

Prudent walks and polygons

Timothy M Garoni, Anthony J Guttmann, Iwan Jensen and
John C Dethridge

ARC Centre of Excellence for Mathematics and Statistics of Complex Systems, Department of
Mathematics and Statistics, The University of Melbourne, Victoria 3010, Australia

E-mail: T.Garoni@ms.unimelb.edu.au, T.Guttmann@ms.unimelb.edu.au and
I.Jensen@ms.unimelb.edu.au

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Abstract

We have produced extended series for two-dimensional prudent polygons, based on a transfer matrix algorithm of complexity $O(n^5)$, for a series of n -step polygons. For prudent polygons in two dimensions we find the growth constant to be smaller than that for the corresponding walks, and by considering three distinct subclasses of prudent walks and polygons, we find that the growth constant for polygons varies with class, while for walks it does not. We give exact values for the critical exponents γ and α for walks and polygons, respectively. We have extended the definition of prudent walks to three dimensions and produced series expansions, using a back-tracking algorithm, for both walks and polygons. In the three-dimensional case we estimate the growth constant for both walks and polygons and also estimate the usual critical exponents γ , ν and α .

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1. Introduction

A well-known long standing problem in combinatorics and statistical mechanics is to find the generating function for self-avoiding polygons (or walks) on a two-dimensional lattice, enumerated by perimeter. These models are of considerable physical significance, describing as they do the behavior of long-chain polymers in dilute solution and biological vesicles. As a consequence, thousands of papers have been devoted to aspects of their behavior, and yet we still lack an exact solution for any relevant generating function.

Let $F(z)$ be a formal power series in z with coefficients in \mathbb{C} . It is said to be *differentiably finite* or *D-finite* if there exists a non-trivial differential equation:

$$P_d(z) \frac{d^d}{dz^d} F(z) + \cdots + P_1(z) \frac{d}{dz} F(z) + P_0(z) F(z) = 0, \quad (1)$$

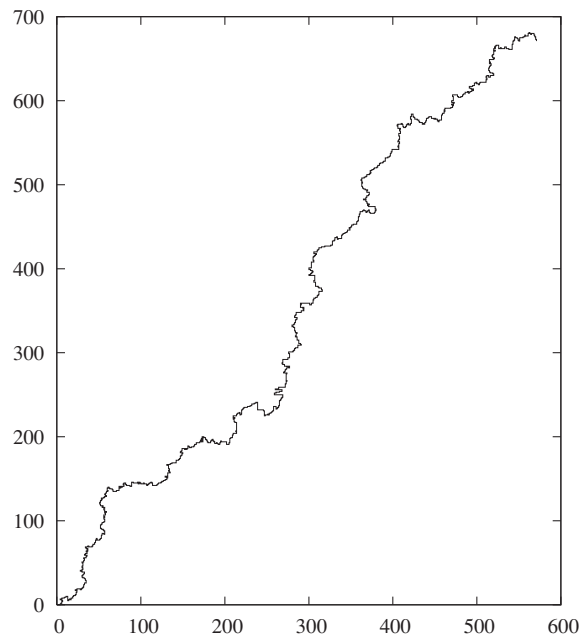


Figure 1. Typical prudent walk of $n = 2000$ steps, generated via Monte Carlo simulation using a pivot algorithm.

with P_j a polynomial in z with complex coefficients [1, 2]. Recently, we have gained a greater understanding of the difficulty of this problem, as Rechnitzer [3] has *proved* that the (anisotropic) generating function for square lattice self-avoiding polygons is not differentially finite (D-finite), confirming a result that had been previously *conjectured* on numerical grounds [4].

The definition of D-finite functions can be extended beyond functions of one variable. Let $G(x, y)$ be a formal power series in y with coefficients that are rational functions of x . Such a series is said to be D-finite if there exists a non-trivial differential equation:

$$Q_d(x, y) \frac{\partial^d}{\partial y^d} G(x, y) + \cdots + Q_1(x, y) \frac{\partial}{\partial y} G(x, y) + Q_0(x, y) G(x, y) = 0, \quad (2)$$

with Q_j a polynomial in x and y with complex coefficients [2].

There are many non-trivial simplifications of the self-avoiding walk or the polygon problem that are solvable [5], but all the simpler models impose an effective directedness or an equivalent constraint that reduces the problem, in essence, to a one-dimensional problem, and all such problems are known to have D-finite solutions.

Prudent walks were introduced to the mathematics community by Pr ea in an unpublished manuscript [6] and more recently have been reintroduced by Duchi [7]. 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 can be generalized 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 [8].

Note the roughly linear behavior—it is believed, although unproven, that the mean-square end-to-end distance grows like n^2 for prudent walks, i.e. that $\nu = 1$.

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 two-dimensional prudent walks is that the end-point of a prudent walk 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 characterization of prudent walks. There are walks such that each step lies on the perimeter of the bounding box that are not prudent. We call such walks *perimeter walks*, and they will be the subject of a future publication [9]. The simplest example of a perimeter walk which is *not* a prudent walk is the walk with steps NEESW, that is the walk, \square , where the last 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, *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 in the aforementioned publication [9].

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.

A related, but not identical, model was proposed more than 20 years ago in the physics literature [10], where it was named the *self-directed walk*. In [10] the authors conducted a Monte Carlo study and found that $\nu = 1$, where $\langle R^2 \rangle_n \sim cn^{2\nu}$. Here $\langle R^2 \rangle_n$ is the mean square end-to-end distance of a walk of length n . They also sketched an argument that the critical exponent γ , characterizing the divergence of the walk generating function $C(x) = \sum c_n x^n \sim A(1 - \mu x)^{-\gamma}$, should be exactly 1, corresponding to a simple pole singularity. This model differs from prudent walks in that different probabilities are assigned to different walks of equal length, depending on the number of allowable choices that can be made at each step. For the problem of prudent walks, all realizations of n -step walks are taken to be equally likely.

The problem proposed by Pr ea was subsequently revived by Duchi [7] who also studied two proper subsets, called *prudent walks of the first type* and *prudent walks of the second type* (see figure 2 for examples). Prudent walks of the first type 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. Equivalently, prudent walks of the first type must end on the northern or eastern sides of the bounding box. Such walks are sometimes referred to as *two-sided prudent walks*.

Prudent walks of the second type 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 to be followed by a north step when the walk visits the bottom of its bounding box. Equivalently, prudent walks of the second type must end on the northern, eastern or southern sides of their bounding box. Such walks are sometimes referred to as *three-sided prudent walks*. Duchi found the solution for prudent walks of the first type and gave functional equations for the generating function of (unrestricted) prudent walks. More recently the problem has been revisited by Bousquet-M elou [11], who gave a systematic treatment of all three types, and in particular gave a solution for the generating function for prudent walks of the second type.

Numerical results for prudent walks (unrestricted) can be found in [12].

In the following section, we give a description of the transfer matrix algorithm used to enumerate prudent walks and polygons. In section 3 we give a summary of known results

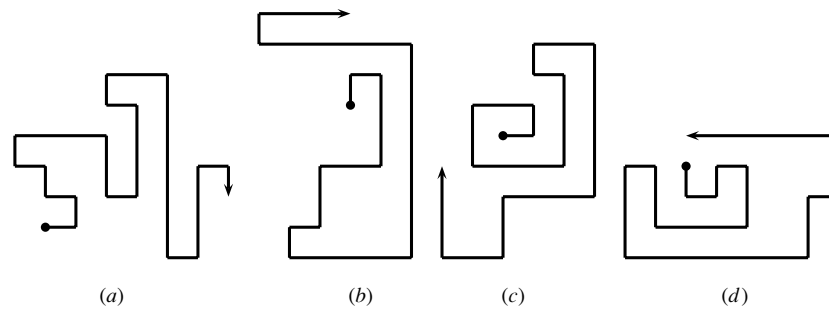


Figure 2. Typical examples of (a) a type-1 prudent walk, (b) a type-2 prudent walk, (c) a general prudent walk and (d) a prudent polygon.

for prudent walks including expressions for the exact generating functions for prudent walks of the first and second kinds as well as a functional equation for the unrestricted problem. Section 4 gives a summary of exact results for two- and three-sided prudent polygons and numerical results from the analysis of the unrestricted prudent polygon generating function. In section 5 we study prudent walks and polygons on the cubic lattice. We give a brief description of the back-tracking algorithm used to calculate the series for the generating functions and analyze these series to obtain numerical estimates for the critical points and exponents α , γ and ν . Finally in section 6 we summarize our findings.

2. Computer enumeration

In two dimensions, we use transfer-matrix algorithms to count the number of prudent walks and polygons. Consider the enumeration of n -step unrestricted prudent walks. Any partially completed walk of say $m < n$ steps is contained within a bounding box, which is the smallest rectangle into which we can fit the walk. It is easy to show that the end-point of the walk must be on a side of this box. The next step must either move away from the box, making it larger, or along the current side, which is possible only if the walk has not already visited vertices lying in that direction.

The transfer-matrix algorithm proceeds by adding a single step to the prudent walk at a time. Given a prudent walk, only a small amount of information about the walk is required in order to determine how to extend the walk by a single step so as to form a longer prudent walk. This information is called a *configuration*. Any partially completed prudent walk corresponds to a unique configuration and there is only a finite number of such configurations. The information needed to describe the configuration of prudent walks is the dimensions of the bounding box, which side of the box the walk end-point is on, the location of the end-point on that side and an integer representing the directions in which the walk is allowed to be extended, i.e. whether there are sites of the walk along the side to the left of the end, to the right of the end or neither (both is not possible.)

For a given configuration, there are three possible steps a walk can take:

- a step outward away from the current side;
- a step to the left along the current side, if there are no walk sites in that direction;
- a step to the right along the current side, if there are no walk sites in that direction.

When we move from a side to a corner of the bounding box, we consider the end point of the walk to have moved to the other side only if that side has been moved outward by the step.

Starting from a walk of size 1 the algorithm progresses by adding a single step at a time until a given maximal length n is reached. During this computation we count the number of walks of intermediate length $m < n$ corresponding to each possible configuration. Any given configuration thus corresponds to an equivalence class of partially completed prudent walks, and when adding a single step to each configuration we are adding a step to each walk in the equivalence class. We keep a list of the possible configurations and the number of walks in the equivalence class of that configuration. The algorithm steps through the list, and for each source configuration s , generates the new target configurations t_j that can be obtained by adding a single step (there are at most three new target configurations t_j per source configuration). We then add the number of walks c_s with the source configuration s to the number of walks c_{t_j} of each of the target configurations t_j . The length of a walk is equal to the number of iterations of the algorithm and the total number of walks of a given length is found by summing the number of walks c_s in the list of source configurations.

Without loss of generality, we can assume that the end-point of the walk is on the top side of the bounding box, since direction is not important for unrestricted prudent walks. We can also assume that the end of the walk is not farther from the left side than from the right side, since the number of ways in which a walk can be completed is invariant under reflection.

For prudent polygons, the position of the end-point of the walk is not enough information to determine if the walk can be extended to create a prudent polygon. The position of the start-point of the walk is also required. So we have to extend a configuration to include the coordinates of the start-point of the walk.

A prudent walk can only be extended to form a prudent polygon if the starting point of the walk either lies on one of the sides of the bounding box or is adjacent to a site on the current side of the bounding box that is in a direction in which the walk can extend. Configurations that do not satisfy this restriction can be discarded since such walks can never lead to prudent polygons.

If we are enumerating polygons of size n , and for a given configuration of m -step walks we cannot reach a site adjacent to the end-point in $n - m$ steps or less, we can ignore that configuration.

When calculating the number of polygons of a given size, we sum the number of walks only for those configurations s where the end-point is adjacent to the start-point.

The number of configurations grows like n^4 . The width w of the bounding box can vary from 1 to n while the length l can vary from 1 to $n-w$. Some smaller boxes cannot occur because for $w \times l < n$ the walk cannot fit within the box, but we shall ignore this effect for simplicity. In a box of size $w \times l$ the end-point can be in any of the w positions on the top edge while the starting point can be in $3w + 2l$ positions, so up to constant factors (arising from the restrictions on the directions the walk may take etc) we have that the number of configurations must be proportional to

$$\sum_{w=1}^n \sum_{l=1}^{n-w} w(3w + 2l) < \sum_{w=1}^n \sum_{l=1}^n w(3w + 2l) < \sum_{w=1}^n (3w^2n + 2wn^2) = O(n^4).$$

As indicated above we do not have to keep all configurations but can discard some because they would not give a prudent polygon of size $\leq n$. This however does not help reduce the asymptotic growth in the number of configurations which remains at $O(n^4)$, and the computational complexity of the algorithm is thus $O(n^5)$.

For prudent walks and polygons of types 1 and 2, we cannot ignore the direction of the current edge in our configuration, since some steps may be disallowed depending on their direction. So we cannot assume that the end-point is on the top edge, or arbitrarily reflects the configuration, since rotations and reflections of a configuration are not equivalent. However,

for type 1 walks and polygons we can reflect about the southwest-to-northeast axis; and for type 2 walks we can reflect about the east–west axis.

Apart from the precise information required in the configuration, the test for which steps are valid from a given configuration and which configurations should be accumulated to give the result, the algorithm to enumerate each of these six objects (type 1, type 2 and full walks and polygons) is identical. So we produced one program to solve all of these problems. The lists are stored in hash tables for efficiency. The number of walks for each configuration and the total number of walks or polygons are computed modulo a large prime number close to the computer’s word size. The computation is repeated for several primes and the final result is calculated by use of the Chinese remainder theorem. This is more efficient than performing the whole calculation using numbers larger than the computer’s word size.

In the following sections, we remark that for prudent walks and polygons of types 1 and 2 the generating functions can be derived rigorously or found from relatively short series. The exceptions are unrestricted prudent walks and polygons, and in the former case the number of walks can be calculated efficiently by the iteration of a functional equation. So the only case requiring serious computational effort is that of unrestricted prudent polygons. We enumerated the number of prudent polygons up to size 1004. The calculation was performed on the SGI Altix cluster of the Australian Partnership for Advanced Computing (APAC). This cluster has a total of 1920 1.6 GHz Itanium2 processors.

The algorithm was parallelized in a fairly straightforward manner with configurations distributed across processors using a basic hashing scheme. As in the basic algorithm, we step through the list of source configurations and generate all the new target configurations. For each target we check, using our hashing scheme, on which processor the target should reside. If this is not the current processor the configuration and its count are stored in a temporary stack. At regular intervals we pause in the main calculation in order to distribute the configurations from the temporary stacks to their designated processors. We found experimentally that it was advantageous to do the ‘parallel’ hashing using only the bounding box and starting point information from the configuration. Also doing the updating of the walk counts is fairly cheap and for this reason we did several primes simultaneously in a single run. To reproduce the integer coefficients correctly up to 1004 steps required some 36 primes so in practice we did four runs with each run using 9 primes. Each run utilized 160 processors and took about 9 h with about 1/3 of this time used in the communication part of the algorithm. In total we used some 5500 CPU hours. Note that for prudent SAW it is more efficient to iterate equation (6), but for prudent polygons this is the most efficient algorithm.

3. Prudent walks

In this section we summarize the known results for prudent walks. More detail can be found in [11, 12]. We denote the generating function of prudent walks of the first type by

$$C^{(1)}(x) = \sum c_n^{(1)} x^n,$$

where $c_n^{(1)}$ is the number of n -step prudent walks of the first type. Then [7]

$$C^{(1)}(x) = 1 + x \frac{(1 - 2x - x^2)(3 + 2x - 3x^2) + (1 - x)\sqrt{(1 - x^4)(1 - 2x - x^2)}}{(1 - 2x - x^2)(1 - 2x - 2x^2 + 2x^3)}. \tag{3}$$

It is clear that the dominant singularity is a simple pole located at the smallest real positive zero of the polynomial $1 - 2x - 2x^2 + 2x^3$, that is at $x = x_c = 0.403\,031\,7168\dots$

Thus the critical exponent $\gamma = 1$, and the asymptotic form of the coefficients is [13] (theorem IV.10)

$$c_n^{(1)} = \lambda^{(1)} / x_c^n + o(\rho^{-n}),$$

for any $\rho < \sqrt{2} - 1$, where $\lambda^{(1)} = \frac{x_c(3x_c-1)}{(3x_c+1)(5x_c-2)} = 2.5165\dots$

We denote the generating function of prudent walks of the second type by

$$C^{(2)}(x) = \sum c_n^{(2)} x^n,$$

where $c_n^{(2)}$ is the number of n -step prudent walks of the second type.

An explicit expression for the generating function was first found by Bousquet-Mélou [11] and it is much more complicated than that for prudent walks of the first type. First, we define

$$q \equiv q(x) = \frac{1 - x + x^2 + x^3 - \sqrt{(1 - x^4)(1 - 2x - x^2)}}{2x}. \tag{4}$$

Then

$$C^{(2)}(x) = \frac{1}{1 - 2x - x^2} \left(2x^2 q T(x; 1) + \frac{(1+x)(2-x-x^2q)}{1-xq} \right) - \frac{1}{1-x},$$

where

$$T(x) \equiv T(x; w) = \sum_{k \geq 0} (-1)^k \frac{\prod_{i=0}^{k-1} \left(\frac{x}{1-xq} - U(q^{i+1}) \right)}{\prod_{i=0}^k \left(\frac{xq}{q-x} - U(q^i) \right)} \times \left(1 + \frac{U(q^k) - x}{x(1-xU(q^k))} + \frac{U(q^{k+1}) - x}{x(1-xU(q^{k+1}))} \right) \tag{5}$$

and

$$U(w) \equiv U(x; w) = \frac{1 - wx + x^2 + wx^3 - \sqrt{(1-x^2)(1+x-wx+wx^2)(1-x-wx-wx^2)}}{2x}.$$

In this case the asymptotics are much more difficult to establish. Bousquet-Mélou [11] has confirmed that the dominant singularity is precisely as for type-1 prudent walks. The factor

$$\prod_{i=0}^k \left(\frac{xq}{q-x} - U(q^i) \right)$$

appearing in the denominator of (5) gives rise to an infinite sequence of poles on the real axis, lying between x_c and $\sqrt{2} - 1$, which are not canceled by zeros of the numerator. This accumulation of poles is enough to prove that the generating function cannot be D-finite.

We denote the generating function for prudent walks as

$$C(x) = \sum c_n x^n,$$

where c_n is the number of n -step prudent walks. Duchi gave two coupled equations which can be iterated to give the series coefficients of prudent walks in polynomial time. Rechnitzer¹ pointed out that these equations can be combined into a single equation,

$$\frac{1}{xw} H(u, v, w) = 1 + H(u, v, w) + H(u, v, w) + H(u, v, w) + \frac{xu}{v-xu} (H(u, v, w) - H(u, xu, w)) + \frac{xv}{u-xv} (H(u, v, w) - H(v, xv, w)), \tag{6}$$

¹ Private communication.

which can be iterated, and the generating function obtained by setting $u = v = w = 1$. A closed-form solution for this problem has not been found. In earlier work [12] the first 400 series coefficients were obtained and analyzed, and it was conjectured that the critical point and the critical exponent remain unchanged from those of prudent walks of types 1 and 2. That is to say, type 1, type 2 and unrestricted prudent walks have the same critical point and the same critical exponent $\gamma = 1$, corresponding to a simple pole.

The anisotropic generating function can be defined as follows: if $c_{m,n}$ denotes the number of prudent walks with m horizontal and n vertical steps, the anisotropic generating function can be written as

$$C(x, y) = \sum_{m,n} c_{m,n} x^m y^n = \sum_n R_n(x) y^n,$$

where $R_n(x) = \frac{M_n(x)}{N_n(x)}$ is the (rational [14]) generating function for prudent walks with n vertical steps.

We [12] calculated the first 10 generating functions $R_1(x), \dots, R_{10}(x)$ and found a regular pattern in the denominators $N_n(x)$ with factors corresponding to cyclotomic polynomials of steadily increasing degree. If this pattern persists, the generating function cannot be D-finite, as the pattern of cyclotomic polynomials of increasing degree implies a buildup of zeros on the unit circle in the complex x plane, and such an accumulation is incompatible with D-finite functions. This follows from the following theorem (from [15]) which shows that such functions cannot have a dense set of singularities:

Theorem. *Let $f(x, y) = \sum_{n \geq 0} H_n(x) y^n$ be a D-finite series in y with coefficients $H_n(x)$ that are rational functions of x . Let S_n be the set of poles of $H_n(x)$ and $S = \cup_n S_n$. Then S has only a finite number of singularities.*

As noted above, isotropic type-2 prudent walks are not D-finite, and the numerical evidence here allows us to conjecture that (anisotropic) unrestricted prudent walks are also not D-finite.

4. Prudent polygons

Polygon analogs of these three classes of walks can be naturally defined as walks of the given class that end at a vertex adjacent to their starting vertex. The relevant generating functions are

$$P^{(1)}(x) = \sum p_n^{(1)} x^n,$$

where $p_n^{(1)}$ is the number of $2n$ -step prudent polygons of the first type,

$$P^{(2)}(x) = \sum p_n^{(2)} x^n,$$

where $p_n^{(2)}$ is the number of $2n$ -step prudent polygons of the second type and

$$P(x) = \sum p_n x^n,$$

where p_n is the number of $2n$ -step prudent polygons. See figure 2 for an example of a prudent polygon. We have generated extensive isotropic and anisotropic series expansions for prudent polygons.

Just as we did for prudent walks above, if we distinguish between steps in the x and y directions, and let $p_{m,n}$ denote the number of prudent polygons with $2m$ horizontal and $2n$ vertical steps, then the anisotropic generating function for polygons can be written as

$$P(x, y) = \sum_{m,n} p_{m,n} x^m y^n = \sum_n H_n(x) y^n,$$

where $H_n(x) = \frac{R_n(x)}{S_n(x)}$ is the (rational [14]) generating function for prudent polygons with $2n$ vertical steps.

4.1. Type 1 or 2-sided prudent polygons

We generated more than 100 terms of the series for type 1 polygons, as described in the previous section, which was more than sufficient to identify the generating function.

For prudent walks of the first type, we found experimentally that the generating function satisfies a second-order linear homogeneous ODE,

$$\sum_{i=0}^2 P_i(x) f^{(i)}(x) = 0,$$

where

$$\begin{aligned} P_0(x) &= (-18 + 72x - 99x^2 + 42x^3 - 30x^4 + 32x^5 - 7x^6 + 2x^7), \\ P_1(x) &= (1 - x)(-12 + 78x - 148x^2 + 97x^3 - 39x^4 + 47x^5 - 9x^6 + 4x^7), \\ P_2(x) &= x(1 - x)^2(1 - 3x - x^2 - x^3)(3 - 7x + 2x^2 - x^3), \end{aligned}$$

which can be solved to yield

$$xP^{(1)}(x) = \sum p_n^{(1)} x^{n+1} = \frac{(1 - 3x + x^2 + 3x^3)}{(1 - x)} - \sqrt{(1 - x)(1 - 3x - x^2 - x^3)}. \quad (7)$$

This result has recently been proved by Schwerdtfeger [16], who showed that it can be derived from the known results for the generating function of bar-graph polygons, as type-1 prudent polygons are essentially bar-graph polygons. From (7) it can be seen that [13] (theorem IV.10)

$$p_n^{(1)} = \text{const. } \mu_1^{2n} \times n^{-3/2}(1 + O(1/n)),$$

where $1/\mu_1^2$ is the positive real root of the polynomial $1 - 3x - x^2 - x^3$. This root is at $x_c = 0.295\,597\,74\dots$, so $\mu_1 = 1.839\,2867\dots$. This should be compared to $\mu = 2.481\,1943\dots$ for type-1 prudent walks. Clearly, prudent polygons are exponentially rare among prudent walks, unlike the analogous situation for ordinary SAW, for which it is known that the growth constants of SAW and SAP are the same.

Using the conventional exponent notation and denoting by $P_s^{(k)}(x)$ the singular part of $P^{(k)}(x)$, we have $P_s^{(1)}(x) \sim \text{const. } (1 - \mu_1^2 x)^{2-\alpha}$, we see that $\alpha = 3/2$.

4.2. Type 2 or 3-sided prudent polygons

For prudent polygons of the second type, we again generated long series, but were unable to find the generating function by numerical experimentation. Given the complexity of the known generating function for type-2 prudent walks, this is perhaps not surprising. Nevertheless, we were able to obtain quite precise numerical results, allowing us to conjecture

$$P_s^{(2)}(x) \sim \text{const. } (1 - \mu_2^2 x)^{2-\alpha},$$

where, again, $\alpha = 3/2$. However, for μ_2 we find $\mu_2 = 2.023\,896 \pm 0.000\,002$, which is greater than μ_1 and shows that type-1 prudent polygons are exponentially rare among type-2 prudent polygons, which are in turn exponentially rare among type-2 prudent walks.

Very recently Schwerdtfeger [16] has obtained an explicit expression for the generating function for these polygons, incidentally confirming our numerical conjectures. He finds the generating function to be

$$P^{(2)}(x) = 2 \left(\frac{x^2}{1 - x} + B(x, 1) + R(x) \right)$$

where

$$B(x, u) = \frac{1 - x - u(1+x)x - \sqrt{x^2(1-x)^2u^2 - 2x(1-x^2)u + (1-x)^2}}{2xu}$$

and

$$R(x) = \sum_{k \geq 0} L((xq^2)^k) \prod_{j=0}^{k-1} K((xq^2)^j),$$

where

$$q = \frac{1 + x^2 - \sqrt{1 - 4x + 2x^2 + x^4}}{2x},$$

$$L(x) = \frac{(1 + x^2 - (1 - 2x + 2x^2 + x^4)q)(B(x, q) + x)}{1 - x(1+x)q - (x(1-x-x^3)q + x^2)(B(x, q) + x)}$$

and

$$K(x) = \frac{(1-x)q - 1 - ((1-x+x^2)q - 1)(B(x, q) + x)}{1 - x(1+x)q - (x(1-x-x^3)q + x^2)(B(x, q) + x)}.$$

Asymptotic analysis of this expression [16] shows that the dominant singularity is given by the real positive zero of $x^5 + 2x^2 + 3x - 2$, which occurs at $x = x_c = 0.49409642\dots = 1/2.0238964\dots$, and the singularity of the generating function is a square-root singularity, just as for type-1 prudent polygons. Both the location of the singularity and its exponent confirm our earlier numerical work.

Turning to the anisotropic generating function, we find numerically that

$$H_n = \frac{2x P_{2n-2}(x)}{(1-x)^{2n-1}}.$$

However, three-sided walks (and polygons) are not x - y symmetric, and so we can view the data in an alternative way by defining generating functions $R_m(y)$ through

$$P(x, y) = \sum_{m,n} p_{m,n} x^m y^n = \sum_m R_m(y) x^m,$$

where $R_m(y)$ is the (rational [14]) generating function for three-sided prudent polygons with $2m$ horizontal steps. When we look at the behavior of $R_m(x)$, we find

$$R_m = \frac{2y P_{2m-1}(y)}{(1-y)^{2m-1}},$$

for $m \leq 3$, but for $m \geq 4$ higher order cyclotomic polynomials appear in the denominator. As we have seen, this pattern, if it persists, is incompatible with a D-finite (anisotropic) generating function. That the isotropic generating function is also not D-finite is confirmed by Schwertfeger [16].

4.3. Unrestricted or four-sided prudent polygons

Again we resorted to a numerical study. The methods we used to analyze and estimate the asymptotic behavior of the series have all been described in [17]. We found from our analysis that the series expansion is quite badly behaved, with evidence of very strong sub-dominant asymptotic behavior that masks the dominant asymptotic behavior until quite large values of n are reached. Our initial attempts at a differential approximant analysis were not as convincing as they usually are. This was not really surprising, as there is evidence of a large number of singularities on the real axis, just beyond the critical point. This is the known situation for

type 2 polygons, where there is an infinite number of poles in a small range of the real axis, just beyond the critical point. It is unremarkable that unrestricted prudent polygons behave similarly. Nevertheless, using third-order inhomogeneous approximants and a series of 125 coefficients, corresponding to a maximum perimeter of 250, we were able to estimate the critical point at $x_c = 1/\mu_p^2 = 0.2267 \pm 0.0004$ or $\mu_p = 2.100 \pm 0.002$. The singularities appeared to be double roots, and we could not get a consistent estimate of the exponent.

Accordingly, we based our analysis on ratio-type methods, which generally are much more slowly convergent than differential approximant methods, but have the advantage that convergence, when it eventually does take place, is more evident.

Indeed, we had to generate some 500 terms in the series (corresponding to polygons with perimeter of up to 1000 steps), before we could get a reasonably clear picture of the asymptotics, and even then it is not as unequivocal as we would like. To estimate the critical point, we used a range of extrapolation methods to extrapolate the ratio of successive terms. We first used Wynn's algorithm, which is known to be slowly convergent, but robust. The first iterates of the ratios were monotonically increasing, beyond 4.3987. This sequence should converge to μ_p^2 . The second iterate was also steadily increasing, suggesting that $\mu_p^2 > 4.4038$. Higher iterates were unstable.

We next used Brzezinski's θ algorithm, which is known to be rapidly convergent under optimal circumstances. The first iterates of the ratios were monotonically increasing for 84 terms, then decreasing until 187 terms, then increasing again, beyond 4.4155. This sequence may continue to exhibit oscillatory behavior, so we are reluctant to use it as anything other than a guide. The second iterates started oscillating quite early in the sequence. Higher iterates were unstable.

We next used the Levin u -transform, which is also known to be rapidly convergent in ideal circumstances. The first iterates of the ratios were monotonically increasing for the first 122 ratios, then steadily decreasing and seemingly approaching an asymptote at a value of 4.4157. The second iterates reached a minimum at 198 terms, then steadily increased and also approached an asymptote around 4.4157, though this is of no significance, as the previous iterates were all around that value, so one would expect an iteration of an almost constant sequence to give that constant value. Higher iterates were unstable.

Finally, a Neville table gave monotone first and second iterates. The first iterates were steadily increasing suggesting $\mu_p^2 > 4.4107$, while the second iterates increased more slowly and gave $\mu_p^2 > 4.4128$. The third iterates reached a maximum at 116 terms, and then a minimum at 201 terms and then steadily increased. If this monotone trend continues, we can conclude $\mu_p^2 > 4.4136$. Combining all these methods, we estimate $\mu_p^2 = 4.415 \pm 0.001$ or $\mu_p = 2.1012 \pm 0.00025$ which encompasses all the results.

In figure 3 we show a plot of the ratios of successive terms plotted against $1/n$. Assuming the singular part of the generating function behaves as $P_s(x) \sim \text{const.} (1 - \mu_p^2 x)^{2-\alpha}$, then asymptotically, the ratios should approach μ_p^2 , with gradient $\mu_p^2(\alpha - 3)$. From the ratio plot, a limit around 4.415 is very plausible, though there is still a small amount of curvature in the locus of ratios. This is almost certainly due to the presence of exponentially small corrections due to one or more nearby singularities on the real axis. Extrapolating this locus to the estimated limit $\mu_p^2 \approx 4.415$, we estimate the slope in the vicinity of the y -axis to be -20 , so that $\alpha \approx -1.5$. We have also used biased differential approximants with the critical point biased at $\mu_p^2 = 4.415$, and while this signaled a confluent singularity at the critical point, it gave a consistent value for the exponent, $\alpha - 2$ as -3.5 ± 0.1 , so that again $\alpha \approx -1.5$.

In summary, we find for the singular part of the generating function, $P_s(x) \sim \text{const.} (1 - \mu_p^2 x)^{2-\alpha}$, where now $\alpha \approx -1.5$. We do not quote error bars as this estimate

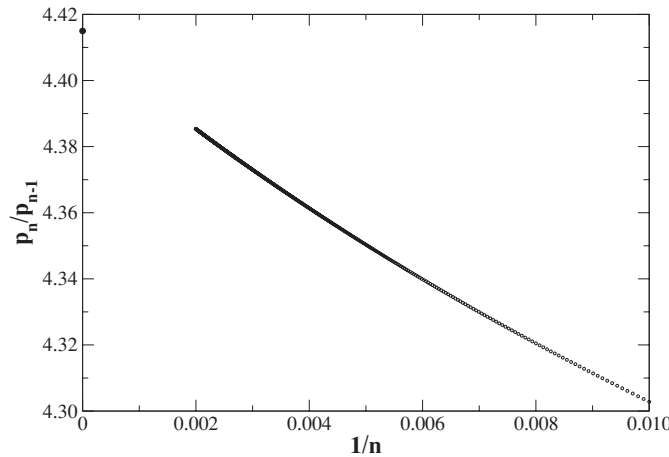


Figure 3. Plot of successive ratios of terms p_n/p_{n-1} against $1/n$ for prudent polygons of half-perimeter n . Our best estimate for the critical point $\mu_p^2 = 4.415$ is marked with a large dot on the y-axis.

of α is very sensitive to the estimate of the critical exponent used to bias the results. If we bias the critical point at $\mu_p^2 = 4.416$, a change of only 1 in the least significant digit, the exponent estimate from differential approximants changes to -4.2 ± 0.02 . Thus our estimate of α can only be taken as indicative rather than precise. What is clear however is that the singularity is unlikely to be of square-root type, as is the case for types 1 and 2 polygons, but of course there is no obvious reason why it should be.

For the anisotropic case, we write the generating function as

$$P(x, y) = \sum_{m,n} p_{m,n} x^m y^n = \sum_n H_n(x) y^n,$$

where the first few $H_n(x)$ are

$$H_1(x) = \frac{2x}{(1-x)}$$

$$H_2(x) = \frac{x(2+2x-x^2)}{(1-x)^3}$$

$$H_3(x) = \frac{x(2+9x+6x^2+x^4+x^5)}{(1-x)^5(1+x)}$$

$$H_4(x) = \frac{x(2+19x+42x^2+37x^3+18x^4+21x^5+11x^6-x^8)}{(1-x)^7(1+x)^2}$$

$$H_5(x) = \frac{V_{14}(x)}{(1-x)^9(1+x)^4(1+x+x^2)},$$

$$H_6(x) = \frac{V_{22}(x)}{(1-x)^{11}(1+x)^6(1+x+x^2)^2},$$

$$H_7(x) = \frac{V_{32}(x)}{(1-x)^{13}(1+x)^8(1+x+x^2)^4(1+x^2)},$$

where $V_i(x)$ denotes a polynomial of degree i . From the above, we see the relentless buildup of cyclotomic polynomials of increasingly high order. As explained above, if this pattern persists, the underlying generating function cannot be D-finite. While this does not *a priori* prove that

the isotropic generating function is not D-finite, we know of no combinatorial problem where this is the case. That is to say, where the isotropic generating function is D-finite, while the anisotropic generating function is not.

5. Three-dimensional prudent walks and polygons

We have enumerated all prudent walks of up to $n = 23$ steps on the three-dimensional simple cubic lattice using a simple backtracking algorithm. As for the case of ordinary SAW, it is a far more difficult task to perform enumerations in three dimensions than it is in two. To take advantage of the inherent symmetry in the problem we only explicitly counted walks whose first step was in the positive x direction, whose first step out of this line (if any) was in the positive y direction and whose first step out of this plane (if any) was in the positive z direction. In addition, we *trivially parallelized* the backtracking algorithm: In three dimensions there are 16 four-step prudent walks whose first two steps are precisely East then North. We independently enumerated the completions to n -step walks of each of these prefixes. Similarly there are 4 four-step prudent walks whose first three steps are East, East, North. Again we independently enumerated the n -step completions of each of these prefixes. Finally, the prudent walks whose first three steps are East, East, East were all enumerated together in the same computation. Thus, for each value of n we ran a total of 21 independent computations. The enumerations for $n = 23$ took a total of around 2377 h (roughly 100 h per independent computation). The computations were performed on *tango*, a 95-node Linux cluster at the Victorian Partnership for Advanced Computing (VPAC). Each node consists of two AMD Barcelona 2.3 GHz quad core processors. In principle, it is probably possible to obtain another term or two by applying the two-step method [18], but we have not pursued this here.

For each $1 \leq n \leq 23$ we computed the number of prudent walks, c_n , the number of prudent polygonal returns, u_{n+1} and the sum of squared end-to-end distances $c_n \langle R^2 \rangle_n$, summed over all prudent walks. The results of our enumerations are presented in table 1.

We analyzed the various series by the method of differential approximants, as well as variants of the ratio method, as used in the analysis of the polygon generating function in the previous section [17]. For the prudent walk generating function, for which we expect

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

we found a singularity on the positive real axis at $x_c = 0.22265 \pm 0.0003$ with the corresponding exponent $\gamma = 1.68 \pm 0.03$. Biasing the value of the critical point at the central estimate, that is setting $x_c = 0.22265$ gives the corresponding biased estimate of $\gamma = 1.67$ from first-order differential approximants and $\gamma = 1.68$ from second-order differential approximants. For SAW, the analogous values are $x_c(\text{SAW}) \approx 0.2134907$ and $\gamma_{\text{SAW}} \approx 1.1567$, so prudent walks are exponentially rare among SAW, and the two models have different critical exponents.

Additionally, for three-dimensional prudent walks we find that there is a singularity in the generating function $C(x)$ on the negative real axis that appears to be at, or just beyond, $x = -x_c$. For the corresponding self-avoiding walk model, it is known that there is a singularity (the analog of an anti-ferromagnetic singularity for a magnetic model) exactly at $x = -x_c(\text{SAW})$, but the argument for the location of that singularity in the case of SAW does not translate to prudent walks. The corresponding exponent is, very approximately, the same magnitude as that of the physical singularity, but opposite in sign. That is to say, there appears to be a singularity of the form

$$\text{const.} (1 + x/x^*)^{\gamma^*},$$

Table 1. Exact enumeration data on the simple cubic lattice. Here c_n denotes the number of n -step prudent walks, u_{n+1} , the number of $(n + 1)$ -step prudent polygonal returns and $\langle R^2 \rangle_n$ the average squared end-to-end distance of n -step prudent walks.

n	c_n	$c_n \langle R^2 \rangle_n$	u_{n+1}
0	1	0	0
1	6	6	0
2	30	72	0
3	150	582	24
4	726	4032	0
5	3510	25542	240
6	16734	153048	0
7	79518	881118	2544
8	375246	4925616	0
9	1766382	26909934	31800
10	8278638	144356280	0
11	38721366	762839334	435864
12	180556206	3981064368	0
13	840524742	20556000822	6323352
14	3903866526	105173637672	0
15	18106798830	533839505646	95647104
16	83832778110	2690761186608	0
17	387690560718	13478479905486	1493934516
18	1790330065854	67142893855752	0
19	8259528315558	332807521103670	23934001600
20	38059497518214	164221451827040	0
21	175228328442174	8070246610372494	391427518152
22	805959153119262	39511166688322248	0
23	3704270575724550	192780251992208934	6511949001648

where $x^* \geq x_c$ and $\gamma^* \approx \gamma$, as well as the physical singularity. For two-dimensional prudent walks, there is also evidence of a singularity on the negative real axis, but located considerably further away from the origin than the physical singularity. That is to say, $x^*(2d) > x_c(2d)$.

To calculate the exponent ν characterizing the mean-square end-to-end distance, $\langle R^2 \rangle_n \sim \text{const. } n^{2\nu}$ we analyzed the series for the sum of the squared end-to-end distances, which diverges at x_c with exponent $\gamma + 2\nu$. From a differential approximant analysis we found $x_c \approx 0.22265$ with $\gamma + 2\nu \approx 3.20$, so that $\nu \approx 0.76$. We also analyzed the series $\langle R^2 \rangle_n$ directly and obtained an estimate for ν consistent with that just quoted, but less precise.

The polygonal returns u_n include a factor $2n$ corresponding to n possible starting points, and a factor of 2 as the path may be traversed clockwise or anticlockwise. We have analyzed the series with coefficients $p_n = u_n/2n$. We only have 11 coefficients, which is not really enough for any but the crudest analysis. From a differential approximant analysis, we find that the generating function $P(z) = \sum_n p_n z^n$ is singular at $z = z_c = 0.0499 \pm 0.0006$ with an exponent 2.3 ± 0.5 . That is to say, $P_s(z) \sim \text{const. } (1 - z/z_c)^{2.3}$. Note that from our analysis of the corresponding walk series, $x_c^2 = 0.04957 \pm 0.00014$. Thus from the numerical data, it is entirely possible that $z_c = x_c^2$ for three-dimensional prudent polygons, just like the analogous situation for three-dimensional SAW, but unlike the situation for two-dimensional prudent

walks and polygons, for which, as discussed above, prudent polygons are exponentially rare among prudent walks.

In two dimensions, the condition of prudency severely limits the number of walks that are also polygons, as the prudency constraint tends to drive the end-point away from the origin. In three dimensions, the prudency constraint is much less severe. In particular, the end-point of the walk does not have to be on the surface of the minimum bounding box. However we have been unable to prove that three-dimensional prudent walks and polygons have the same growth constant. In particular, the proof of the corresponding result for standard SAW and SAP does not carry over to the prudent case. In higher dimensions it is increasingly likely that prudent walks and polygons have coincident growth constants, though we have no numerical data to investigate this point. If it is true that $z_c = x_c^2$ for three-dimensional prudent polygons, then we can carry out a biased analysis in which we fix z_c at x_c^2 . In that case we find that the estimate for the exponent $2 - \alpha$ of the polygon generating function is a little higher at 2.5 ± 0.2 so that $\alpha = -0.5 \pm 0.2$.

6. Conclusion

We have defined and analyzed series for prudent walks and polygons in both two and three dimensions. In two dimensions, we also discussed two subsets, which are exactly solvable. We found that two-dimensional prudent polygons are exponentially rare among prudent walks, unlike the situation for two-dimensional SAW. We gave numerical arguments in support of the conjecture that the anisotropic generating function for two-dimensional prudent polygons is not D-finite.

We derived extensive series for three-dimensional prudent walks and polygons. As far as we are aware, this problem has not been studied previously. We have given estimates of the critical point and critical exponents. In terms of the usual notation we found that the growth constant for walks is $\mu \approx 4.491$, with exponents $\gamma \approx 1.68$, $\nu \approx 0.76$ and $\alpha \approx -0.3$ based on an unbiased estimate of the critical point. For SAW $\mu_{\text{SAW}} \approx 4.68404$, $\gamma \approx 1.1567$, $\nu \approx 0.5875$ and $\alpha \approx 0.2375$. For SAW we have the hyper-scaling relation $d\nu = 2 - \alpha$. While there is no *a priori* reason to expect this hyper-scaling relation to hold for three-dimensional prudent walks, as it is not a statistical mechanical model derived from a Hamiltonian, we nevertheless note that $3\nu \approx 2.28$ while $2 - \alpha \approx 2.28$. The uncertainties in our exponent estimates are too great to attach much significance to this approximate equality, except to flag it as a possibility.

In terms of physical significance, the model of prudent walks, while exponentially rare among SAW in both two and three dimensions, is nevertheless exponentially abundant compared to any other solved or numerically estimated model. Other variants of the model that relax the prudency constraint to some extent are likely to have growth constants even closer to that of SAW, and these will be the subject of a future publication [9].

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