GEOMETRY OF PENTAGONS AND VOLUMES OF FULLERENES

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Abstract

We provide new proofs of some known facts from geometry of pentagons and hexagons and prove some new facts and formulas concerning areas. We reprove the Gauss pentagon formula, the hexagon analogue and show some consequences. We also give a new proof of the Robbins area formula for cyclic pentagons (and hexagons). This proof is intrinsic.We also prove formulas relating area, circumradius and side lengths of such polygons. The obtained results we apply to get an efficient algorithm for computing surface areas and volumes of inscribed "fullerenes", i.e. 3-polytopes (solids) inscribed in a sphere of given radius, whose faces are at most hexagons and knowing only the graph and edge lengths of the fullerene.

1 Introduction

In this paper we prove some new and reprove some known facts from geometry of pentagons and hexagons. The main topic is how to efficiently compute the area of such polygons.

The main application of the above mentioned results is to obtain an efficient procedure to compute the surface area and volume of certain (3-dimensional) polytopes. We call a (mathematical) "fullerene" a polytope whose faces are only triangles, quadrilaterals, pentagons and hexagons in any possible combination. In general, computing volume of a polytope is a hard problem, and again, of course, it depends on the available data. And so is with general fullerenes. However, in section 5 we show how to compute in a rather efficient way the volume (and surface area) of a fullerene inscribed in a sphere of a given radius R, knowing only the combinatorial structure (i.e. the graph) of the fullerene and its edge lengths.

2 Triangles and quadrilaterals

Here we briefly recall and provide short proofs of some of the facts from geometry of triangles and quadrilaterals which we shall use later. One of the hallmarks is the famous *Heron's formula* from the 1st century (known also to Archimedes in the 3th century B.C.). Here is a "one-sentence proof". Let T be the area of a triangle ΔABC with side lengths a, b, c (in the standard way, i.e., a opposite to A etc.), and let C be the angle at the vertex

C. Then by laws of sines and cosines we have $4T = 2ab\sin C$ and $a^2+b^2-c^2 = 2ab\cos C$. By squaring and adding the last two formulas we get

$$(4T)^2 + (a^2+b^2-c^2)^2 = (2ab)^2 \ , \tag{1}$$

hence

$$(4T)^2 = (2ab)^2 - (a^2+b^2-c^2)^2 \ . \tag{2}$$

More symmetrically, (2) can be written as

$$(4T)^2 = 4[(ab)^2+(bc)^2+(ca)^2] - (a^2+b^2+c^2)^2, \tag{3}$$

or as $(4T)^2 = 4e_2 - e_1^2$, where e_1, e_2 are the elementary symmetric functions of a^2, b^2, c^2.

In the very recognizible form of square root, the Heron formula reads as

$$T = \sqrt{s(s-a)(s-b)(s-c)} \ , \tag{4}$$

where $s = (a+b+c)/2$ is the triangle's semiperimeter.

Now we turn to quadrilaterals (or quadrangles). Let $ABCD$ be a convex quadrilateral with side lengths $a = AB$, $b = BC$, $c = CD$, and $d = DA$, and lengths of diagonals $e = AC$ and $f = BD$. Denote by A, B, C, D the interior angles by vertices by the same letter, i.e. $A = \angle DAB$, $B = \angle ABC$, etc. Let $Q = \text{area}(ABCD)$ be the area of the quadrilateral $ABCD$. Then the following *Bretschneider's formula* (from around 1840) holds

$$(4Q)^2 = (2ef)^2 - (a^2-b^2+c^2-d^2)^2. \tag{5}$$

Another quadrilateral area formula is the following.

$$Q = \sqrt{(s-a)(s-b(s-c)(s-d) - abcd\cos^2\frac{A+C}{2}} \ , \tag{6}$$

where $s = (a+b+c+d)/2$ is again the semiperimeter.

The Bretschneider's formula can also be written in the following form:

$$Q = \sqrt{(s-a)(s-b)(s-c)(s-d) - \frac{1}{4}(ac+bd+ef)(ac+bd-ef)}. \tag{7}$$

Consider (simultaneously) three different cyclic quadrilaterals inscribed in a circle of radius R, all having side lengths a, b, c, d and diagonals e, f, g. But, if a, b, c, d is the cyclic order of the side lengths, then e, f is the diagonal pair and e separates the pair a, b from the pair c, d. Similarly, for the cyclic order a, c, b, d the diagonal pair is g, f, and for the cyclic order a, b, d, c the diagonal pair is e, g. Then clearly all three of these qudrilaterals have the same area Q, the same semiperimeter s and the same circumradius R.

Proposition 2.1 *The following (equivalent) relations hold.*
1) $4QR = (ab+cd)e = (ad+bc)f = (ac+bd)g$ *;*
2) $4QR = efg$ *;*
3) $ef = ac+bd, fg = ab+cd, eg = ad+bc$ *(Ptolemy formula);*
4) $(4QR)^2 = (ab+cd)(ac+bd)(ad+bc)$*,*
or, expanded by powers of a: $(4QR)^2 = pa^3 + ta^2 + pqa + p^2$ *,*
where $p = bcd$*,* $q = b^2+c^2+d^2$*, and* $t = (bc)^2+(cd)^2+(db)^2$*;*

5) $e^2 = \dfrac{(ad+bc)(ac+bd)}{ab+cd}$, $\quad f^2 = \dfrac{(ab+cd)(ac+bd)}{ad+bc}$, $\quad g^2 = \dfrac{(ab+cd)(ad+bc)}{ac+bd}$;

6) $R^2 = \dfrac{(ab+cd)(ac+bd)(ad+bc)}{4(ac+bd)^2-(a^2-b^2+c^2-d^2)^2}$;

7) $(4Q)^2 = 4[(ab)^2+(ac)^2+(ad)^2+(bc)^2+(bd)^2+(cd)^2]-(a^2+b^2+c^2+d^2)^2+8abcd =$
$= 4(ac+bd)^2-(a^2-b^2+c^2-d^2)^2 =$
$= 16(s-a)(s-b)(s-c)(s-d)$ *(Brahmagupta's formula, 7th century).*

3 The Gauss pentagon area formula

A rather forgotten "gem" of Gauss (from 1823) is the pentagon area formula. Let us briefly recall it and provide its short proof. Let $ABCDE$ be a convex pentagon. A vertex triangle of a pentagon is called any triangle with three consecutive vertices. Denote the area of a *vertex triangle* by the middle vertex enclosed by (). So, let $(A) = \text{area}(EAB)$, $(B) = \text{area}(ABC)$, $(C) = \text{area}(BCD)$, $(D) = \text{area}(CDE)$, and $(E) = \text{area}(DEA)$.

The Gauss formula says that to compute the area of a (convex) pentagon, it is enough to know only the areas of its vertex triangles. More precisely, the following holds, see [6], [7], [19].

Theorem 3.1 ***(The Gauss pentagon formula).***
Let K be the area of a convex pentagon $ABCDE$. Denote by c_1 and c_2 the first and second cyclic symmetric function of the areas of the vertex triangles of the pentagon, respectively. Precisely,

$$c_1 = (A)+(B)+(C)+(D)+(E),$$

and

$$c_2 = (A)(B)+(B)(C)+(C)(D)+(D)(E)+(E)(A) \ .$$

Then K is given by

$$K^2 - c_1 K + c_2 = 0 \ . \tag{8}$$

4 Cyclic pentagons and hexagons and the Robbins formula

We shall consider now cyclic pentagons and hexagons and give a new proof of the Robbins formula. The *Robbins formula* is the formula for the area of a cyclic pentagon (and hexagon) in terms of its side lengths. So, it is next in the sequence of formulas of Heron and Brahmagupta. Robbins proved it in 1994, see [12] and [13].

Theorem 4.1 ***(The Robbins pentagon formula).*** *The area K of a cyclic pentagon satisfies the following monic heptic (i.e. degree 7) equation in $(4K)^2$ in terms of elementary symmetric functions e_k $(1 \le k \le 5)$ of squares of its side lengths:*

$$B^2[(4K)^2B + H_1^2] - 128e_5[16H_1^3 + 18(4K)^2H_1B + 2^7 3^3 e_5 (4K)^4] = 0 \ . \tag{9}$$

Here:

$$\begin{aligned} H &:= (4K)^2 + e_1^2 - 4e_2 \quad \text{(H for "Heron")}, \\ H_1 &:= e_1 H + 8e_3, \\ B &:= H^2 - 64e_4 \quad \text{(B for "Brahmagupta")}. \end{aligned} \tag{10}$$

Proposition 4.2 *Let K and R be the area and circumradius of a cyclic pentagon. Then $Z = 4KR$ satisfies the following heptic equation in terms of monomial functions $m_{\lambda_1\lambda_2\ldots}$ of squares of side lengths $a, \ldots, e$ and the product $\eta = abcde$:*

$$\begin{aligned}
&-Z^7 + 2m_{111}Z^5 + (m_2 + 6m_{11})\eta Z^4 + \\
&+(m_{3111} - m_{222} + 17m_{21111})Z^3 + (m_{311} - 2m_{221} + 3m_{2111} + 44m_{11111})\eta Z^2 + \\
&+(m_{31} - 2m_{22} - m_{211} + 12m_{1111})\eta^2 Z + (m_3 - m_{21} + 2m_{111})\eta^3 = 0 \ .
\end{aligned} \tag{11}$$

Theorem 4.3 ***(The Robbins hexagon formula).*** *Let K be the area of a cyclic hexagon, e_k, $k = 1, \ldots, 6$ the elementary symmetric functions of its squared side lengths, $\eta = \sqrt{e_6}$, and let quantities H, B and H_1 as before. Then $(4K)^2$ satisfies the following monic heptic equation with either upper or lower signs*

$$\begin{aligned}
&(B \pm 64e_1\eta)^2[(4K)^2(B \pm 64e_1\eta) + (H_1 \mp 16\eta)^2] - (128e_5 \pm 32H\eta)[16(H_1 \mp 16\eta)^3 + \\
&18(4K)^2(H_1 \mp 16\eta)(B \pm 64e_1\eta) + 27(128e_5 \pm 32H\eta)(4K)^4] = 0.
\end{aligned} \tag{12}$$

As in the pentagon case, here also there is an expression (heptic equation) in $(4KR)^2$ in terms of side lengths analogous to (11). One also starts here by using twice formula 4) from Proposition 2.1. And finally, the "hexagon R^2-equation" can also be derived similarly.

In fact, long ago Möbius in [10] proved the existence of a polynomial equation in R^2 in terms of squared side lengths of a cyclic n-gon of degree Δ_k for $n = 2k+1$, and $2\Delta_k$ for $n = 2k+2$, where

$$\Delta_k = \frac{1}{2}[(2k+1)\binom{2k}{k} - 2^{2k}] = \sum_{i=0}^{k-1}(k-i)\binom{2k+1}{i}, \tag{13}$$

It was only recently proved (see [9] and [4]) that there is also a monic irreducible polynomial equation for $(4K)^2$ in terms of (symmetric functions of) squared side lengths of a cyclic n-gon of the same degree as above Δ_k (or $2\Delta_k$). The coefficients are integers, and the polynomial is unique (up to sign). In the same paper [9] an explicit area formula for a heptagon and octagon was given as well. In this context, see also [11] and [2].

5 Surface area and volumes of fullerenes

With this model in mind we call a *mathematical fullerene* (which we still call simply a *fullerene*) a convex polytope P whose faces make any possible mixture of triangles, quadrilaterals, pentagons and hexagons. *Inscribed fullerene* is a fullerene which is inscribed in a sphere (i.e. all vertices lie on a sphere).
Suppose we know the combinatorial structure of P, i.e. the graph $G(P)$ of P, the lengths of all edges of P, $l(P) = \{a_{ij}\}$, and in the case of an inscribed fullerene, the radius R of the circumscribed sphere. Based only on these data, we want to compute the surface area of P and volume of P, $vol(P)$. And we want to do it in an efficient way.

Of course, for a general fullerene these data are not sufficient. If we, instead know the areas of all vertex triangles of all faces of P, then an efficient way to compute the surface area of P is to use the Gauss formula for pentagons and analogous formula for hexagons (provided we know an additional triangle area in every hexagon).

When only edge lengths are available, we can get an upper bound for the area using the isoperimetric inequality for an n-gon which relates the perimeter L and the area K of the n-gon:

$$\frac{L^2}{K} \geq 4n \tan\frac{\pi}{n}, \tag{14}$$

with equality if and only if the polygon is regular (see [5]). An upper bound for the volume V of the polytope in terms of its surface area S is given by the following "isoperimetric inequality" for a convex polytope P with

m faces:

$$\frac{S^2}{V^3} \geq 54(m-2)(4\sin^2\alpha_m - 1)\tan\alpha_m, \tag{15}$$

where $\alpha_m = \frac{\pi}{6}\frac{m}{m-2}$. Equality here occurs if and only if P is the regular tetrahedron, cube or dodecahedron (see [5]).

Suppose now that beside edge lengths of a fullerene we know in every quadrilateral one diagonal and in every pentagon two touching diagonals. Then three Heron's formulas computes the area of the pentagon, and if two crossing diagonals are given then after solving a quadratic equation we again use Heron's formula three times (or once Heron's and once Breitschneider's formula) to get the area of a pentagon.

A bit more complex computation is needed to get hexagon's area when in addition to all side lengths three more lengths of diagonals are given.

Consider now a fullerene P inscribed in a sphere of radius R. Then all of its faces are cyclic polygons and to compute area(P), the surface area of P, we have to add all face areas area(F) for all faces F of P. If we know $G(P)$ and $l(P)$, then by using formulas of Heron, Brahmagupta or Robbins, depending on the face F, we can do the job.
This time, however, we can compute the volume $vol(P)$ of P also in the exact terms. It is equal to the sum of volumes of pyramides whose apex is in the circumsphere center. So,

$$\mathrm{vol}(P) = \frac{1}{3}\sum_F \mathrm{area}(F)\cdot h_F,$$

where the sum runs over all faces F of P, and where h_F is the height of the corresponding pyramide. Every term area(F) we compute in terms of side lengths as explained above. Next, since every face is a cyclic polygon, let r_F be the circumradius of the face F. If F is a triangle or quadrilateral, then this radius is easy to compute (by using Proposition 2.1 6)). But, for a pentagon or hexagon we use a heptic in r_F^2 as explained in section 4. Finally, the height is given by $h_F = \sqrt{R^2 - r_F^2}$.
However, the volume of an inscribed fullerene P can be, in fact, computed more efficiently in the following way:

$$\mathrm{vol}(P) = \frac{1}{12}\sum_F \sqrt{R^2(4\,\mathrm{area}(F))^2 - (4r_F\,\mathrm{area}(F))^2}. \tag{16}$$

To compute $(4\,\mathrm{area}(F))^2$ we use again the corresponding formula of Heron, Brahmagupta or Robbins (Theorems 4.1, or 4.3) and for computing the term $(4r_F\,\mathrm{area}(F))^2$ we use Proposition 2.1, formula 4) for quadilaterals, Proposition 4.2 for pentagons and the procedure explained in section 4 for hexagons.
So, this relatively simple algorithm computes (or, at least relates) in an exact and efficient way the volume vol(P), in terms of the graph $G(P)$, the edge lengths $l(P)$ and circumradius R of an inscribed fullerene P.
Let v, e and f be the numbers of vertices, edges and faces of P, respectively, $v - e + f = 2$, and let f_k be the number of k-gon faces of P, $k = 3, 4, 5, 6$. By neglecting the basic operations (additions etc.), the algorithm complexity roughly amounts to solving $2(f_5 + f_6)$ heptic equations and taking about $4f$ square roots, i.e. solving quadratics. Of course, often these equations could be solved only numerically but with any precision.
Finally, just note that for some special fullerenes we don't need the full machinery described above to compute the surface area and volume; examples are affine regular, affine semiregular and other special kinds of fullerenes.

And one final remark is that by results of [9], we can, at least theoretically include heptagons and octagons as faces of fullerenes, and still be able, in principle, to compute volume of such an inscribed "quasi fullerene".

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