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On the number of *k*-faces of primitive parallelohedra

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Dehn–Sommerville relations for simple (simplicial) polytopes are applied to primitive parallelohedra. New restrictions on numbers of k-faces of non-principal primitive parallelohedra are explicitly formulated for five-, six- and seven-dimensional parallelohedra.

1. Introduction

Recently Baburin & Engel (2013) gave an interesting table listing the numbers N_k of k-faces of primitive parallelohedra[1] in E^d, $2 \le d \le 6$. For principal primitive parallelohedra these numbers were found by Voronoï (1908*a*,*b*) but for $d \ge 5$ there exist non-principal parallelohedra and, apparently, as numerical results show for $d = 5, 6$, there are serious restrictions on the numbers of k-faces (abbreviated below as f-vectors) for non-principal parallelohedra. The aim of this short note is to combine known facts about f-vectors of simple polytopes, namely the Dehn–Sommerville relations (Barvinok, 2002), together with some general properties of primitive parallelohedra in order to get restrictions on possible values of f-vectors for non-principal primitive parallelohedra. The restrictions thus obtained are collected in Table 1. They are not very sharp and become less interesting with increasing dimension. Nevertheless, the author hopes that some additional simple but general relations can be added for primitive parallelohedra to improve significantly the freedom in the choice of possible f-vectors. That is why the author finds it useful to bring this (not well solved) problem to the attention of the crystallographic community.

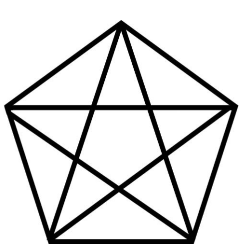
The next two sections briefly summarize useful properties of primitive parallelohedra and of simple polytopes. The last section presents the results and speculations about possible generalizations and improvements.

2. Primitive parallelohedra

A parallelohedron P in a facet-to-facet tiling of E^d is named primitive if in every k-face of P, $k = 0, 1, \ldots, d-1$, exactly $d - k + 1$ adjacent parallelohedra meet. In particular, each vertex, v, of a primitive parallelohedron in E^d is determined by the intersection of d facets. Let $\{\mathbf{f}_{l_1}, \ldots, \mathbf{f}_{l_d}\}$ be the set of the corresponding facet vectors[2] whose corresponding facets meet in a common vertex v of a lattice L. These vectors are linearly independent and determine a sublattice of the lattice L of

[1] Parallelohedra are convex bodies which tile space by translations. Parallelohedra appear naturally in crystallography, for example, as Voronoï cells of lattices.

[2] Facet vectors $\pm\mathbf{f}_i$ of a Voronoï cell of a lattice L are the shortest vectors in their $L/2L$ coset.



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index $\omega(v)$. It was shown by Voronoï (1908*a*,*b*) that the upper bound for the number of vertices is reached exactly if, for each vertex v of a primitive parallelohedron, $\omega(v) = 1$. Ryshkov & Baranovskii (1998) gave upper bounds for the index $\omega(v)$, namely, they have proved that for dimensions $d = 2, 3, 4, 5, 6$ the maximal values of the index $\omega(v)$ are 1, 1, 1, 2, 3, respectively.

The primitive parallelohedron with $\omega(v) = 1$ for each of its vertices is called principal primitive. Voronoï has shown that the number of k-faces N_k, $0 \le k \le d$, of a parallelohedron in E^d satisfies the following inequality:

$$N_k \le (d+1-k) \sum_{l=0}^{d-k} (-1)^{d-k-l} \binom{d-k}{l} (1+l)^d. \qquad (1)$$

For the number of facets (*i.e.* for $k = d-1$), equation (1) becomes an equality *for all primitive* parallelohedra:

$$N_{d-1} = 2(2^d - 1) \qquad (2)$$

and coincides with the upper bound in the inequality for the number of facets given by Minkowski (1907) for a d-dimensional parallelohedron:

$$2d \le N_{d-1} \le 2(2^d - 1). \qquad (3)$$

The equality sign in (1) holds for principal primitive parallelohedra for any k.

Another important property of primitive parallelohedra which is used below is the divisibility property of the k-face numbers. Namely, the number of k-faces of primitive parallelohedra should be a multiple of $2(d-k+1)$ for $k < d-1$ (Engel *et al.*, 2004).

3. Dehn–Sommerville relations for simple polytopes

A d-dimensional polytope P is called *simple* if every vertex v of P belongs to exactly d facets of P.

The class of simple polytopes is larger than the class of primitive parallelohedra defined in terms of primitive tilings. For example, the d-dimensional cube is a simple but not primitive parallelohedron. For a simple d-dimensional polytope the system of linear relations between numbers of k-faces (known as Dehn–Sommerville relations) consists of $\lfloor (d+1)/2 \rfloor$ relations, where $\lfloor x \rfloor$ is the integer part of x. The simplest way to introduce these relations is to use the so-called h-vectors of the polytope (Barvinok, 2002).

Definition. h-vector: let P be a d-dimensional simple polytope and $N_k(P)$ be the number of k-dimensional faces of P [we agree that $N_d(P) = 1$]. Let

$$h_k(P) = \sum_{i=k}^{d} (-1)^{i-k} \binom{i}{k} N_i(P) \text{ for } k = 0, \ldots, d. \qquad (4)$$

The $(d+1)$-tuple $[h_0(P), \ldots, h_d(P)]$ is called the h-vector of P.

It can be proved that numbers of k-faces, N_k, can be uniquely determined from $h_k(P)$:

Table 1
Restrictions on possible values of f-vectors for primitive parallelohedra.

For the boundaries of the domain of variation of α, β, γ parameters, see the text.

d	2	3	4	5	6	7
N_0	6	24	120	$720 - 12\alpha$	$5040 + 12\alpha - 40\gamma$	$40320 + 48\alpha - 16\beta$
N_1	6	36	240	$1800 - 30\alpha$	$15120 + 36\alpha - 120\gamma$	$141120 + 168\alpha - 56\beta$
N_2	1	14	150	$1560 - 24\alpha$	$16800 + 30\alpha - 120\gamma$	$191520 + 204\alpha - 72\beta$
N_3		1	30	$540 - 6\alpha$	$8400 - 40\gamma$	$126000 + 90\alpha - 40\beta$
N_4			1	62	$1806 - 6\alpha$	$40824 - 8\beta$
N_5				1	126	$5796 - 6\alpha$
N_6					1	254

$$N_i(P) = \sum_{k=i}^{d} \binom{k}{i} h_k(P) \text{ for } i = 0, \ldots, d. \qquad (5)$$

Now we formulate without proof the following important proposition.

Proposition (Dehn–Sommerville relations). Let P be a simple d-dimensional polytope. Then

$$h_k(P) = h_{d-k}(P) \text{ for } k = 0, \ldots, d \qquad (6)$$

and

$$1 = h_0 \le h_1 \le \ldots \le h_{\lfloor d/2 \rfloor}. \qquad (7)$$

For centrally symmetric simple d-polytopes Stanley (1996) improved inequality (7), namely:

$$h_i - h_{i-1} \ge \binom{d}{i} - \binom{d}{i-1}, \text{ for } i \le \lfloor d/2 \rfloor. \qquad (8)$$

For primitive parallelohedra (which form a subclass of simple polytopes) we can apply Dehn–Sommerville relations together with explicit expression (2) for the number of facets of primitive parallelohedra and the upper bound for the number of k-faces of primitive parallelohedra given by Voronoï [equation (1)]. Also we take into account that the number of k-faces of primitive parallelohedra should be a multiple of $2(d-k+1)$ for $k < d-1$.

4. Restrictions on the number of k-faces for primitive parallelohedra

In this section we apply Dehn–Sommerville relations separately to primitive parallelohedra of different dimensions.

4.1. d = 2 primitive parallelohedra

We start with the trivial case of two-dimensional primitive parallelohedra. For $d = 2$, the only Dehn–Sommerville relation coincides with the Euler equation of the polytope. Together with $N_1 = 6$ which follows from the general bound (2) this determines the unique f-vector of numbers of faces $(N_1 = 6, N_0 = 6)$ for primitive two-dimensional parallelohedra.

4.2. $d = 3$ primitive parallelohedra

For $d = 3$ the second Dehn–Sommerville relation appears which can be written in a form applicable for any $d \geq 3$,

$$dN_0(P) = 2N_1(P) \text{ for } d \geq 3. \quad (9)$$

Applying two Dehn–Sommerville relations to three-dimensional simple polytopes we get the following expression for the *f*-vector:

$$(N_0 = 2N_2 - 4, \quad N_1 = 3N_2 - 6, \quad N_2), \quad (10)$$

which includes one free parameter, N_2. For primitive three-dimensional parallelohedra the number of facets is $N_2 = 14 = 2(2^3 - 1)$ [this follows from (2)] and we get the unique possible *f*-vector for three-dimensional primitive parallelohedra: $(N_0 = 24, N_1 = 36, N_2 = 14)$.

4.3. $d = 4$ primitive parallelohedra

The same two general linear Dehn–Sommerville relations exist for four-dimensional simple polytopes. This means that we can express numbers of *k*-faces for four-dimensional simple polytopes in terms of two free parameters, say N_3 and N_2:

$$(N_0 = N_2 - N_3, \quad N_1 = 2N_2 - 2N_3, \quad N_2, \quad N_3). \quad (11)$$

It follows that for primitive 4-parallelohedra after imposing $N_3 = 30 = 2(2^4 - 1)$ and $N_2 = 150 - 6\alpha$, taking into account that primitive parallelohedra have only sixfold belts (*i.e.* N_{d-2} should be a multiple of 6), we get for the *f*-vector and for the *h*-vector the following expressions which depend on one free integer parameter α:

$$(N_0 = 120 - 6\alpha, \quad N_1 = 240 - 12\alpha, \quad N_2 = 150 - 6\alpha, \quad N_3 = 30, \quad N_4 = 1); \quad (12)$$

$$(h_0 = 1 = h_4, \quad h_1 = 26 = h_3, \quad h_2 = 66 - 6\alpha). \quad (13)$$

Applying relation (7) we get immediately that α can take only a small number of values, namely $\alpha = 0, 1, 2, 3, 4, 5, 6$. But among these values only $\alpha = 0$ and $\alpha = 5$ give the number of vertices divisible by 10 and among these two possible values only $\alpha = 0$ gives the number of edges divisible by 8. Consequently, we get that the only possible *f*-vector for primitive four-dimensional parallelohedra is $(N_0 = 120, N_1 = 240, N_2 = 150, N_3 = 30, N_4 = 1)$. Note that there are three combinatorially different primitive parallelohedra for $d = 4$. All three are principal primitive. There exists also one combinatorial type of $d = 4$ parallelohedra which has the maximal number of facets but which is non-primitive.

4.4. $d = 5$ primitive parallelohedra

For five-dimensional simple polytopes there are three Dehn–Sommerville linear relations which we give explicitly below:

$$N_0 - N_1 + N_2 - N_3 + N_4 - 2 = 0; \quad (14)$$

$$N_1 - 2N_2 + 3N_3 - 5N_4 + 10 = 0; \quad (15)$$

$$N_2 - 4N_3 + 10N_4 - 20 = 0. \quad (16)$$

For primitive parallelohedra $N_4 = 62 = 2(2^5 - 1)$ and we can express N_{d-2} as $N_3 = 540 - 6\alpha$, taking into account again that primitive parallelohedra have only sixfold belts (*i.e.* N_{d-2} should be a multiple of 6). This allows us to express all numbers of faces in terms of one free parameter α:

$$(N_0 = 720 - 12\alpha, \quad N_1 = 1800 - 30\alpha, \quad N_2 = 1560 - 24\alpha, \quad N_3 = 540 - 6\alpha, \quad N_4 = 62) \text{ with } \alpha = 0, 1, \ldots. \quad (17)$$

For the components of the *h*-vector we have

$$(h_0 = 1 = h_5; \quad h_1 = 57 = h_4; \quad h_2 = 302 - 6\alpha = h_3). \quad (18)$$

It is easy to see that N_k (for $k < d - 1 = 4$) are divisible by $2(d - k + 1)$ for any integer $\alpha = 0, 1, \ldots$. The *f*-vectors found by Baburin & Engel (2013) correspond to $\alpha = 0, 1$. The restriction imposed by inequality (7) applicable to any simple polytopes gives upper boundary $\alpha \leq 40$, which is very far above the observed values.

4.5. $d = 6$ primitive parallelohedra

For six-dimensional simple polytopes there are again three linear Dehn–Sommerville relations. Together with $N_5 = 126 = 2(2^6 - 1)$ this gives for six-dimensional primitive parallelohedra the following expression for the *f*-vector depending on two free parameters:

$$(N_5 = 126; \quad N_4 = 1806 - 6\alpha; \quad N_3 = 8400 - 8\beta; \quad N_2 = 16800 + 30\alpha - 24\beta; \quad N_1 = 15120 + 36\alpha - 24\beta; \quad N_0 = 5040 + 12\alpha - 8\beta). \quad (19)$$

We see that for any integer α, β the N_4 is divisible by 6, the N_3 is divisible by 8, the N_1 is divisible by 12. At the same time N_2 becomes a multiple of 10 only for $\beta = 5\gamma$, with $\gamma = 0, 1, 2, \ldots$. Replacing β by 5γ we get

$$(N_5 = 126; \quad N_4 = 1806 - 6\alpha; \quad N_3 = 8400 - 40\gamma; \quad N_2 = 16800 + 30\alpha - 120\gamma; \quad N_1 = 15120 + 36\alpha - 120\gamma; \quad N_0 = 5040 + 12\alpha - 40\gamma). \quad (20)$$

But we still need to check that N_0 is divisible by 14. This is equivalent to the requirement for $(3\alpha - 10\gamma)$ to be a multiple of 7. This is possible only for $\alpha = 0$, $\gamma = 0, 7, 14, \ldots$; $\alpha = 1$, $\gamma = 1, 8, 15, \ldots$; $\alpha = 2$, $\gamma = 2, 9, 16, \ldots$ *etc.* More generally we should have $\gamma - \alpha = 7k$.

Taking into account that for any set of two free parameters, α, γ, the numbers of faces cannot exceed their values for principal primitive parallelohedra, we get general restrictions on possible values of free parameters $0 \leq 3\alpha \leq 10\gamma$. Together with the divisibility constraint $\gamma = \alpha + 7k$, with k being any integer, it follows that for $\gamma = 0$ the only possible value of the second parameter is $\alpha = 0$. Similarly, for $\gamma = 1$ we should have $\alpha = 1$ and for $\gamma = 2$, $\alpha = 2$. Only starting from $\gamma = 3$, several values of the second parameter are possible; in particular formal solutions are $(\gamma = 3, \alpha = 3)$ and $(\gamma = 3, \alpha = 10)$. Numerical results given by Baburin & Engel (2013) correspond to *f*-vectors with $\alpha = \gamma = 0, 1, \ldots, 16$. These results indicate that for six-dimensional primitive parallelohedra the whole observed set of *f*-vectors can be described as only a one-parameter family. This allows us to suggest that there exists an additional property of primitive parallelohedra which is not taken into account in the present analysis.

It is clear that with increasing dimension the number of free parameters for the *f*-vectors obtained within the scheme adopted above increases. For seven-dimensional parallelohedra we still have two free parameters but for eight-dimensional parallelohedra there are three such parameters *etc*. The question whether the exact solution for *f*-vectors of primitive parallelohedra in any dimension can be described by a one-parameter family or a multi-parameter family is an interesting open problem.

4.6. $d = 7$ primitive parallelohedra

To go a little bit beyond results for the *f*-vectors of primitive parallelohedra communicated in Baburin & Engel (2013) we give here a short comment about solutions for $d = 7$ which are listed in Table 1 together with solutions for $d = 2, 3, 4, 5, 6$.

For $d = 7$ there are four Dehn–Sommerville linear relations which can be explicitly rewritten from (6) as

$$N_0 - N_1 + N_2 - N_3 + N_4 - N_5 + N_6 - 2 = 0; \qquad (21)$$

$$N_1 - 2N_2 + 3N_3 - 4N_4 + 5N_5 - 7N_6 + 14 = 0; \qquad (22)$$

$$N_2 - 3N_3 + 6N_4 - 11N_5 + 21N_6 - 42 = 0; \qquad (23)$$

$$N_3 - 5N_4 + 15N_5 - 35N_6 + 70 = 0. \qquad (24)$$

Replacing $N_6 = 254 = 2(2^7 - 1)$, $N_5 = 5796 - 6\alpha$ and $N_4 = 40824 - 8\beta$ we get the following set of components of *f*-vectors depending on two free parameters:

$$(N_0 = 40320 + 48\alpha - 16\beta, \quad N_1 = 141120 + 168\alpha - 56\beta, \quad N_2 = 191520 + 204\alpha - 72\beta, \quad N_3 = 126000 + 90\alpha - 40\beta, \quad N_4 = 40824 - 8\beta, \quad N_5 = 5796 - 6\alpha, \quad N_6 = 254). \qquad (25)$$

Now for any integer α and β the N_k, $k < d - 1$, numbers are always divisible by $2(d - k + 1)$. Taking into account that N_k numbers for any choice of α and β parameters cannot be larger than the limiting values for principal primitive parallelohedra, we get the following restriction of parameters: $\beta \geq 3\alpha \geq 0$. Whether an additional linear inequality between possible values of α and β parameters exists for primitive parallelohedra in a way similar to the situation observed for six-dimensional parallelohedra is a very interesting question. To find sharper lower boundaries for the numbers of faces of primitive parallelohedra (or equivalently the upper boundary on free parameters $\alpha, \beta, \gamma, \ldots$) is another challenge.

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References

Baburin, I. A. & Engel, P. (2013). *Acta Cryst.* A**69**, 510–516.
Barvinok, A. (2002). *A Course in Convexity*. Providence: AMS.
Engel, P., Michel, L. & Senechal, M. (2004). *Lattice Geometry*. IHES preprint P/04/45.
Minkowski, H. (1907). *Diophantische Approximationen*. Leipzig: Teubner. Reprinted by Chelsea, New York, 1957.
Ryshkov, S. S. & Baranovskii, E. P. (1998). *Proc. Inst. Math. Acad. Sci. Ukraine*, **21**, 115–124.
Stanley, R. P. (1996). *Combinatorics and Commutative Algebra*. Boston: Birkhäuser.
Voronoï, G. M. (1908*a*). *J. Reine Math.* **134**, 198–287.
Voronoï, G. M. (1908*b*). *J. Reine Math.* **135**, 67–181.