-tu}-\frac{tu}{u-t}+u^2t^3)T(t,u)=\frac{1}{1-tu}-u^2t^2+\frac{u-2t}{u-t}tT(t,t).$$

We do not have a solution to this equation.

References

[1] M. Bousquet-Mélou, A.J. Guttmann and I. Jensen, Self-avoiding walks crossing a square, J. Phys. A **38** (2005) 9159–9181.

[2] M. Bousquet-Mélou, Families of prudent self-avoiding walks, J. of Combinatorial Theory, Series A **117** (2010) 313–344.

[3] A.R. Conway and A.J. Guttmann, Square lattice self-avoiding walks and corrections to scaling, Phys. Rev. Lett. **77** (1996), 5284–5287.

[4] J.C. Dethridge and A.J. Guttmann, Prudent self-avoiding walks, Entropy **10** (2008), 309–318.

[5] K.E. Donald, Science **194** (1976) 1235.

[6] E. Duchi, On some classes of prudent walks. In Proceedings of the FPSAC'05, Taormina, Italy, (2005).

[7] T.M. Garoni, A.J. Guttmann, I. Jensen and J.C. Dethridge, Prudent walks and polygons, J. Phys. A **42** (2009), 095205.

[8] L.F. Gregory, Intersections of Random Walks. Birkhäuser (1996).

[9] A.J. Guttmann (Ed.), Polygons, Polyominoes and Polycubes, Springer (2009).

[10] J. Iwan, Enumeration of self-avoiding walks on the square lattice J. Phys. A **37** (2004) 5503-5524.

[11] E.J. Janse van Rensburg, Monte Carlo methods for the self-avoiding walk, (Topical Review) J. Phys. A **42** (2009), 323001.

[12] M. Neal and S. Gordon, The Self-Avoiding Walk. Birkhäuser (1996).

[13] P. Préa, Exterior self-avoiding walks on the square lattice, (1997) (manuscript).

[14] R. P. Stanley, Enumerative Combinatorics I, Wadsworth & Brooks/Cole (1986).