

LETTER TO THE EDITOR

Perimeter Generating Functions For The Mean-Squared Radius Of Gyration Of Convex Polygons

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Abstract. We have derived long series expansions for the perimeter generating functions of the radius of gyration of various polygons with a convexity constraint. Using the series we numerically find simple (algebraic) exact solutions for the generating functions. In all cases the size exponent $\nu = 1$.

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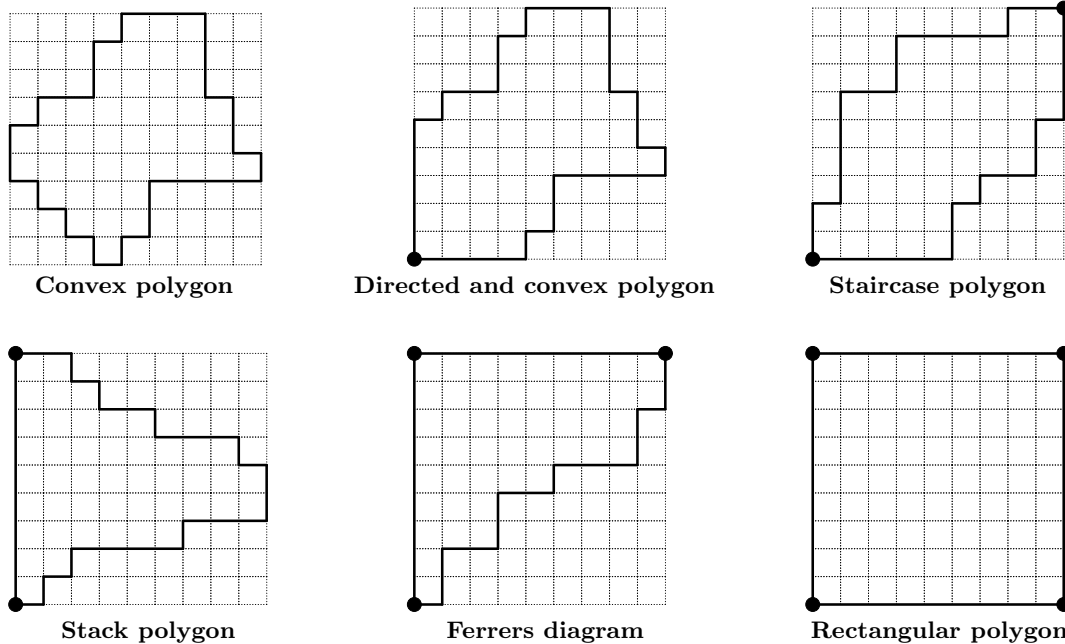


Figure 1. Examples of the types of convex polygons we consider in this paper.

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. The models are of tremendous inherent interest as well as serving as simple models of polymers and vesicles [1, 2, 3]. Despite strenuous effort over the past 50 years or so this problem has not been solved on any regular two dimensional lattice. However, there are many simplifications of this problem that are solvable [4], but all the simpler models impose an effective directedness or other constraint that reduces the problem, in essence, to a one-dimensional problem.

One particular class of exactly solved polygon models are those with a convexity constraint (see figure 1). On the square lattice a polygon is said to be *convex* if it is convex with respect to both vertical and horizontal lines, i.e., any vertical line will intersect the polygon at zero or two horizontal edges while similarly any horizontal line will intersect the polygon at zero or two vertical edges. Alternatively a convex polygon is a SAP of a length equal to the perimeter of its minimal bounding rectangle. If we further demand that the polygon must include the vertices in some of the corners of the minimal bounding rectangle we can define a further five polygon models as illustrated in figure 1. The full perimeter and area generating functions are known for all these models [4]. Also of great interest is the mean-square radius of gyration, $\langle R^2 \rangle_n$, which measures the typical size of a polygon with perimeter n . In this paper we report on work leading to conjectured exact solutions for the generating functions associated with the mean-square radius of gyration for the class of convex polygons.

An n -step self-avoiding walk ω is a sequence of *distinct* vertices $\omega_0, \omega_1, \dots, \omega_n$ such that each vertex is a nearest neighbour of its predecessor. SAWs are considered distinct up to translations of the starting point ω_0 . A self-avoiding polygon of length n is an $n - 1$ -step SAW such that ω_0 and ω_{n-1} are nearest neighbours and a closed loop can be formed by inserting a single additional step joining the two end-points. We shall use the symbol Ω_n to mean the set of all SAPs of perimeter length n . Generally SAPs are considered distinct up to a translation, so if there are p_n SAPs of length n there are $2np_n$ walks (the factor of two arising since the walk can go in two directions). One expects in general that $p_n \sim A\mu^n n^{\alpha-3}$, where μ is the so-called connective constant while α is a critical exponent. In our cases μ and α are known from the exact solutions for the perimeter generating functions

$$\mathcal{P}(x) = \sum_n p_{2n} x^n \sim A(x)(1 - \mu^2 x)^{2-\alpha}, \quad (1)$$

where we took into account that polygons on the square lattice have even length. The generating functions thus have a singularity at the critical point $x_c = 1/\mu^2$ with critical exponent $2 - \alpha$. The function $A(x)$ is analytic at $x = x_c$. Note that both μ and α are model dependent.

The mean-square radius of gyration of n -step polygons is defined by,

$$\langle R^2 \rangle_n = \frac{1}{2n^2 p_n} \sum_{\Omega_n} \sum_{i,j=0}^{n-1} (\omega_i - \omega_j)^2, \quad (2)$$

where we expect that $\langle R^2 \rangle_n \sim Bn^{2\nu}$. It is advantageous to look at the quantity $r_n = n^2 p_n \langle R^2 \rangle_n$, which is an integer, and in particular we shall study the associated generating function

$$\mathcal{R}(x) = \sum_n r_{2n} x^n \sim B(x)(1 - \mu^2 x)^{-(\alpha+2\nu)}, \quad (3)$$

where we again used that r_n is non-zero only when n is even.

The values for the critical exponents are known exactly, though non-rigorously, for self-avoiding polygons due to the work by Nienhuis [5], $\alpha = 1/2$ and $\nu = 3/4$. As we shall demonstrate later, the exponent α takes on several different values for the convex polygons studied in this paper, but the exponent $\nu = 1$ in all cases.

In the next section we briefly describe the algorithm used to calculate r_n and in the following section we list the various perimeter generating functions.

2. Computer enumeration

The first terms in the series for the polygon generating function are calculated using transfer matrix techniques to count the number of polygons spanning rectangles $W + 1$ edges wide and $L + 1$ edges long. The transfer matrix technique involves drawing a line through the rectangle intersecting a set of edges. For each configuration of occupied or empty edges along the intersection we maintain a (perimeter) generating function for

partial polygons cutting the intersection in that particular pattern. Due to the convexity constraint a vertical line will intersect the polygon exactly twice. The upper edge of the convex polygon performs a directed walk taking steps to the right and up until it reaches the top of the rectangle where it turns and then performs a directed walk with steps to the right and down. Likewise the lower edge performs a directed walk with right and down steps until it hits the bottom of the rectangle where it turns and takes only right and up steps. A convex polygon is formed once the two walks meet. In order to specify a configuration we just need to know the positions of the edges and whether or not the top and bottom of the rectangle has been touched. All the possible configurations can then be encoded by four $(W + 1) \times (W + 1)$ -matrices, one matrix for each possibility of touched borders. As the vertical boundary line is moved one step forwards the matrices are updated to allow for all the legal moves of the edge-walks (the walks must be directed as described above and never cross). The updating involves simple double sums over the indices. This approach was used by Guttmann and Enting [6] and is very efficient. However, in one iteration many steps can be inserted and this makes the calculation of the contributions to the radius of gyration somewhat cumbersome. We find it more convenient to use an algorithm in which the convex polygons in a given rectangle are enumerated by moving the intersection so as to add one vertex at a time. The method we used to enumerate convex polygons on the square lattice is a specialisation of the method originally devised by Enting [7] for the enumeration of self-avoiding polygons. As noted earlier, convex polygons can be viewed as SAPs with a number of steps equal to the perimeter of the minimal bounding rectangle. So we could simply take our previous algorithm [8, 9], which we generalised in order to calculate the radius of gyration, and only extract the terms counting convex polygons. Due to the convexity constraint we were able to simplify the algorithm somewhat and make it more efficient. However, the algorithm is still quite similar to the SAP enumeration algorithm so we won't describe it further. Suffice to say that the method for calculating the radius of gyration coefficients r_n has been described in [9].

Using this algorithm we quickly (a few hours of CPU time) calculated the radius of gyration of the polygon models of figure 1 to length $n = 110$, giving us 56 terms in the half-perimeter series. The first few terms p_n and r_n are listed in table 1. The full series for the generating functions studied in this paper can be obtained by sending a request to the author or via the web at <http://www.ms.unimelb.edu.au/~iwan/>.

3. The exact generating functions

In this section we use the series for r_n to find (numerically) the exact perimeter generating functions for the radius of gyration of convex polygons.

The perimeter generating function for convex polygons was first obtained by Delest and Viennot [10] using the method of algebraic languages and later by several other

Table 1. The number of polygons p_n and their mean-squared radius of gyration $r_n = n^2 p_n \langle R^2 \rangle_n$.

Convex polygons			Directed and convex polygons		Staircase polygons	
n	p_n	r_n	p_n	r_n	p_n	r_n
4	1	8	1	8	1	8
6	2	66	2	66	2	66
8	7	600	6	522	5	444
10	28	5164	20	3772	14	2710
12	120	41768	70	25138	42	15512
14	528	317584	252	157212	132	84756
16	2344	2280792	924	935140	429	446952
18	10416	15573120	3432	5343160	1430	2291718
20	46160	101743312	12870	29541450	4862	11485760
22	203680	639664960	48620	158920172	16796	56486716
24	894312	3889101336	184756	835390460	58786	273405288
26	3907056	22961959168	705432	4305416136	208012	1305401916
28	16986352	132118984560	2704156	21812985652	742900	6159651344
30	73512288	743046249664	10400600	108875244952	2674440	28766573800
32	316786960	4095077270128	40116600	536326527048	9694845	133128274320
34	1359763168	22163717040384	155117520	2611304032624	35357670	611143639110
36	5815457184	118021533366432	601080390	12582098181466	129644790	2785335811920
38	24788842304	619313064407680	2333606220	60058408242252	477638700	12612104460780
40	105340982248	3206924122635928	9075135300	284257070075212	1767263190	56773091159400

Stack polygons			Ferrers diagrams		Rectangular polygons	
n	p_n	r_n	p_n	r_n	p_n	r_n
4	1	8	1	8	1	8
6	2	66	2	66	2	66
8	5	444	4	366	3	288
10	13	2541	8	1640	4	900
12	34	12840	16	6404	5	2280
14	89	59113	32	22696	6	4998
16	233	253600	64	74832	7	9856
18	610	1029802	128	233312	8	17928
20	1597	4002112	256	695680	9	30600
22	4181	15005189	512	2000128	10	49610
24	10946	54603436	1024	5578752	11	77088
26	28657	193743969	2048	15166464	12	115596
28	75025	672725072	4096	40336384	13	168168
30	196418	2292470170	8192	105256960	14	238350
32	514229	7685026612	16384	270135296	15	330240
34	1346269	25392243845	32768	683188224	16	448528
36	3524578	82826447752	65536	1705443328	17	598536
38	9227465	267077278409	131072	4207935488	18	786258
40	24157817	852322922488	262144	10274078720	19	1018400

authors using different methods [6, 11, 12]:

$$\mathcal{P}_{\text{Convex}}(x) = \frac{x^2 - 6x^3 + 11x^4 - 4x^5}{(1 - 4x)^2} - \frac{4x^4}{(1 - 4x)^{3/2}}. \tag{4}$$

From this we see that the critical point $x_c = 1/4$ (and thus $\mu = 2$) while the critical exponent $2 - \alpha = -2$ (and thus $\alpha = 4$), corresponding to the dominant double pole at $x = x_c$. In addition there is a sub-dominant square root correction. Informed by this result it is natural to assume that the generation function for the mean-squared radius of gyration has a similar form. That is we assume that $\mathcal{R}(x) = [A(x) + B(x)\sqrt{1 - 4x}]/(1 - 4x)^\gamma$, where $A(x)$ and $B(x)$ are polynomials. Using the method of differential approximants [13] we easily established that $\gamma = 6$. Next we wrote a simple Maple routine to find

such a solution, that is we solve for the unknown coefficients a_i and b_i of $A(x)$ and $B(x)$. We simply form the series expansion for $[A(x) + B(x)\sqrt{1-4x}]$, match the series coefficients to those of $\mathcal{R}(x)(1-4x)^6$ and solve the resulting set of linear equations in the coefficient a_i and b_i . In this fashion we found a solution with polynomials of degree 10 requiring no more than 22 unknown coefficients. Since we have more than 50 known terms r_{2n} there are at least 30 unused series coefficients which serve as strong checks on the correctness of our solution. The generating function for the mean-squared radius of gyration of convex polygons is:

$$\mathcal{R}_{\text{Convex}}(x) = \frac{2x^2(1-2x)(4-55x+388x^2-1058x^3+956x^4+2064x^5-6592x^6+6400x^7)}{(1-4x)^6} - \frac{4x^4(15+22x-408x^2+1664x^3-3720x^4+3456x^5)}{(1-4x)^{11/2}}. \quad (5)$$

From this we see that the critical exponent $\alpha + 2\nu = 6$ and thus $\nu = 1$. This should be compared to the result for self-avoiding polygons $\nu = 3/4$ [5]. Physically, there is a simple argument for $\nu = 1$. Convex polygons are relevant to the description of vesicles in the *inflated* regime, where they are space-filling, and since the radius of gyration measures a typical size of a polygon $\langle R^2 \rangle_n$ is proportional to a typical area and hence $\nu = 1$ for convex polygons. The value $\nu = 3/4$ means that SAPs are much more ramified.

Directed and convex polygons was considered by Lin and Chang [11]. They calculated the full anisotropic generating function for directed and convex polygons. In the isotropic case which we consider here their result reduces to the very simple form

$$\mathcal{P}_{\text{DirConv}}(x) = \frac{x^2}{(1-4x)^{1/2}}, \quad (6)$$

so we have $x_c = 1/4$ while $2 - \alpha = -1/2$ and thus $\alpha = 5/2$. As for the convex case we start by looking for a solution to $\mathcal{R}(x)$ of the same form, that is $\mathcal{R}(x) = A(x)/(1-4x)^\gamma$, with $\gamma = 9/2$ determined from differential approximants. However we were not successful at first, so next we tried a solution of the same form as for convex polygons and found that

$$\mathcal{R}_{\text{DirConv}}(x) = \frac{-x^2 + 20x^3 - 48x^4 + 24x^5 - 168x^6 + 384x^7}{(1-4x)^{9/2}} + \frac{9x^2 - 44x^3 + 72x^4 - 32x^5}{(1-4x)^3}. \quad (7)$$

So in this case we find the critical exponent $\alpha + 2\nu = 9/2$ and thus as before $\nu = 1$.

The model of staircase polygons is very well-known and much studied, dating back at least to the work by Pólya [14] who showed that $p_{2n} = \frac{1}{4n-2} \binom{2n}{n}$ for $n \geq 2$. This result was obtained by Delest and Viennot [10] in the more elegant form $p_{2n+2} = C_n = \frac{1}{n+1} \binom{2n}{n}$, where C_n are the famous and ubiquitous Catalan numbers. Consequently the generating function is

$$\mathcal{P}_{\text{Stair}}(x) = (1-2x-\sqrt{1-4x})/2, \quad (8)$$

and $x_c = 1/4$, while $2 - \alpha = 1/2$ and thus $\alpha = 3/2$. As per the previous cases we quite readily find the radius of gyration generation function

$$\mathcal{R}_{\text{Stair}}(x) = \frac{x(1 - 6x + 24x^2 - 60x^3 + 64x^4)}{(1 - 4x)^{7/2}} - x, \quad (9)$$

and we see that $\alpha + 2\nu = 7/2$ and once again $\nu = 1$.

Stack polygons were also considered by Lin and Chang [11] and their result for the generating function is

$$\mathcal{P}_{\text{Stack}}(x) = \frac{x^2(1 - x)}{(1 - 3x + x^2)}. \quad (10)$$

The critical point is now given by the zero of $1 - 3x + x^2$ namely $x_c = 0.381966011\dots$ and the critical exponent is $2 - \alpha = -1$ or $\alpha = 3$. In this case the radius of gyration generation function is of the same form and again we have $\nu = 1$. Explicitly we find that

$$\mathcal{R}_{\text{Stack}}(x) = \frac{8x^2 - 54x^3 + 214x^4 - 489x^5 + 605x^6 - 386x^7 + 177x^8 - 120x^9 + 19x^{10} - x^{11}}{(1 - 3x + x^2)^5}. \quad (11)$$

The generating function for Ferrers diagrams is trivial in that these polygons are simply formed from a directed walk with $n - 2$ right or up steps, extended at the starting point with a horizontal step and at the end-point with a vertical step, and then closed by straight lines to form a polygon with $2n$ steps. It immediately follows that the generating function is

$$\mathcal{P}_{\text{Ferrers}}(x) = \frac{x^2}{(1 - 2x)}, \quad (12)$$

and we have $x_c = 2$ and $\alpha = 3$. The radius of gyration generation function is of the same form and with $\nu = 1$,

$$\mathcal{R}_{\text{Ferrers}}(x) = \frac{2x^2(4 - 7x + 13x^2 - 10x^3 + 2x^4)}{(1 - 2x)^5}. \quad (13)$$

Rectangular polygons are obviously the simplest case and the generating function is simply

$$\mathcal{P}_{\text{Rect}}(x) = \frac{x^2}{(1 - x)^2}, \quad (14)$$

so that $x_c = 1$ and $\alpha = 4$. The radius of gyration generating function is found to be

$$\mathcal{R}_{\text{Rect}}(x) = \frac{2x^2(1 + x)^2(4 + x)}{(1 - x)^6}, \quad (15)$$

and again we have $\nu = 1$.

Now that these results for the radius of gyration of convex polygons are known from the numerical work presented here it should be easier to prove them rigorously.

Acknowledgments

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