A census of flag-vectors of 4-polytopes

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How close to a complete description are the known conditions on the flag-vectors of 4-dimensional convex polytopes? We present a computational study (in the POLYMAKE framework) of this question. For small numbers of vertices the conditions are pretty good: only one "impossible flag-vector" satisfies the conditions for $f_0 \leq 7$, and only 12 for $f_0 = 8$.

(1) The set of all f-vectors of (convex, bounded) d-polytopes has dimension $d-1$: the only linear relation is given by the Euler-Poincaré equation. The corresponding set $\mathcal{F}(\mathcal{P}^d)$ of all the flag-vectors of d-polytopes has dimension $F_d - 1$, where F_d is the d-th Fibonacci number ($F_0 = F_1 = 1$, $F_k = F_{k-1} + F_{k-2}$): their linear relations are given by the generalized Dehn-Sommerville equations of Bayer & Billera [6].

(2) For $d = 3$, both the f-vector and the flag-vector of a 3-polytope is determined by (f_0, f_2). In these coordinates, the set of all f-vectors, and of all flag-vectors of 3-polytopes is completely described by

$$\{(f_0(P), f_2(P)) : P \in \mathcal{P}_3\} \quad = \quad \{(f_0, f_2) \in \mathbb{Z}^2 : \begin{array}{l} f_0 \leq 2f_2 - 4, \\ f_2 \leq 2f_0 - 4\}, \end{array}$$

a classical result of Steinitz [12]. In particular, $\mathcal{F}(\mathcal{P}^3)$ has a finite linear description, so the convex hull $\mathrm{conv}(\mathcal{F}(\mathcal{P}^3))$ is closed, and all the integral points in this set are f-vectors, that is, $\mathrm{conv}(\mathcal{F}(\mathcal{P}^3)) \cap \mathbb{Z}^3 = \mathcal{F}(\mathcal{P}^3)$. A complete characterization (involving non-linear

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relations) is also available for *simplicial* d-polytopes with the "g-Theorem" of Stanley and Billera & Lee, but not for *general* d-polytopes and any $d \geq 4$.

(3) For $d = 4$, the flag-vector $\mathcal{F}(P)$ of a 4-polytope $P \in \mathcal{P}^4$ is given by

$$\mathcal{F}(P) := (f_0, f_1, f_3, f_{03})$$

together with the linear relations quoted in **(1)**. In these coordinates, the known conditions and restrictions on possible flag-vectors may be summarized as follows (see [5] and [7]):

(3.0) $(f_0, f_1, f_3, f_{03}) \in \{1, 2, 3, \dots\}^4 \subseteq \mathbb{R}^4$

(3.1) Linear inequalities

$$\begin{array}{lrrrrcr}
(3.1.1) & -\ f_0 & +\ f_1 & +3f_3 & -\ f_{03} & \leq & 0 \\
(3.1.2) & 2f_0 & +\ f_1 & & -\ f_{03} & \leq & 0 \\
(3.1.3) & 3f_0 & & +3f_3 & -\ f_{03} & \leq & 10 \\
(3.1.4) & 4f_0 & -4f_1 & & +\ f_{03} & \leq & 0 \\
(3.1.5) & f_0 & & & & \geq & 5 \\
(3.1.6) & & & f_3 & & \geq & 5
\end{array}$$

(3.2) Nonlinear inequalities

$$\begin{array}{lrrrrcr}
(3.2.1) & 2f_0 & -\ f_1 & -6f_3 & +2f_{03} & \leq & \binom{f_0}{2} \\
(3.2.2) & -5f_0 & -\ f_1 & +\ f_3 & +2f_{03} & \leq & \binom{f_3}{2} \\
(3.2.3) & & f_1 & -4f_3 & +\ f_{03} & \leq & \binom{f_0}{2} \\
(3.2.4) & -5f_0 & +\ f_1 & +\ f_3 & +\ f_{03} & \leq & \binom{f_3}{2}
\end{array}$$

(3.3) Excluded values

$$\begin{array}{llll}
\mathcal{F}(P) \notin \{ & (7,15,7,32), & (7,16,8,35), & \\
 & (8,17,7,35), & (8,18,8,38), & (8,18,8,39), \\
 & (8,19,10,44), & (8,20,11,47), & (8,20,11,48), \\
 & (10,21,8,44), & (11,23,8,47), & (11,23,8,48) \quad \}.
\end{array}$$

(4) Here are some comments on the conditions in **(3)**.

(4.1) The solution set of (3.1) is a 4-dimensional cone whose apex is $\mathcal{F}(\Delta_4) = (5, 10, 5, 20)$. It has six facets and seven extreme rays, see Bayer [5].
The conditions $f_0 \geq 5$ and $f_3 \geq 5$ can be derived from the other conditions:
(3.1.1), (3.1.4), (3.2.1) and (3.2.3) together yield $f_0(f_0 - 3) \geq 10f_3$, so (3.0) yields $f_0 \geq 5$. Dually, one obtains $f_3 \geq 5$.

(4.2) The four quadratic conditions of (3.2) are *concave*, that is, the complements of the solution sets are (strictly) convex. For example, using coordinates that include $x_1 = f_0$ and

$x_2 = -2f_1 - 12f_3 + 4f_{03}$, the condition (3.2.1) is $2x_1 + \frac{1}{2}x_2 \le \binom{x_1}{2}$, that is, $x_2 \le x_1^2 - 5x_1$. This implies for flag-vectors with equality that no non-trivial convex combination may be a flag-vector. For example, $\mathcal{F}^1 = \mathcal{F}(\Delta_4) = (5, 10, 5, 20)$ and $\mathcal{F}^2 = (8, 22, 11, 50)$ are flag-vectors of simple 4-polytopes with equality in both (3.2.1) and (3.2.3), and hence the convex combinations $\frac{2}{3}\mathcal{F}^2 + \frac{1}{3}\mathcal{F}^2 = (6, 14, 7, 30)$ and $\frac{1}{3}\mathcal{F}^1 + \frac{2}{3}\mathcal{F}^2 = (7, 18, 9, 40)$ violate the same conditions.

In particular, $\mathcal{F}(\mathcal{P}^4)$ is not convex:

$$\mathcal{F}(\mathcal{P}^4) \quad \neq \quad \operatorname{conv} \mathcal{F}(\mathcal{P}^4) \cap \mathbb{Z}^4.$$

(It is also known that $\operatorname{conv} \mathcal{F}(\mathcal{P}^4)$ is not closed.)

(4.3) For all $i < j$, the possible pairs (f_i, f_j) for 4-polytopes were determined by Grünbaum [10], Barnette [2] and Barnette & Reay [3], see [7]. We comment on three specific values:

- Barnette [2] proved $(f_1, f_2) \neq (18, 16)$. This value has to be added to the list of special "impossible pairs" in [2] and in [7].
- In Barnette's paper, no proof is given for $(f_1, f_2) \neq (26, 21)$. However, this can be derived from the inequalities in (3), see [11, page 48].
- [2] lists $(f_1, f_2) = (32, 25)$ as an impossible pair, but polytopes with these values exist.

The impossible pairs from the above characterizations allow one to exclude eleven integer vectors that satisfy the conditions of (3.0)–(3.2). These are the ones listed in (3.3). All these "excluded" flag-vectors satisfy $f_0 \le 20$ and $f_3 \le 20$.

(5) For our computational study, we have enumerated all the "potential flag-vectors" that satisfy the conditions of (3) in the range $f_0 \le 20$ and $f_3 \le 20$: There are exactly

$$n(f_0 \le 20, f_3 \le 20) \quad = \quad 54768$$

such potential flag-vectors.

In particular, note that $f_0 \le 8$ implies $f_3 \le 20$ by the Upper Bound Theorem. There are

4 potential flag-vectors for $f_0 = 6$,
20 potential flag-vectors for $f_0 = 7$, and
86 potential flag-vectors for $f_0 = 8$.

We managed to generate 8363 flag-vectors in the range $\max\{f_0, f_3\} \le 20$ by combining the following methods:

- generation of random polytopes whose vertices have small integer coordinates,

- generation of all 19 flag-vectors of simplicial polytopes in the range, according to the g-theorem,
- generation of all 165 flag-vectors of pyramids and bipyramids over 3-polytopes,
- generation of all 4-dimensional 0/1-polytopes, which yields 139 different flag-vectors,
- generation of flag-vectors by "cutting off simple vertices" whenever existence of such a vertex was established, and
- dualization: with each flag-vector we included the flag-vector of the dual polytope.

A great part of the analysis, in particular, the generation and the analysis of random polytopes and of the 0/1-polytopes, was performed in the POLYMAKE system of Gawrilow & Joswig [9].

(6) For small numbers of vertices, we obtained actual polytopes for nearly all potential flag-vectors.

Theorem. *All potential flag-vectors (that satisfy the conditions of section* **(3)**) *with* $f_0 \leq 7$ *occur as flag-vectors of convex 4-polytopes, with the sole exception of*

$$(7, 17, 9, 39).$$

For $f_0 = 8$*, convex polytopes exist for all potential flag-vectors, except for the following twelve:*

$(8, 19, 9, 42)$	$(8, 20, 8, 40)$	$(8, 20, 9, 43)$
$(8, 20, 10, 46)$	$(8, 21, 8, 39)$	$(8, 21, 12, 51)$
$(8, 22, 13, 55)$	$(8, 23, 14, 59)$	$(8, 24, 15, 63)$
$(8, 21, 12, 52)$	$(8, 22, 8, 38)^*$	$(8, 22, 13, 56)$

Of these twelve, the first nine lie in the interior of the convex hull of actual flag-vectors of 4-polytopes, while the last three lie outside the convex hull.

Proof. The potential flag-vector $(7, 17, 9, 39)$ was found by Bayer [5]; it is impossible since it is not assumed in the complete classification of all 4-polytopes with 7 vertices [10, Sect. 6.2]. The non-realizability of the twelve vectors above follows from the classification of 4-polytopes with 8 vertices by Altshuler & Steinberg [1]. For this, we have computed the flag-vectors of all 4-polytopes with 8 vertices from the data of the combinatorial types that are given in Tables 1 and 3 of [1]. There are 1294 different combinatorial types, but they have only 74 different flag-vectors — the 12 "potential flag-vectors" listed above are non-realizable.

It is an interesting challenge to provide *new* flag-vector inequalities that would "cut off" some of the twelve potential flag-vectors given above. See [11, page 74] for more non-realized potential flag-vectors. □

(7) There is still a long way to go until we can claim to "understand" the flag-vectors, or even just the f-vectors of 4-polytopes. For example, the "diagonal" case of polytopes with

$f_0 = f_3$ shows our ignorance. This case is also relevant for the question about "fat-lattice" 4-polytopes, as asked by Avis, Bremner & Seidel [4]: how large is

$$f(n) \quad := \quad \max\{f_1 : (f_0, f_1, f_3, f_{03}) \in \mathcal{F}(\mathcal{P}^4),\ \ f_0, f_3 \le n\}\,?$$

This question is of considerable importance for the complexity of convex-hull algorithms!

Here we note the following: addition of (3.1.1) and (3.2.3) yields

$$2f_1 \ \le\ f_0 + f_3 + \tbinom{f_0}{2} \ =\ \frac{f_0^2 + f_0 + 2f_3}{2} \ \le\ \frac{(\max\{f_0, f_3\})^2 + 3\max\{f_0, f_3\}}{2}$$

and thus

$$f_1 \ \le\ \left\lfloor \frac{n^2 + 3n}{4} \right\rfloor \qquad \text{for} \quad n := \max\{f_0, f_3\}.$$

And indeed, this inequality is sharp for *potential* f-vectors: for example, for $f_0 = f_3$ we have the potential f-vectors.

$$\begin{array}{ll}
(4k, 4k^2+3k, 4k, 4k^2+11k) & \text{for } k \ge 2,\\
(4k+1, 4k^2+5k+1, 4k+1, 4k^2+13k+3) & \text{for } k \ge 1,\\
(4k+2, 4k^2+7k+2, 4k+2, 4k^2+15k+6) & \text{for } k \ge 2,\\
(4k+2, 4k^2+7k+2, 4k+2, 4k^2+15k+7) & \text{for } k \ge 1,\\
(4k+3, 4k^2+9k+4, 4k+3, 4k^2+17k+10) & \text{for } k \ge 2, \text{ and}\\
(4k+3, 4k^2+9k+4, 4k+3, 4k^2+17k+11) & \text{for } k \ge 1.
\end{array}$$

However, these vectors are *potential*: for $f_0 = 8$ ($k = 2$), the flag-vector $(8, 22, 8, 38)$ does **not** appear for any polytope (see the theorem above), and the maximal f_1 (assuming $f_0 = f_3$) is obtained by $(8, 21, 8, 38)$. Similarly, for $f_0 = 18$ the largest f_1 for a *potential* flag-vector is attained by $(18, 94, 18, 130)$, while the largest f_1 we actually *found* was in $(18, 61, 18, 102)$. So the gap (measured, e. g., in the ratio $\frac{f_1}{f_0}$), widens as $f_0 = f_3$ gets larger. And indeed, a result of Edelsbrunner & Sharir [8] implies that

$$f_{03} \ =\ O({f_0}^{2/3}{f_3}^{2/3}),$$

which is $f_{03} = O({f_0}^{4/3})$ in the "diagonal case" where $f_0 = f_3$. Unfortunately, it seems to be hard to get an explicit value for the constant hidden in the "O" of this result.

Here is a conjectured inequality for flag-vectors by M. Bayer [5, p. 149]:

$$2f_0 - f_1 + 3f_3 \quad \ge \quad 15.$$

We found no actual polytopes that would violate this conjecture. However, counter-examples can be found among the sequences of flag-vectors listed above, where f_1 grows quadratically with $n := f_0 = f_3$. As specific examples, we note the potential flag-vectors

$$\begin{array}{lllrl}
(13, 51, 13, 77) & \text{yields} & 2f_0 - f_1 + 3f_3 = & 14, & \\
(18, 91, 18, 127) & \text{yields} & = & -1, & \text{and}\\
(20, 115, 20, 155) & \text{yields} & = & -15. &
\end{array}$$

Here is another conjectured inequality for flag-vectors [5, p. 145]:

$$2f_0 + f_1 + 3f_3 - f_{03} \quad \geq \quad 15.$$

Again we found no actual polytopes that violate this conjecture, but there are counter-examples among the potential f-vectors, such as

$$\begin{array}{llrl} (15,41,15,102) & \text{yields} \quad 2f_0 + f_1 + 3f_3 - f_{03} = & 14, & \\ (20,61,20,162) & \text{yields} \qquad\qquad\qquad\qquad = & -1, & \text{and} \\ (20,62,20,166) & \text{yields} \qquad\qquad\qquad\qquad = & -4. & \end{array}$$

A much stronger inequality, in some sense the "strongest possible" one, which would imply all those just mentioned from [5] and from [8], was suggested by Billera and Ehrenborg (personal communication):

$$2f_0 - f_1 + 9f_3 - 2f_{03} \quad \geq \quad 45.$$

Again, our data give lots of "potential f-vectors" that violate this, but no real counter-example.

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