Three-Dimensional Convex Polygons

Mireille Bousquet-Mélou
LaBRI, Université Bordeaux 1

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[summary by Eithne Murray]

Abstract

A method to enumerate self-avoiding convex polygons, which in theory will work for all dimensions, is presented. The generating series for polygons of dimensions 2 (already known) and 3 are given. They are both the quotients of two D-finite series, and it appears that this property might hold for higher dimensions.

1. Introduction

A very old open problem is to enumerate self-avoiding walks (self-avoiding polygons) in dimension d. This talk answers a slightly more restricted problem by presenting a method of enumerating convex self-avoiding polygons. The 2-dimensional case has already been solved in [3] and [6], but this method works in higher dimensions, and provides a combinatorial interpretation of the 2-dimensional result.

Some basic definitions are required. An *(oriented) polygon* of perimeter $2n$ is a closed path $(s_1, s_2, \ldots, s_{2n})$ of vertices on $\mathbb{Z}^d$ such that s_i and s_{i+1} are neighbours for $1 \le i \le 2n$ and $s_{2n+1} = s_1$. It is defined up to cyclic permutations of its vertices. The *rooted* polygon $(s_1, s_1, \ldots, s_{2n})$ *represents* all the polygons formed by the cyclic permutations. A *self-avoiding polygon* is such that $s_i \neq s_j$ for $1 \le i \neq j \le 2n$; in other words, it never crosses itself except at the start/end point. A non-empty self-avoiding polygon is also called a *loop*. Note that the polygon (s_1, s_2) is a loop.

Polygons are often represented as words over an alphabet. This representation means the polygons are defined up to a translation in $\mathbb{Z}^d$, which is a requirement for counting them, and also gives a convenient method to define additional properties of the polygons. Thus a rooted polygon of perimeter $2n$ will often be regarded as a word $u = u_1 u_2 \cdots u_{2n}$ on the alphabet $\mathcal{A} = \{1, 2, \ldots, d\} \cup \{\bar{1}, \bar{2}, \ldots, \bar{d}\}$. Then if $(e_1, \ldots, e_d)$ is the canonical basis of $\mathbb{Z}^d$, and $u_i = k$ (resp. $\bar{k}$), then u_i is a unitary step from the vertex s_i to s_{i+1} along e_k (resp. $-e_k$). Note that for all $k \le d$, the number of occurrences of k in u, denoted $|u|_k$, is equal to the number of occurrences of $\bar{k}$ in u. Conversely, any word u on $\mathcal{A}$ that satisfies $|u|_k = |u|_{\bar{k}}$ for $1 \le k \le d$ is a rooted polygon. For example, the polygon $12\bar{1}\bar{2}$ would be a unit square. More examples can be seen in figure 1.

This representation is used to define *dimension*, *unimodal polygon* and *convex polygon* (see below). These concepts are important since the method to count the convex polygons involves decomposing them into their unimodal parts, and counting their loops of each dimension.

The *dimension* of a polygon is the dimension of its convex hull, which is equal to the number of k such that $|u|_k > 0$. For example, the loop (s_1, s_2), represented by $u = k\bar{k}$, has dimension 1.

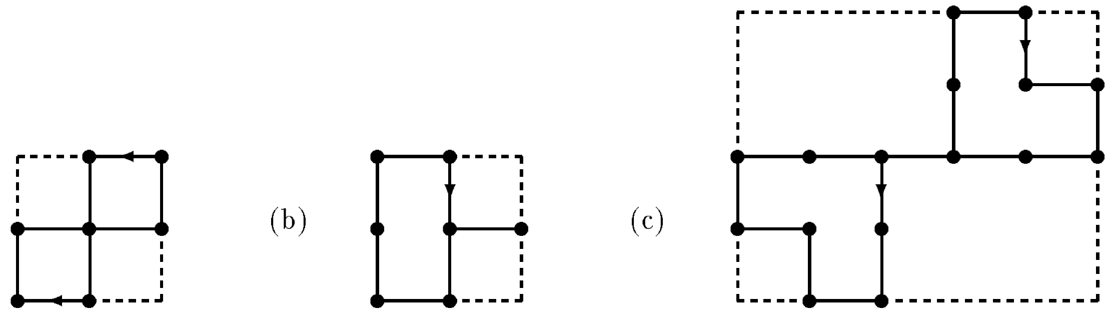

FIGURE 1. (a) staircase (b) unimodal (c) convex polygons

A polygon is *unimodal* if, for each direction k, the polygon can be written $u = vw$ with $|v|_{\bar{k}} = |w|_k = 0$. In other words, all the k's come before all the $\bar{k}$'s in its representative word u, and so all the steps taken in a given direction occur before all the steps taken to return from that direction.

A polygon is *convex* if for each k there is a cyclic permutation of the polygon such that all the k's come before all the $\bar{k}$'s. More intuitively, for each k, and each $a \in \mathbb{R}$, the intersection of a convex polygon with the half-space $\{(a_1, \ldots, a_d) : a_k \leq a\}$ is connected. Another characteristic is that the length of the perimeter of a convex polygon is equal to the length of the perimeter of the smallest bounding box of the polygon. A unimodal polygon is a convex polygon that contains the vertex of minimal coordinates of its smallest bounding box. See figure 1.

2. Enumeration Method

To count the self-avoiding convex polygons, the idea is to count all convex polygons and then remove those that are not self-avoiding. Let P represent the number of all convex polygons of dimension d, and P_k be the number of convex polygons of dimension d with a k-dimensional loop but no loops of dimension $< k$. Then

$$P = P_1 + P_2 + \cdots + P_d. \tag{1}$$

Polygons will be enumerated by using a generating function based on their perimeters. If $\mathcal{P}$ is a set of polygons, then the *perimeter generating function* for the elements of $\mathcal{P}$ is

$$\sum_{u \in \mathcal{P}} t^{|u|/2},$$

where $|u|$ stands for the number of letters of u; and the *multi-perimeter generating function* is

$$\sum_{u \in \mathcal{P}} x_1^{|u|_1} \cdots x_d^{|u|_d}.$$

A *staircase polygon* is a pair of directed paths having the same end-points, so all the steps taken in positive directions (words on $\{1, \ldots, d\}$) occur before all the steps taken in negative directions (words on $\{\bar{1}, \ldots, \bar{d}\}$). The multi-perimeter generating function for staircase polygons, where n_i is the number of steps taken in direction e_i in $\mathbb{Z}^d$, is

$$Z_d(x_1, \ldots, x_d) = \sum_{n_1, \ldots, n_d} \binom{n_1 + \cdots + n_d}{n_1, \ldots, n_d}^2 x_1^{n_1} \cdots x_d^{n_d}$$

(see [4]). This series is D-finite, that is, it satisfies a linear differential equation with polynomial coefficients [7]. Moreover,

$$(2) \qquad Z_2(x_1,x_2) = \sum_{n_1,n_2} \binom{n_1+n_2}{n_1,n_2}^2 x_1^{n_1} x_d^{n_2} = \frac{1}{\sqrt{1-2x_1-2x_2-2x_1x_2+x_1^2+x_2^2}}$$

is algebraic. This series has a generalization to Z_λ where λ is a partition [4].

THEOREM 1. *The multi-perimeter generating function of the number of d-dimensional convex polygons that have no 1-dimensional loops is*

$$P - P_1 = E\left[\frac{(d-1)!x_1\cdots x_d(1-x_1)^2\cdots(1-x_d)^2}{(1-x_1-\cdots-x_d)^d}\right]$$

where if $f(x_1,\ldots,x_d) = \sum_{n_1,\ldots,n_d} a_{n_1,\ldots,n_d} x_1^{n_1}\cdots x_d^{n_d}$, *then the* even part *of f is*

$$E\left[f(x_1,\ldots,x_d)\right] = \sum_{n_1,\ldots,n_d} a_{2n_1,\ldots,2n_d} x_1^{2n_1}\cdots x_d^{2n_d}.$$

The proof of this theorem uses the inclusion/exclusion principle and a decomposition of the word-representations of the polygons.

The following gives the formula which will be applied to count convex loops. The idea is that for a convex polygon having loops of dimension d, two cases can occur: either it has only one loop (it itself is a d-dimensional loop), or it can have two loops. There are 2^d possible loop structures, and the loops are unimodal. If the polygon is represented by ul_1vl_2, where the l_i are loops, then uv is essentially a staircase polygon, and so counted by Z_d. Details are presented in [2].

THEOREM 2. *In dimension d, let P_d and Z_d be defined as above, and let U_d be the multi-perimeter generating function for unimodal polygons having only loops of dimension d, and C_d be the generating function for convex polygons having only loops of dimension d. Then*

$$P_d = C_d + 2^{d-1} Z_d U_d^2.$$

Since a convex polygon of dimension d which has only loops of dimension d is self-avoiding, C_d counts the d-dimensional self-avoiding convex polygons. Now U_d can be calculated for all d by rewriting it in terms of Z_d using induction. An important element of the proof is that a loop of a rooted unimodal polygon is unimodal, and hence if a rooted unimodal polygon $u_0l_1u_1l_2u_2$ has loops l_i in $I_i \subset \{1,\ldots,d\}$, then $I_1 \cap I_2 = \emptyset$. Thus a unimodal polygon is made up of a sequence of unimodal loops separated by staircase polygons where the structure of the distribution of the loops can be described by a partition of d. The generating function for unimodal polygons having loops corresponding to this partition can be expressed in terms of Z_λ, λ the partition of d, and U_k, $k \leq d$. Then this result, together with equation (1) and theorem 2 gives a means of calculating the number of self-avoiding convex polygons.

3. 2-D Polygons

In dimension $d = 2$, $P - P_1 = P_2$, so combining theorems 1 and 2 gives

$$E\left[\frac{x_1x_2(1-x_1)^2(1-x_2)^2}{(1-x_1-x_2)^2}\right] = C_2 + 2Z_2U_2^2$$

Setting $\Delta = 1 - 2x_1 - 2x_2 - 2x_1x_2 + x_1^2 + x_2^2$, and solving for C_2 using $U_2 = 2\frac{x_1x_2}{\sqrt{\Delta}}$ and (2) gives

$$C_2 = \frac{2x_1x_2A}{\Delta^2} - \frac{8x_1^2x_2^2}{\Delta^{3/2}}$$

where

$$A = 1 - 3x_1 - 3x_2 + 3x_1^2 + 3x_2^2 + 5x_1x_2 - x_1^3 - x_2^3 - x_1^2x_2 - x_1x_2^2 - x_1x_2(x_1 - x_2)^2.$$

This was first proved by Lin and Chang [6], and is a refinement of a result by Delest and Viennot [3]. Alternate proofs are found in [1] and [5]. This work gives a nice combinatorial interpretation of each of the two parts of C_2 in terms of convex polygons having no one-dimensional loops, thereby solving an open problem due to Viennot.

4. 3-D Polygons

This time, the situation is more complicated. Given $P - P_1 = P_2 + P_3$, where $P - P_1$ is calculated using theorem 1, and $P_3 = C_3 + 4Z_3U_3^2$ by theorem 2, it remains to find a way to count P_2, the number of polygons in $\mathbb{Z}^3$ having 2-dimensional loops but no 1-dimension loops. This can be done by a case-by-case analysis of the 7 possible loop structures. The result is

$$C_3 = A(t) + \frac{B(t)}{Z_3}$$

where $A(t)$ and $B(t)$ are algebraic in t, and Z_3 is D-finite. $A(t)$ is of degree 16, and $B(t)$ has degree 8. (The exact value of C_3 would take up a quarter of the page.)

5. Conclusion

This method works because the loops of unimodal polygons are non-overlapping. In theory this method is extensible to higher dimensions, though of course in practice the calculation of the P_i's for $i < d$ would become difficult. Since for each d the series Z_d is D-finite and the series U_d can be written in terms of Z_d, is seems reasonable from the formula to believe that the result will continue to be a quotient of two D-finite series. There may be generalizations to polygons that are convex along $d - 1$ directions, and 3-choice polygons.

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