Some new self-avoiding walk and polygon models

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Abstract

We study the behaviour of prudent, perimeter and quasi-prudent self-avoiding walks and polygons in both two and three dimensions, as well as some solvable subsets. Our analysis combines exact solutions of some simpler cases, careful asymptotic analysis of functional equations which can be obtained in more complicated cases and extensive numerical studies based on exact series expansions for less tractable cases, augmented by long Monte Carlo runs in some cases.

1 Introduction

A long standing problem in combinatorics is to find the generating function for self-avoiding walks (SAW) on a two-dimensional lattice, enumerated by length, and of self-avoiding polygons (SAP) enumerated by either perimeter or area or both. At first sight it is surprising that, for these problems, an exact solution has not been found. Recently, we have gained a greater understanding as to the difficulty of these problems, as Rechnitzer [14] has *proved* that the (anisotropic) generating function for square lattice self-avoiding polygons is not differentiably finite (D-finite) [16], confirming a result that had been previously *conjectured* on numerical grounds [11].

In the absence of an exact solution, researchers have looked for simpler, solvable models that hopefully still preserve many of the essential features of the original problem. Furthermore, many of those simpler models are of interest in their own right. There are many non-trivial simplifications of the self-avoiding walk or polygon problem that are solvable [3], but most of the simpler models impose an effective directedness or equivalent constraint that reduces the problem, in essence, to a one-dimensional problem, and most such problems are known to have D-finite solutions.

We have recently studied several families of walks and polygons that are closer, in some sense, to SAW and SAP than most previously solved models. The models

+This article is dedicated to the memory of Philippe, who sadly passed away on March 22, 2011, before this paper was completed.

considered are called *prudent walks* (and polygons), *perimeter walks* (and polygons) and *quasi-prudent walks* (and polygons).

2 Prudent walks and polygons

2.1 Prudent walks

Prudent walks were introduced to the mathematics community by Préa in an unpublished manuscript [13] and more recently reintroduced by Duchi [6]. A prudent walk is a connected path on the square lattice $\mathbb{Z}^2$ 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. We enumerate prudent walks by the number of steps n. We take the empty walk of length zero, given by the vertex $(0,0)$, to be a prudent walk. The definition of prudent walks extends naturally to hyper-cubic lattices $\mathbb{Z}^d$. Figure 1 shows a typical prudent walk of $n = 2000$ steps, generated via Monte Carlo simulation using a pivot algorithm [12]. Note the roughly linear behaviour – it is believed, although unproven, that the mean-square end-to-end distance grows like n^2 for prudent walks. An equivalent statement is that the fractal dimension is 1. (For SAW it is 4/3.)

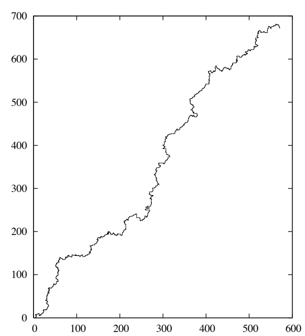


Figure 1: Typical prudent walk of $n = 2000$ steps, generated via Monte Carlo simulation using a pivot algorithm.

The *bounding box* of a prudent walk is the minimal rectangle containing the walk. The bounding box may reduce to a line or even to a point in the case of the empty walk. One significant feature of any two-dimensional prudent walk is that the end-point is always on the boundary of the bounding box. Each step either lies along the boundary perimeter, or extends the bounding box. Note that this is not a characterisation of prudent walks – there are walks such that each step lies on the perimeter of the bounding box that are not prudent. This observation led to the definition of *perimeter walks*, defined by the requirement that each step lies on the perimeter of the bounding box, which are discussed below. The simplest example of a perimeter walk which is *not* a prudent walk is the walk with steps NEESW, that is the walk, , where the last

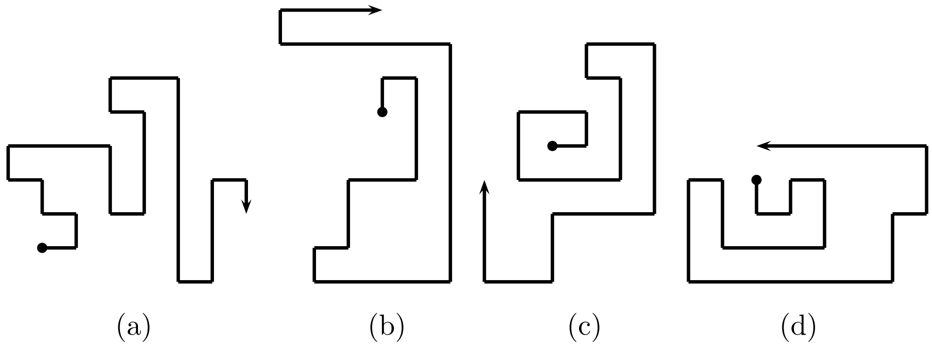


Figure 2: Typical examples of: (a) a two-sided prudent walk, (b) a three-sided prudent walk, (c) a general prudent walk, and (d) a four-sided prudent polygon.

west step breaks the prudent restriction since it steps in the direction of the occupied vertex at the origin.

Furthermore, if one extends the definition of prudent walks to three-dimensional walks, then *it is not true* that each step of the walk lies on the perimeter of the bounding box. Again, one can define three-dimensional walks with the property that each step lies on the perimeter of the bounding box, and these too will be discussed.

Another feature of prudent walks that should be borne in mind is that they are, generally speaking, not reversible. If a path from the origin to the end-point defines a prudent walk, it is unlikely that the path from the end-point to the origin will also be a prudent walk. Ordinary SAW are of course reversible.

The problem proposed by Préa was subsequently revived by Duchi [6] who also studied two proper subsets, called *two-sided prudent walks* and *three-sided prudent walks* (see Figure 2 for examples). Two-sided prudent walks are prudent walks which, after every step, must end on the north or east sides of the current bounding box. Equivalently, they are prudent walks in which it is forbidden for a west step to be followed by a south step, or a south step to be followed by a west step.

Three-sided prudent walks must end on the north, east or south sides of their bounding box. Equivalently, three-sided prudent walks are prudent walks in which it is forbidden for a west step to be followed by a south step when the walk visits the top of its bounding box and a west step followed by a north step when the walk visits the bottom of its bounding box. Duchi found the solution for two-sided prudent walks, and gave functional equations for the generating function of (unrestricted) prudent walks. More recently the problem has been revisited by Bousquet-Mélou [4], who gave a systematic treatment of all three types, and in particular gave a solution for the generating function of three-sided prudent walks, and also gave the solution for the analogous problem on the triangular lattice.

For unrestricted prudent walks, the functional equation has three catalytic variables, and we have been unable to solve it. However it yields a polynomial-time algorithm for the generation of the coefficients, and Guttmann and Dethridge [5] analysed the series given by the first 400 terms of the generating function. For all three cases, two-sided, three-sided and unrestricted prudent walks it was found that the generating function had a simple-pole singularity, located at the real, positive zero of the polynomial $1 - 2x - 2x^2 + 2x^3$, or numerically at $x_c = 0.4030317\ldots$[1] (this is a rigorous statement only for the two solvable cases. For unrestricted prudent SAW it is a consequence of numerical analysis). One has

$$c_n^{(a)} \sim \lambda^{(a)} (x_c^{(a)})^{-n}$$

where $a = 2, 3, 4$ corresponds to two-, three- and unrestricted prudent SAW respectively. We have $\lambda^{(2)} = 2.5165\ldots$, $\lambda^{(3)} = 6.33\ldots$, $\lambda^{(4)} = 16.12\ldots$.

The generating function for two-sided prudent walks is an algebraic function, while for three-sided prudent walks it is not algebraic, and not D-finite. It is a function of q-series, and there is an infinite sequence of poles lying on the positive real axis between x_c and $x = \sqrt{2} - 1$. The nature of the solution for unrestricted prudent walks is not known, but is likely to be at least as complicated as that for three-sided prudent walks.

We have also carried out numerical studies of prudent walks in three dimensions, by enumerating them by a simple backtracking algorithm [9]. Let c_n denote the number of n-step prudent walks on the three-dimensional simple-cubic lattice. We found for the generating function

$$C(x) = \sum c_n x^n \sim const.(1 - x/x_c)^{-\gamma}, \tag{1}$$

where $x_c = 0.22265 \pm 0.00001$ (where the error bars are confidence limits, rather than rigorous bounds), and $\gamma = 1.68 \pm 0.03$, and is unlikely to be rational. For SAW, the analogous critical values are $x_c \approx 0.2134907$ and $\gamma \approx 1.1567$, so again we see that prudent walks are exponentially rare among SAW. Another property of interest is the mean square end-to-end distance,

$$\langle R_e^2 \rangle_n = \sum_\omega r_\omega^2 / c_n,$$

where ω labels the set of all c_n n-step SAW. This property defines a critical exponent $\nu = 1/d_f$, where d_f is the *fractal dimension* of the object from the relation

$$\langle R_e^2 \rangle_n \sim const. \cdot n^{2\nu}.$$

Series analysis allows us to estimate $\nu \approx 0.76$ for three-dimensional prudent walks. As already mentioned, two-dimensional prudent walks (and perimeter and quasi-prudent walks, considered below), all have $\nu = 1$. This is a conjecture which is undoubtedly true, but has not been proved.

2.2 Prudent polygons: two- and three-sided

2.2.1 Perimeter generating function

We define n-step prudent polygons, as usual, as $(n-1)$-step prudent walks that end at a vertex adjacent to their starting point. Then the addition of a single bond gives an n-step polygon. The polygon version of the problem was introduced in [9] and studied

[1] For SAW the corresponding singularity is located at $x_c = 0.37905227\ldots$, so prudent walks are an exponentially small subset of SAW.

in detail by Schwerdtfeger [15] who solved the problem in the case of the *perimeter* generating function of two-sided and three-sided prudent polygons, using a method of solution similar to that used by Bousquet-Mélou for the walk case.

Let $p_n^{(a)}$ denote the number of n-step prudent polygons, where a indexes the number of sides. For $a = 2$ these are simply bargraph polygons, and as shown by Schwerdtfeger, the perimeter generating function required is [15]

$$P_2(x) = \frac{1}{x}\left(\frac{1-3x+x^2+3x^3}{1-x} - \sqrt{(1-x)(1-3x-x^2-x^3)}\right) = \sum_n p_n^{(2)} x^n.$$

So the asymptotics are given by

$$p_n^{(2)} \sim const. \cdot n^{-3/2} (x_c^{(2)})^{-n} \quad (n \text{ even})$$

and $p_n^{(a)} = 0$ for n odd. Here $x_c^{(2)} = 0.54368902\ldots$ is the square-root of the positive root of $1-3x-x^2-x^3$. For three-sided prudent polygons, Schwerdtfeger showed that the solution was a non D-finite function of q-series, just as for three-sided prudent walks. The dominant asymptotics are similar to those of two-sided prudent polygons, with the same exponent but a different critical point. One has

$$p_n^{(3)} \sim const. \cdot n^{-3/2} (x_c^{(3)})^{-n} \quad (n \text{ even}),$$

where $x_c^{(3)} = 0.494096\ldots$, which is the positive root of $x^5 + 2x^2 + 3x - 2$.

2.2.2 Area generating function

Next we consider the behaviour of prudent polygons enumerated by *area* rather than perimeter. That case is in one sense easier, in that as we move from two-sided, to three-sided to four-sided, the exponential growth factor $\mu = 1/x_c$ remains unchanged (at exactly 2). For perimeter enumeration, x_c changes as we move through the same cycle of models. While for the four-sided case, enumerated by area, we cannot solve the problem, we do at least know (more precisely, conjecture) the exact value of x_c. This makes the series analysis more precise than in the perimeter enumeration case.

Two-sided prudent polygons must end at $(0, 1)$ or $(1, 0)$, and since reflection in the line $y = x$ converts polygons ending at one of those points to the other, we need only consider those ending at $(0, 1)$. Polygons traversed in a clockwise direction are just a row of cells and thus have a trivial generating function; those traversed in an anti-clockwise direction are bargraphs, whose generating function is

$$B(q) = \frac{q}{1-2q}.$$

So the overall area generating function for two-sided prudent polygons is

$$A_2(q) = \frac{2q(2-3q)}{(1-q)(1-2q)} = \sum_{n\geq 0} (2^n + 2) q^n,$$

and hence the generating function singularity is a simple pole at $q = 1/2$, and the amplitude is exactly 1. An example of a prudent SAW leading to a two-sided prudent polygon is shown in Figure 3.

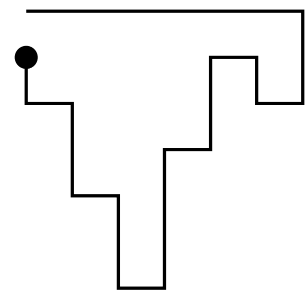


Figure 3: A prudent SAW corresponding to a two-sided prudent SAP.

We turn now to the more interesting case of three-sided prudent polygons, an example of which is shown in Figure 4. These can end at $(0,1),(1,0)$ or $(-1,0)$. Those ending at $(0,1)$ (in either direction) are just bargraphs, whose generating function is given above. Polygons ending at $(-1,0)$ or $(1,0)$ are related by reflection in the y-axis, so we consider only the former case.

A polygon ending at $(-1,0)$ in a clockwise direction is just a single column, and thus has a trivial area generating function. The anti-clockwise case, however, is the interesting one – here, we divide the polygons into two classes and use a recursive algorithm. In order to implement this algorithm we need to keep track of the *width* of each polygon, and so we introduce a new *catalytic variable* u to do so.

The first class consists of those polygons which never step above the line $y = 1$: these are just bargraphs whose first column has height one. The generating function of these objects is the first term on the RHS of (2).

On the other hand, polygons which *do* step above the line $y = 1$ can be constructed by adding a row to the top of another three-sided polygon, and possibly an additional bargraph to the rightmost end of this new row. In order to ensure that the extra bargraph does not violate the prudent condition, we must first make sure that the new row is at least as wide as the polygon below it – hence the need to track the width of each polygon. The generating function of these polygons is given by the second and third terms on the RHS of (2).

Since all polygons ending at $(-1,0)$ in an anti-clockwise direction fall into one of these two classes, adding their generating functions must give the overall generating function A_3^*, and so we obtain

$$A_3^*(q,u) = \frac{qu(1-q)}{1-q-qu} + \frac{q}{1-q}(A_3^*(q,u) - A_3^*(q,qu)) + \frac{qu(1-q)}{1-q-qu}A_3^*(q,qu) \qquad (2)$$

This functional equation can be solved by iteration, and after setting $u = 1$ and accounting for the other simpler cases (polygons ending at $(0,1)$ etc.), we find

$$A_3(q) := A_3(q,1) = \frac{-2q^3(1-q)^2}{(1-2q)^2}\sum_{n=1}^{\infty}\frac{(-1)^n q^{2n}}{(1-2q)^n}a(q;q^n) + \frac{2q(3-10q+9q^2-q^3)}{(1-2q)^2(1-q)}, \quad (3)$$

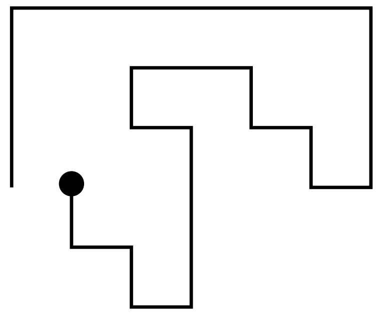


Figure 4: A prudent SAW corresponding to a three-sided prudent SAP.

where

$$a(q;z) = \frac{-(1-2q)(v;q)_\infty(uz;q)_\infty}{q^2(1-q-qz)(vz;q)_\infty(u;q)_\infty};\ u = \frac{q}{1-q},\ v = \frac{1-q+q^2}{1-q}. \tag{4}$$

As usual

$$(u;q)_\infty = \prod_{n=0}^{\infty}(1-uq^n).$$

To determine the asymptotics, our first line of attack was to generate 500 terms in the series expansion, and apply the usual methods of series analysis [10]. The results of that analysis gave $a_n^{(3)} \approx \lambda \times n^g \times 2^n$, with $\lambda \approx 0.108$ and $g \approx 1.585$. This seemed such an unlikely exponent that we decided to perform a careful asymptotic analysis of the generating function, using the Mellin transform methods described in Appendix B.7 of [8].

The details of these calculations can be found in [1, 2]; the salient point is that the relevant singularities of the Mellin transform of $A_3(q)$, which determine the singular behaviour of the generating function near the singularity $q = 1/2$, occur at

$$s_k = \log_2 3 - 1 + 2k\pi i,\ k \in \mathbb{Z}. \tag{5}$$

The largest contribution to the singular behaviour comes from the real Mellin transform singularity s_0, which leads to the approximation

$$A_3(q) \underset{q\to 1/2}{\sim} \frac{\pi(3/2;1/2)_\infty(1/3;1/2)_\infty}{9\log 2\sin\pi s_0(1/2;1/2)_\infty^2} \times \frac{1}{(1-2q)^{s_0}}. \tag{6}$$

Thus we expect the asymptotics to behave, in the usual way, as

$$a_n^{(3)} \sim \kappa \cdot n^g \cdot 2^n$$

where

$$\kappa = \frac{\pi(3/2;1/2)_\infty(1/3;1/2)_\infty}{9\log 2\sin\pi s_0(1/2;1/2)_\infty^2\Gamma(s_0+2)} = 0.1083842947\ldots \tag{7}$$

and

$$g = s_0 + 1 = \log_2 3 = 1.584962501\ldots$$

in seemingly good agreement with our series analysis. However there are two surprises. The first is the transcendental value of the exponent. This is very rare for two-dimensional lattice models. What is even rarer is seen if we consider further terms in the asymptotics. In particular, recall that only the the term $k = 0$ in (5) was taken. If we now include the next two terms, corresponding to $k = \pm 1$ we get an additional term, to be added to our first approximation, of the form

$$\kappa' \cdot n^g \cdot 2^n$$

where

$$\kappa' \approx c(\cos(2\pi \log_2 n) + \sin(2\pi \log_2 n)) \tag{8}$$

where $c \approx 10^{-9}$. Taking $k = \pm 2$ adds a further oscillatory term with an even smaller amplitude. Thus we see that the leading amplitude does not, in fact exist. That is to say, the limit

$$\lim_{n\to\infty} \frac{a_n^{(3)}}{n^g \cdot 2^n}$$

doesn't exist! Numerically, we would be unlikely to ever observe this (without prior knowledge of this behaviour), as the "effective amplitude" is indeed given by (7), and varies from this value as n increases by no more than about 1 part in 10^8. Knowing that this term is present, and having available very long series of hundreds of terms, it is possible to see clear numerical evidence of this [1]. Such oscillatory behaviour is classical in the analysis of digital trees and related structures [7], but to the best of our knowledge this is the first time it has been shown to occur in the context of lattice models.

The sub-dominant term in the asymptotic expansion is expected to be proportional to $n \cdot 2^n$. It is possible to calculate the coefficient of this term also, and it is identically zero. It is not subject to an additional oscillatory component. The next terms we expect are proportional to $n^{g-1} \log n$ and n^{g-1}, and the 'coefficients' of these terms will oscillate in a similar manner to the leading term. In fact, it is relatively straightforward to calculate the constant (non-oscillating) components of arbitrarily many sub-dominant terms – see [2] for further details. Consequently, if we ignore the minute oscillatory components, the asymptotic expansion of $a_n^{(3)}$ has the form

$$\begin{aligned} a_n^{(3)} \sim 2^n(0.1083842947 \cdot n^g - 0.3928066917 \cdot n^{g-1} \log n \\ + 0.5442458535 \cdot n^{g-1} + \mathrm{O}(n^{g-2} \log n)) \end{aligned}$$

2.3 The full problem: four-sided prudent polygons

For the unrestricted, or four-sided case, Garoni et al [9] used a transfer-matrix formulation to generate the first 500 terms in the generating function (equivalent to 1000 step polygons). Schwerdtfeger [15] subsequently gave an equivalent, but more elegant, functional equation for the four-sided case. A prudent SAW leading to a four-sided prudent polygon is shown in Figure 2(d).

In the perimeter case, Garoni et al gave an analysis of the 500 term series. Despite the substantial length of the series, the results were not as precise as one might have expected. The number of polygons of perimeter n was found to grow like

$$p_n^{(4)} \sim const. \cdot n^{-\gamma}(x_c^{(4)})^{-n} \quad (n \text{ even}),$$

where $x_c^{(4)} \approx 0.4759$, and $\gamma \approx 3.5$ were estimated. In [9] an analysis of the critical behaviour of three-dimensional prudent polygons was also given, but because only 11 non-zero terms in the generating function are known, the results are rather imprecise.

For unrestricted prudent polygons enumerated by area, we have constructed a functional equation. Polygons ending at $(1,0)$ in a clockwise direction can be rotated and/or reflected to give all other four-sided polygons, so the generating function for these polygons is precisely $1/8$ of the overall generating function. We partition this sub-class of polygons into three classes $\mathcal{X}, \mathcal{Y}$ and $\mathcal{Z}$, with respective generating functions $X(q,u,v), Y(q,u,v)$ and $Z(q,u,v)$. In all three cases q measures area; for $\mathcal{X}$, u measures width and v measures height; for $\mathcal{Y}$, u measures height and v measures width; and for $\mathcal{Z}$, $(u+1)$ measures width and v measures height. We find that

$$\begin{aligned} X(q,u,v) = \frac{qv}{1-q}[X(q,u,v) - X(q,qu,v)] + \frac{qv}{1-q}[Y(q,v,u) - Y(q,v,qu)] \\ + \frac{quv}{1-q}[Z(q,u,v) - qZ(q,qu,v)] \end{aligned} \tag{9}$$

$$\begin{aligned} Y(q,u,v) = quv + \frac{qv}{1-q}[Y(q,u,v) - Y(q,qu,v)] + \frac{qv^2}{1-q}[Z(q,v,u) - Z(q,v,qu)] \\ + quv[X(q,qv,u) + Y(q,u,qv) + qvZ(q,qv,u)] \end{aligned} \tag{10}$$

$$Z(q,u,v) = \frac{qv}{1-q}[Z(q,u,v) - Z(q,qu,v)] + qvY(q,qv,u) + quvZ(q,u,qv) \tag{11}$$

An explanation of the sub-classes $\mathcal{X}, \mathcal{Y}$ and $\mathcal{Z}$ and the derivation of this equation is given in [1], and is based on a construction by Schwerdtfeger [15]. We are unable to solve this functional equation, nor extract its asymptotics. Accordingly, we turn to series analysis. The functional equation can be iterated to generate long series, with more than 800 terms, in polynomial time. Indeed, the complexity is $\mathrm{O}(n^4)$. The first few terms $a_1, \ldots, a_{15}$ are

$$8, 16, 40, 96, 232, 560, 1336, 3176, 7480, 17528, 40776, 94336, 216976, 496432, 1130120.$$

The full series can be found at www.ms.unimelb.edu.au/˜tonyg. We cannot say if we will have the same phenomenon of a non-existent critical amplitude in this case, but even if so, it won't affect our numerical study, which is too crude to detect possible effects of the magnitude observed for the three-sided case.

We have used a variety of techniques of series analysis [10], including the method of differential approximants, and standard sequence extrapolation algorithms to estimate the critical exponent. Assuming $a_n \sim \lambda \cdot 2^n \cdot n^{g_4}$, in order to estimate the exponent g_4 we extrapolated the sequence

$$n(a_n/(2 \cdot a_{n-1}) - 1)n \sim g_4.$$

This sequence is very slowly converging, despite the fact that we have some 800 terms in the sequence. The best we can do is estimate $2.58 < g_4 < 2.61$, where, as is usual in series analysis, the bounds are confidence limits and are not rigorous. It is tempting to conjecture that the exponent g_4 in this case is just 1 greater than that for the three-sided case, so that $g_4 = 1 + \log_2(3) = 2.58496\ldots$.

We have investigated this conjecture with some success. Firstly, we considered the Hadamard quotient of the series for four-sided polygons and that of the derivative of the series for three-sided polygons. Differentiation increases the exponent by 1. If the conjecture is true, the coefficients of the Hadamard product should tend to a constant. With 800 terms in the quotient series, the ratio does seem to be approaching a constant. If $p_n^{(3)}$ denotes the number of three-sided polygons of area n and $p_n^{(4)}$ denotes the number of four-sided polygons of area n, extrapolating the Hadamard product $h_n = n \cdot p_n^{(3)}/p_n^{(4)}$ against $1/\sqrt{n}$, we find a limit of 3.25 ± 0.05. Next, we tested the assumption that the asymptotics for the four-sided case is just given by the derivative of the three-sided case. We fitted successive quartets of coefficients $a_j, a_{j+1}, a_{j+2}, a_{j+3}$ to

$$2^n(\kappa \cdot n^{g_4} + \kappa_1 \cdot n^2 + \kappa_2 \cdot n^{g_4-1} \log n + \kappa_3 \cdot n^{g_4-1}).$$

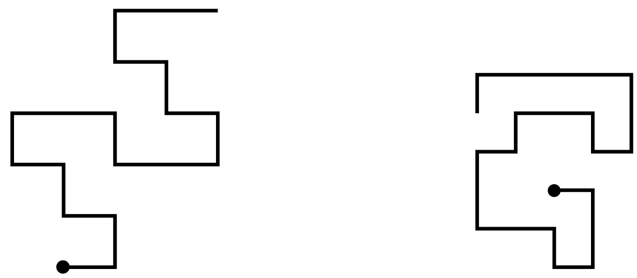
Estimates of κ are well-converged to $\kappa \approx 0.03341 \pm 0.00003$. This implies that the "amplitude" of the three-sided polygons should be $0.03341 \pm 0.00003 \times 3.25 \pm 0.05 = 0.108 \pm 0.002$ which agrees well with the direct estimate, calculated above, of $0.108384\ldots$. On balance, we believe the conjecture is more likely to be true than not. In the table below we summarise our results for the case of prudent walks, and also polygons enumerated by both perimeter and area. The blank entries could be filled, but are not considered to give much new insight, so we haven't done the necessary calculations.

Prudent model	Walks $A\mu^n \cdot n^g$			Polygons by perimeter $B\kappa^n \cdot n^h$			Polygons by area $C\tau^n \cdot n^f$		
# sides	A	μ	g	B	κ	h	C	τ	f
1 sided		2.4142	0						
2 sided	2.5165	2.481194	0		1.83928	-3/2	1	2	0
3 sided	6.33	2.481194	0		2.02389	-3/2	0.10838	2	1.58496
4 sided	16.12	2.481194	0		2.1013	$\approx -7/2$	0.03341	2	2.58496
3 dim.		4.4913	≈ 0.68		≤ 4.491	≈ -3.5			$\nu \approx 0.76$

3 Perimeter walks and polygons

A feature of prudent walks is that they always lie on the perimeter of their minimum bounding box. This suggests another model, which we call *perimeter walks*, in which the definition is that, at each step, the walk must lie on the perimeter of its bounding rectangle. Thus, such walks are a superset of prudent walks, as every prudent walk is a perimeter walk, but not vice versa[2]. We show examples of two-sided and unrestricted perimeter walks in Figure 5.

[2] This is not true in three dimensions, as prudent walks in $\mathbb{Z}^3$ do not have to have each step on surface of its bounding box.



(a) (b)

Figure 5: Examples of (a) a two-sided perimeter walk and (b) an unrestricted perimeter walk.

For one-sided perimeter walks, the generating function is the same as in the case of one-sided prudent walks. They are just partially directed walks, and the length generating function is

$$C(x) = \frac{1+x}{1-2x-x^2} = \sum c_n^{(1)} x^n,$$

so the generating function has a simple pole singularity. More precisely, $c_n^{(1)} \sim const. \times \mu_1^n$, where $\mu_1 = 1 + \sqrt{2}$.

The perimeter generating function for two-sided perimeter walks, $\sum c_n^{(2)} x^n$, is rather more difficult to calculate. We find it to be a complicated function involving sums and products of rational functions of q-series, and some non-rational terms. Its asymptotic behaviour is however comparatively simple, and it is found to have a simple pole singularity, more precisely $c_n^{(2)} \sim const. \times \mu_2^n$, where $\mu_2 = 2.50399663 \cdots$.

For three-sided and unrestricted perimeter walks we must resort to numerical studies. We can write down (complicated) functional equations, and these can be iterated to obtain many terms in the generating function. There are then standard methods [10] to estimate the asymptotics from the known terms of the generating function. In this way we are able to conjecture (but not prove) that the growth constant μ for both three-sided and unrestricted perimeter walks is the same as that for two-sided walks (which can, in principle, be calculated, to arbitrary accuracy from the solution of the two-sided case, though the calculation is non-trivial). We also find numerically, and conjecture, that the nature of the singularity is just a simple pole. So just as we found for prudent walks, we find that the growth constant for perimeter walks is the same for two-sided, three-sided and unrestricted walks, as is the critical exponent, which corresponds to a simple pole singularity. Only the amplitude changes as we move from two-sided to unrestricted walks.

Just as we did for prudent walks, we can define a polygon subset of perimeter walks. For two sided perimeter polygons, enumerated by perimeter, we have calculated the generating function. It is

$$P(x) = \sum p_n x^n = 1 - 4x + x^2 + \frac{(-1+5x+x^2+x^3)\sqrt{1-x}}{\sqrt{1-3x-x^2-x^3}}. \tag{12}$$

Asymptotically, one has $p_n \sim const. \times \mu^{2n} \cdot n^{-1/2}$, where $1/\mu^2 = 1/3.38297576\ldots$ is the positive root of $1 - 3x - x^2 - x^3$. Thus $\mu = 1.83928675\ldots$. Two-sided perimeter polygons can also be enumerated by area, and we have calculated that generating function. It is

$$A(y) = \sum a_n q^n = \frac{2q(2-4q+q^2)}{(1-2q)^2} = 4q + \sum_{n>1}(n+6)2^{n-2}q^n, \tag{13}$$

from which the asymptotics are obvious. We have also calculated the functional equation for three-sided perimeter polygons, but this has too many catalytic variables for us to solve. For those cases we turn to numerical methods. For three-sided perimeter polygons enumerated by perimeter we have some 170 terms in the series. It is straightforward to analyse this series by standard methods, and we find the asymptotic behaviour

$$p_n^{(3)} \sim const. \times \mu^{2n} \cdot n^{-1/2},$$

where $\mu^2 = 4.096156888\ldots$ and $1/\mu^2$ is conjectured to be the positive root of $2 - 3x - 2x^2 - x^5$. Thus $\mu = 2.02389646\ldots$, exactly as for three-sided *prudent* polygons enumerated by perimeter. As for the two-sided case, we note that this generating function is singular at the same point as the generating function for the corresponding prudent polygon model, but that the exponent differs by 1.

For three-sided perimeter polygons enumerated by area, we have 800 terms in the series. It is clear that the singularity occurs exactly at $q = 1/2$, exactly as for the two-sided case. However the exponent is not easily recognised. Recall that for three-sided prudent polygons enumerated by area we were surprised to find a non-algebraic exponent $(1 + \log_2 3,)$. Here we find the coefficients grow as

$$a_n^{(3)} \sim const. \times 2^n \cdot n^{4.242},$$

where we cannot identify the exponent, except to remark that it is numerically indistinguishable from $3\sqrt{2}$. While this is a useful mnemonic, we have no reason to believe that that is the true exponent. We have also obtained a rough estimate of the amplitude, reported in the Table below.

For four-sided or full perimeter polygons enumerated by perimeter we have only data for polygons of perimeter up to 50 steps (only even numbers of steps are possible). This is too short to obtain reliable estimates of the exponent, though the growth constant we can estimate to be 2.10 ± 0.0, from which we conjecture that it is the same as the growth constant for four-sided prudent polygons, which is known to greater accuracy. It is this latter value we have entered in the table below. Assuming that this is the correct growth constant still does not allow us to give an accurate estimate of the exponent h. Our best estimate is $h \approx -1$, but this is so approximate that we prefer to enter a question mark in the table below.

For full perimeter polygons the exponent estimate is again based on a rather short series, with area up to 44, so should be considered somewhat uncertain, with the last quoted digit being subject to change. We are however confident as to the value of the growth constant. Nevertheless, the uncertainty in the exponent precludes us from giving a useful estimate of the amplitude C in this case.

Perimeter Model	Walks $A\mu^n \cdot n^g$			Polygons by perimeter $B\kappa^n \cdot n^h$			Polygons by area $C\tau^n \cdot n^f$		
# sides	A	μ	g	B	κ	h	C	τ	f
1 sided		2.4142	0						
2 sided		2.503996	0		1.83928	-1/2	1/4	2	1
3 sided	6.33	2.503996	0		2.02389	-1/2	0.0003	2	4.242
4 sided	16.12	2.503996	0		2.1013	?		2	6.2

Our data is still not fully adequate, but a careful study based on the available data supports the view that, as observed for prudent walks, the growth constant and exponent for walks remains unchanged as we change models from two-sided to three-sided to unrestricted perimeter walks.

We have limited data for three-dimensional perimeter walks. We find the asymptotic behaviour of the number of n-step walks to be $const. \cdot \mu^n n^g$, where the growth constant is $\mu \approx 4.33$, and the critical exponent is $g \approx 4$. Thus in three dimensions the perimeter constraint means that the walks are less numerous than prudent walks (for which $\mu \approx 4.4913$), while in two-dimensions they are of course more numerous. This is perfectly understandable, as three-dimensional prudent walks can turn to the interior of the bounding box, whereas perimeter walks cannot. In two dimensions however, prudent walks are a strict subset of perimeter walks.

For perimeter polygons, enumerated by perimeter, the growth constant increases as we move from two-sided to three-sided to unrestricted perimeter polygons, and appears to be the same as for the corresponding prudent model, with an exponent 1 greater.

For perimeter polygons enumerated by area, the critical point remains constant at 1/2 as we move from two- to three- to four-sided polygons, but the exponent increases steadily.

In the Table above we summarise our knowledge of critical points and exponents for perimeter walks and polygons.

4 Quasi-prudent walks and polygons

Quasi-prudent walks are a further superset of perimeter walks. These were, we believe, suggested by Jim Propp in response to a seminar on prudent walks. A quasi-prudent walk is a self-avoiding walk in which it is possible to draw a ray parallel to a lattice axis, from the end-point to infinity, without intersecting the walk. Such walks are, by definition, not trapped. Not all steps lie on the minimum bounding rectangle–they can be in the interior of that rectangle. This complicates the usual definition of one-sided, two-sided etc. Instead, following a suggestion of M Bousquet-Mélou, we consider the *hull* of the walk instead of the box.

The hull is a dynamic construction, and is defined as follows: At each step, one draws the perpendicular bisector of that step. If that bisector hits any other steps of the walk, all sites on the path joining these two steps belong to the hull. Then, if the hull is disconnected, one adds the minimum number of sites to ensure that the hull is connected. One can now define the N side of the hull to be the uppermost row of points in the hull, and similarly for the E, W and S sides. The NE side is then the set of points on the boundary of the hull which connects the N side to the E side,

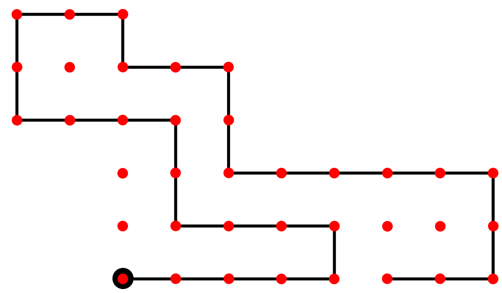


Figure 6: An example of a quasi-prudent walk, showing the *hull* (dotted).

and similarly for NW, SE and SW. A quasi-prudent walk is then one-sided if its hull is empty or if its endpoint always lies on the N side of its hull, and similarly for two-sided, three-sided, etc. So we can talk of k-sided quasi-prudent walks. A quasi-prudent walk and its associated hull is shown in Figure 6.

This problem is significantly more difficult than prudent or perimeter walks. Therefore most of our results are numerical. We have calculated the generating functions for one-sided quasi-prudent walks and polygons. For the former case, the generating function is already a rather complicated algebraic expression. The asymptotics are however quite simple, and we find the number of n-step one-sided quasi-prudent walks grows as

$$c_n \sim const. \times \mu^n,$$

where $\mu = 1 + \sqrt{2}$, and the singularity is a simple pole. For one-sided quasi-prudent polygons, enumerated by perimeter, the asymptotic behaviour is $p_n \sim const. \times \mu^{2n} \cdot n^{-3/2}$, where $1/\mu^2 = 1/4.67589185\ldots$ is the positive root of $4-16x-12x^2-3x^3$. Thus $\mu = 2.16238106\ldots$.

One-sided quasi-prudent polygons enumerated by area can also be calculated. The generating function is

$$A(q) = \sum a_n q^n = 2q\left(\frac{1}{1-q} + \frac{1}{1-3q+q^2}\right) = 4q + 8q^2 + 18q^3 + 44q^4 + 112q^5 + \ldots,$$

so the asymptotic behaviour is $a_n \sim const. \times \mu^n$, where $\mu = (3+\sqrt{5})/2 = 2.61803398\ldots$ is the reciprocal of the smallest positive root of $1 - 3q + q^2$.

To go beyond one-sided walks we need to resort to numerical studies. For unrestricted quasi-prudent SAW, we have generated the first 32 terms of the generating function by a backtracking algorithm. Analysis of those terms allows us to estimate

$$c_n \sim const. \times \mu^n \cdot n^g,$$

where $\mu_1 \approx 2.609$ and $g \approx 1.0$. We conjecture that this is the case for two-sided and three-sided quasi-prudent walks also. We have not yet made further studies of quasi-prudent polygons enumerated by perimeter or area. However our Monte Carlo studies of very long walks (up to 10000 steps) confirm the result that the exponent $\nu = 1$.

5 Conclusion

We have analysed three subsets of self-avoiding walks, prudent, perimeter and quasi-prudent walks. To our disappointment, all appear to have fractal dimension 1, while SAW have fractal dimension 4/3. It would be of great interest to find a solvable model of two-dimensional self-avoiding walks with fractal dimension greater than 1 (and less than 2). However we have found some very interesting properties of three-sided prudent polygons, enumerated by area. This model has an irrational critical exponent, and a non-existent critical amplitude. This last effect is subtle, as the mean amplitude is modified by a periodic additive term that is some 8 or 9 orders of magnitude smaller than the mean. Other models presented involve three (or more) catalytic variables, and present interesting test cases for new methods of solution. Regrettably, we are still no closer to solving the problem of self-avoiding walks and polygons.

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