More bounds on the diameters of convex polytopes

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Dedicated to Professor Kees Roos on the occasion of his 70th birthday.

Let $\Delta(d, n)$ be the maximum possible diameter of the vertex-edge graph over all d-dimensional polytopes defined by n inequalities. The *Hirsch bound* holds for particular n and d if $\Delta(d, n) \leq n - d$. Francisco Santos recently resolved a question open for more than five decades by showing that $\Delta(d, 2d) \geq d + 1$ for $d = 43$; the dimension was then lowered to 20 by Matschke, Santos and Weibel. This progress has stimulated interest in related questions. The existence of a polynomial upper bound for $\Delta(d, n)$ is still an open question, the best bound being the quasi-polynomial one due to Kalai and Kleitman in 1992. Another natural question is for how large n and d the Hirsch bound holds. Goodey showed in 1972 that $\Delta(4, 10) = 5$ and $\Delta(5, 11) = 6$, and more recently, Bremner and Schewe showed that $\Delta(4, 11) = \Delta(6, 12) = 6$. Here, we show that $\Delta(4, 12) = \Delta(5, 12) = 7$.

Keywords: pivoting methods; linear optimization; discrete geometry; combinatorics; convex polytopes

1. Introduction

Finding a good bound on the maximal diameter $\Delta(d, n)$ of the 1-skeleton (vertex-edge graph) of a polytope in terms of its dimension d and the number of its facets n is one of the basic open questions in polytope theory [10]. Although some bounds are known, the behaviour of the function $\Delta(d, n)$ is largely unknown. The Hirsch conjecture, formulated in 1957 and reported in [4], states that $\Delta(d, n)$ is linear in n and d: $\Delta(d, n) \leq n - d$. The conjecture was recently disproved by Santos [18] by exhibiting a counterexample for $\Delta(d, 2d)$ with $d = 43$ which was further improved to $d = 20$ [17]. The conjecture is known to hold in small dimensions, that is, for $d \leq 3$ [15], along with other specific pairs of d and n (Table 1). However, the asymptotic behaviour of $\Delta(d, n)$ is not well understood: the best upper bound – due to Kalai and Kleitman [12] – is quasi-polynomial. For more background on the Hirsch Conjecture, see the survey [14].

The behaviour of $\Delta(d, n)$ is not only a natural question of extremal discrete geometry, but also historically closely connected with the theory of the simplex method. The approach of using

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Table 1. Previously known bounds on $\Delta(d, n)$ [2,9,11,16].

	$n - 2d$				
d	0	1	2	3	4
4	4	5	5	6	7+
5	5	6	7–8	7+	8+
6	6	7–9	8+	9+	9+
7	7–10	8+	9+	10+	11+
8	8+	9+	10+	11+	12+

abstract models [7,8,13] to study linear optimization has recently achieved the exciting result of a subexponential lower bound for Zadeh's rule [8], another long-standing open problem. On the positive side, several authors have recently shown upper bounds for interesting special cases of the simplex method [21] and the diameter problem [5].

In this article, we show the following theorem.

THEOREM 1.1 $\Delta(4, 12) = \Delta(5, 12) = 7$.

The first of these new values continues the pattern of $\Delta(4, n) = n - 5$ for $n \geq 10$. It would be very interesting to establish a general sub-Hirsch bound for $d = 4$. The considered computational approaches might help to narrow the gap between the smallest entries for d and $n - d$ yielding a counterexample and the largest ones for which the Hirsch conjecture still holds.

Our approach is computational and builds on the approach used by Bremner and Schewe [2]. As in [2], we reduce the determination of $\Delta(d, n)$ to a set of simplicial complex realizability problems. Section 2 introduces our computational framework and some related background. A common theme in the SAT literature is that the hardest instances to solve are those that are 'almost satisfiable'; we find a similar classification of our realizability problems. Compared to [2], this work involves significantly more computation, and we discuss a simple but effective parallelization strategy in Section 2. Finally, we discuss our new bounds in Section 3. Again comparing with [2], the results here have the feature that they do not rely on having *a priori* upper bounds on the value of $\Delta(d, n)$ to be computed, but rather on inductive computation of $\Delta(d, n)$ using bounds on $\Delta(d - 1, n - 1)$.

2. General approach

In this section, we give a summary of our general approach. For more on the theoretical background, the reader is referred to [2].

It is easy to see via a perturbation argument that $\Delta(d, n)$ is always achieved by some simple polytope. By a reduction applied from [16], we only need to consider *end-disjoint* paths: paths where the end vertices do not lie on a common facet (*facet-disjointness*). It will be convenient from both an expository and a computational view to work in a polar setting where we consider the lengths of facet paths on the boundary of simplicial polytopes. We apply the term *end-disjoint* equally to the corresponding facet paths, where it has the simple interpretation that two end facets do not intersect.

A *combinatorial facet path* is a simplicial complex with a path as a dual graph, where edges are defined by two d-simplices sharing a $(d - 1)$-simplex. Our general strategy is to show $\Delta(d, n) \neq k$ by generating all non-isomorphic combinatorial facet paths of length k on n vertices in dimension
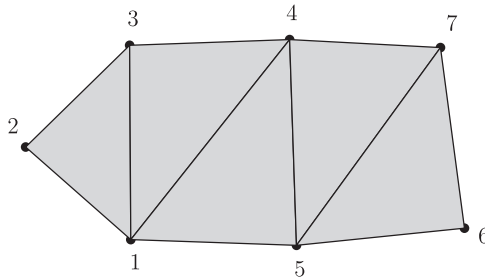
Figure 1. An end-disjoint path on seven vertices, generated by pivot sequence $(2, 4)(3, 5)(1, 7)(4, 6)$.
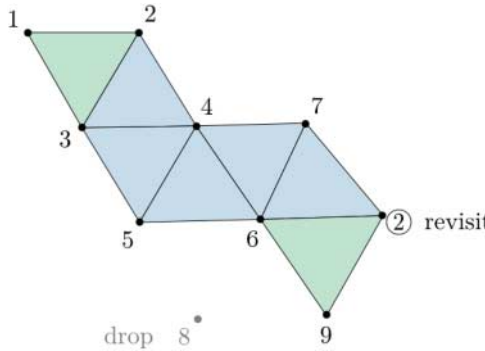

Figure 2. Example of a facet path.

d and showing that none can be embedded on the boundary of a simplicial polytope as a shortest path.

The generation of all possible paths for particular d and n begins with the case where the paths are *non-revisiting*, that is, paths where no vertex is visited more than once. These can be generated via a simple recursive scheme, using a bijection with *restricted growth strings*, that is, k-ary strings where the symbols first occur in order. Each symbol represents a choice of pivot, and the strings can be unpacked into combinatorial facet paths. Figure 1 illustrates a non-revisiting path with $d = 3, n = 7$; we will use this path as a running example in this section.

Multiple revisit facet paths are generated from facet paths with one less revisit by identifying pairs of vertices. Such an identification is valid only if it results in another facet path, that is, does not introduce new ridges, and if the resulting facet path is still end-disjoint.

If a vertex is not used in a facet path, we call this occurrence a *drop*. See Figure 2 for an illustration of a path of length 6 involving 1 revisit (vertex 2) and 1 drop (vertex 8) with $n = 9$ and $d = 3$. We can then classify paths by dimension d, primal facets/dual vertices n, length k, the number of revisits m, and the number of drops l. For end-disjoint paths, a simple counting argument yields:

$$m - l = k + d - n,$$
$$m \leq k - d,$$
$$l \leq n - 2d.$$

Table 2 provides the number of paths to consider for each possible combination of d, n, k, m, and l. It will turn out that each path generates an SAT instance that needs to be shown to be unsatisfiable.

Table 2. Number of paths to consider, SAT instances to solve.

d	n	k	m	l	#
4	10	6	0	0	15
4	10	6	1	1	24
4	10	6	2	2	16
4	11	7	0	0	50
4	11	7	1	1	200
4	11	7	2	2	354
4	11	7	3	3	96
4	12	8	0	0	160
4	12	8	1	1	1258
4	12	8	2	2	5172
4	12	8	3	3	7398
4	12	8	4	4	1512
5	11	7	1	0	98
5	11	7	2	1	98
5	12	8	1	0	1079
5	12	8	2	1	3184
5	12	8	3	2	2904
6	12	7	1	0	11

For any set $Z = \{x_1, \ldots, x_{d-1}, y_1, \ldots, y_4\} \subset \mathbb{R}^{d+1}$, as a special case of the Grassmann–Plücker relations on determinants [1, Section 3.5], we have

$$\det(X, y_1, y_2) \cdot \det(X, y_3, y_4) + \det(X, y_1, y_4) \cdot \det(X, y_2, y_3) - \det(X, y_1, y_3) \cdot \det(X, y_2, y_4) = 0, \tag{1}$$

where $X = \{x_1 \ldots, x_{d-1}\}$. We are, in particular, interested in the case where Z represents $(d + 3)$-points in $\mathbb{R}^d$ in homogeneous coordinates; the various determinants are then signed volumes of simplices. In the case of points drawn from the vertices of a simplicial polytope, we may assume without loss of generality that these simplices are never flat, that is, determinant 0. Thus, if we define $\chi(v_1, \ldots, v_{d+1}) = \text{sign}(\det(v_1, \ldots, v_{d+1}))$, it follows from (1) that

$$\{\chi(X, y_1, y_2)\chi(X, y_3, y_4), -\chi(X, y_1, y_3)\chi(X, y_2, y_4), \chi(X, y_1, y_4)\chi(X, y_2, y_3)\} = \{-1, +1\}. \tag{2}$$

Any alternating map $\chi : E^{d+1} \to \{-, +\}$ satisfying these constraints for all $(d + 3)$-subsets (and all choices of $y_1 \ldots y_4$) is called a *uniform chirotope*; this is one of the many axiomatizations of *uniform-oriented matroids* [1]. In the rest of this paper, we call uniform chirotopes simply chirotopes.

There are $\binom{n}{d+3}\binom{d+3}{4}$ Grassmann–Plücker constraints in their natural encoding, and this further expands by a factor of 16 when converted to conjunctive normal form (CNF) suitable for an SAT solver. In the particular case of $d = 3, n = 7$ (cf. Figure 1), there are 105 constraints of the form (2). The first two (lexicographically) are

$$\{\chi(1, 2, 3, 4) \cdot \chi(1, 2, 5, 6), -\chi(1, 2, 3, 5) \cdot \chi(1, 2, 4, 6), \chi(1, 2, 3, 6) \cdot \chi(1, 2, 4, 5)\} = \{+1, -1\},$$
$$\{\chi(2, 3, 1, 4) \cdot \chi(2, 3, 5, 6), -\chi(2, 3, 1, 5) \cdot \chi(2, 3, 4, 6), \chi(2, 3, 1, 6) \cdot \chi(2, 3, 4, 5)\} = \{+1, -1\}.$$

A *facet* is a d-set $F \subset E$ such that for all $g \in E \setminus F$, $\chi(F, g)$ has the same sign. An *interior point* of a chirotope is some $g \in E$ that is not contained in any facet. We are mainly concerned with *convex* chirotopes, that is, those without interior points.

Facet constraints actually remove variables from the problem, since they define sets of equations. Equations can be removed as a preprocessing step, although most modern SAT solvers deal with equality constraints quite effectively, even when the constraints are transformed to CNF.

Referring back to the example of Figure 1, we can derive the following equations:

$$\alpha = \chi(1,2,3,4) = \chi(1,2,3,5) = \chi(1,2,3,6) = \chi(1,2,3,7),$$
$$\alpha = \chi(1,3,4,2) = \chi(1,3,4,5) = \chi(1,3,4,6) = \chi(1,3,4,7),$$
$$\alpha = \chi(1,4,5,2) = \chi(1,4,5,3) = \chi(1,4,5,6) = \chi(1,4,5,7),$$
$$-\alpha = \chi(4,5,7,1) = \chi(4,5,7,2) = \chi(4,5,7,3) = \chi(4,5,7,6),$$
$$-\alpha = \chi(5,6,7,1) = \chi(5,6,7,2) = \chi(5,6,7,3) = \chi(5,6,7,4).$$

These equations can be substituted into our example Grassmann–Plücker constraints to simplify

$$\{\alpha \cdot \chi(1,2,5,6), -\alpha \cdot \chi(1,2,4,6), \alpha \cdot \chi(1,2,4,5)\} = \{+1, -1\},$$
$$\{\alpha \cdot \chi(2,3,5,6), -\alpha \cdot \chi(2,3,4,6), \alpha \cdot \chi(2,3,4,5)\} = \{+1, -1\}.$$

Since every convex polytope defines a convex chirotope, our diameter bounds can be established by showing that for each candidate combinatorial facet path π there is no alternating sign map $\chi(\cdot)$ that

(P1) satisfies the Grassmann–Plücker constraints, that is, a chirotope,
(P2) forces each d-simplex of the candidate facet path to be a facet of the chirotope,
(P3) does not induce a *shortcut*, that is, a facet path of length shorter than k between the end facets of π. See Figure 3 for an illustration of a shortcut on a three-dimensional polytope.

Each potential shortcut can be eliminated with constraints encoding the fact that some d-simplex of the potential shortcut is not a facet. In principle, one can generate all conceivable shortcuts by considering all short paths in the graph of all possible pivots between d-simplices, but this approach is generally impractical. We therefore use an incremental approach where candidate chirotopes are generated and any shortcuts on the boundary of these candidate solutions are used to generate new constraints. In the case of Figure 3, we need to add (at least) the constraint that both $\{2,3,6\}$ and $\{2,5,6\}$ are not facets. Since we know that $\chi(2,3,6,5) = -\chi(2,5,6,3)$, we can
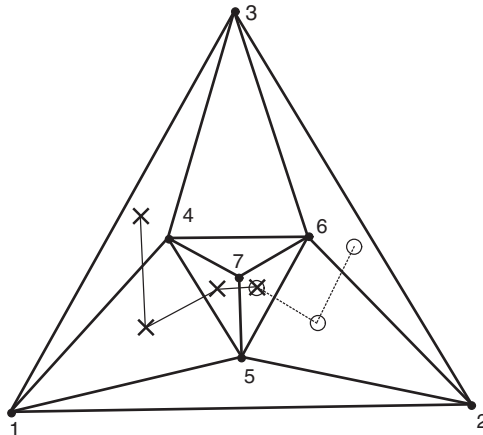

Figure 3. Illustrating a non-shortest embedding of the path from Figure 1. The path $\{\{1,2,3\}, \{2,3,6\}, \{2,5,6\}, \{5,6,7\}\}$ is a shortcut.

combine this into a single high-level constraint (which generates two CNF constraints):

$$\{-\chi(2,3,6,1), -\chi(2,3,6,4), -\chi(2,3,6,5), -\chi(2,3,6,7), \chi(2,5,6,1), \chi(2,5,6,3),$$
$$\chi(2,5,6,4), \chi(2,5,6,7)\} = \{+1, -1\}.$$

A notable omission from the list of constraints above is that we do not explicitly constrain the alternating map $\chi(\cdot)$ to be convex. We note that either every element is in some facet, and thus the chirotope is convex by definition, or there is some interior point not used by the long facet path. A realization with interior points corresponds to a realization on a smaller number of elements. In the work here, we always have bounds for $\Delta(d, j)$ for $j < n$ when working on a bound for $\Delta(d, n)$, so we effectively reduce non-convex cases to smaller convex ones.

Chirotopes can be viewed as a generalization of real polytopes in the sense that for every real polytope, we can obtain its chirotope directly. Therefore, showing the non-existence of chirotopes satisfying properties P1–P3 immediately precludes the existence of real polytopes satisfying the same properties.

The search for a chirotope with properties P1 and P2 is encoded as an instance of SAT [2,19,20], with P3 handled implicitly via adding constraints and resolving. Each SAT problem is solved with MiniSat [6]. MiniSat itself discovers many constraints during the solution process, and these are carried forward between successive subproblems.

With the implementation of [2], we were able to reconfirm Goodey's results for $\Delta(4, 10)$ and $\Delta(5, 11)$ in a matter of minutes. While the number of paths to consider increases with the number of the revisits, in our experiments, these paths are much less computationally demanding than the ones with fewer revisits. For example, the 7398 paths of length 8 on 4-polytopes with 12 facets and involving 3 revisits and 3 drops require only a tiny fraction of the computational effort to tackle the 160 paths without a drop or revisit.

In order to deal with the intractability of the problem as the dimension, number of facets, and path length increased, we proceeded by splitting our original facet embedding problem into subproblems by fixing chirotope signs. We use the non-SAT-based `mpc` backtracking software [3] to backtrack to a certain fixed level of the search tree; every leaf job was then processed in parallel on the Shared Hierarchical Academic Research Computing Network. Figure 4 (a partial trace of the execution of `mpc`) illustrates the splitting process on a problem generated from the octahedron. Note that variable propagation (similar to the *unit propagation* used by SAT solvers) reduces the number of leaves of the tree.
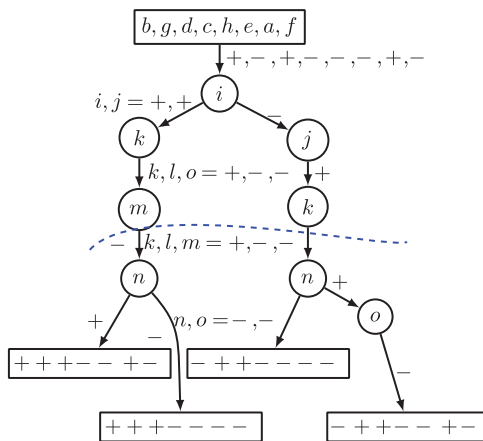

Figure 4. Using partial backtracking to generate subproblems.

Table 3. Number of difficult paths.

d	n	k	m	l	#
4	12	8	0	0	2
5	12	8	1	0	15
5	12	8	2	1	6

Jobs requiring a long time to complete were further split and executed on the cluster until the entire search space was covered. Table 3 provides the number of paths which were computationally difficult enough to require splitting. For example, out of 160 paths of length 8 on 4-polytopes with 12 facets without drop or revisit, 2 required splitting.

3. Results

Summarizing the computational results, we have the following.

PROPOSITION 3.1 *There are no* $(4, 12)$- *or* $(5, 12)$-*polytopes with facet-disjoint vertices at distance* 8.

Note that we actually prove something slightly stronger: for $(d, n) = (4, 12)$ or $(5, 12)$, no (d, n)-chirotope has vertex-disjoint facets at distance 8, where distance is defined by the shortest facet path.

While the non-existence of k-length paths implies the non-existence of $(k + 1)$-length paths, it is not obvious if the non-existence of end-disjoint k-length paths implies the non-existence of $(k + 1)$-length paths. To be able to rule out vertices – not necessarily facet-disjoint – at distance $l > k$, we introduce the following lemma.

LEMMA 3.2 *If* $\Delta(d - 1, n - 1) < k$ *and there is no* (d, n)-*polytope with two facet-disjoint vertices at distance* k, *then* $\Delta(d, n) < k$.

Proof Assume the contrary. Let u and v be the vertices on a (d, n)-polytope at distance $l \geq k$. By considering a shortest path from u to v, there is a vertex w at distance k from u. u and w must share a common facet F to prevent a contradiction. F is a $(d - 1, n - 1)$-polytope with diameter at least k. ∎

By Proposition 3.1 and because $\Delta(3, 11) = 6$ and $\Delta(4, 11) = 6$ [2,15], we can apply Lemma 3.2 to obtain the main theorem.

THEOREM 3.3 $\Delta(4, 12) = \Delta(5, 12) = 7$.

We recall the following result of Klee and Walkup [16]:

PROPERTY 3.4 $\Delta(d, 2d + k) \leq \Delta(d - 1, 2d + k - 1) + \lfloor k/2 \rfloor + 1$ *for* $0 \leq k \leq 3$.

Property 3.4 along with the two new entries for $\Delta(d, n)$ imply the additional upper bounds: $\Delta(5, 13) \leq 9$, $\Delta(6, 13) \leq 8$, $\Delta(6, 14) \leq 11$, $\Delta(7, 14) \leq 9$, $\Delta(7, 15) \leq 12$, and $\Delta(8, 16) \leq 13$ see Table 4 where the new entries and bounds are entered in bold.

Table 4. Summary of bounds on $\Delta(d, n)$.

	$n - 2d$				
d	0	1	2	3	4
4	4	5	5	6	**7**
5	5	6	**7**	**7–9**	8+
6	6	**7–8**	**8–11**	9+	9+
7	**7–9**	**8–12**	9+	10+	11+
8	**8–13**	9+	10+	11+	12+

4. Conclusions

In this paper, we have presented new bounds for the diameter of the 1-skeleton of convex polytopes in dimensions 4 and 5. It remains open to find the smallest n and d for which the Hirsch bound fails to hold; we are also interested if the current trend which shows $\Delta(4, n) = n - 5$ continues beyond $n = 12$. The tools used here are mainly computational as in [2], although further analysis of the relationship between bounds on end-disjoint paths and bounds on more general paths was needed in order to establish new bounds without requiring *a priori* upper bounds. Furthermore, the scale of the computations forced us to solve individual cases in parallel. The simple strategy we used may be effective for other so-called *tree search* problems. Finally, we observe experimentally that among our unrealizable simplicial complexes, the most difficult to show unsatisfiable are those with the simplest topology.

Acknowledgements

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