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# Computational determination of the largest lattice polytope diameter

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#### Abstract

A lattice (d, k)-polytope is the convex hull of a set of points in dimension d whose coordinates are integers between 0 and k. Let  $\delta(d, k)$  be the largest diameter over all lattice (d, k)-polytopes. We develop a computational framework to determine  $\delta(d, k)$  for small instances. We show that  $\delta(3, 4) = 7$  and  $\delta(3, 5) = 9$ ; that is, we verify for (d, k) = (3, 4) and (3, 5) the conjecture whereby  $\delta(d, k)$  is at most  $\lfloor (k+1)d/2 \rfloor$  and is achieved, up to translation, by a Minkowski sum of lattice vectors.

Keywords: Lattice polytope, edge-graph diameter, enumeration algorithm

#### 1. Introduction

Finding a good bound on the maximal edge-diameter of a polytope in terms of its dimension and the number of its facets is not only a natural question of discrete geometry, but also historically closely connected with the theory of the simplex method, as the diameter is a lower bound for the number of pivots required in the worst case. Considering bounded polytopes whose vertices are integer-valued, we investigate a similar question where the number of facets is replaced by the grid embedding size.

The convex hull of integer-valued points is called a lattice polytope and, if all the vertices are drawn from  $\{0, 1, ..., k\}^d$ , it is referred to as a lattice (d, k)-polytope. Let  $\delta(d, k)$  be the largest edge-diameter over all lattice (d, k)-polytopes. Naddef [8] showed in 1989 that  $\delta(d, 1) = d$ , Kleinschmidt and

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Onn [7] generalized this result in 1992 showing that  $\delta(d,k) \leq kd$ . In 2016, Del Pia and Michini [3] strengthened the upper bound to  $\delta(d,k) \leq kd - \lceil d/2 \rceil$  for  $k \geq 2$ , and showed that  $\delta(d,2) = \lfloor 3d/2 \rfloor$ . Pursuing Del Pia and Michini's approach, Deza and Pournin [6] showed that  $\delta(d,k) \leq kd - \lceil 2d/3 \rceil - (k-2)$  for  $k \geq 4$ , and that  $\delta(4,3) = 8$ . The determination of  $\delta(2,k)$  was investigated independently in the early nineties by Thiele [9], Balog and Bárány [2], and Acketa and Žunić [1] showing that  $\delta(2,k) = \frac{6}{(2\pi)^{2/3}}k^{2/3} + O(k^{1/3}\log k)$ .

Investigating the lower bound on  $\delta(d,k)$ , Deza, Manoussakis, and Onn [5] introduced the *primitive lattice polytope*  $H_1(d,2)$  as the Minkowski sum of all the nonzero vectors v drawn from  $\{-1,0,1\}^d$  such that  $||v||_1 \leq 2$  and the first nonzero coordinate of v is positive. They showed that, for any k < 2d, there exists a subset of the generators of  $H_1(d,2)$  whose Minkowski sum is, up to translation, a lattice (d,k)-polytope of diameter  $\lfloor (k+1)d/2 \rfloor$ . Thus, they showed that  $\delta(d,k) \geq \lfloor (k+1)d/2 \rfloor$  for all k < 2d and proposed Conjecture 1.

**Conjecture 1.** For any d and k,  $\delta(d,k)$  is achieved, up to translation, by a Minkowski sum of lattice vectors. In particular, when k < 2d,  $\delta(d,k) = \lfloor (k+1)d/2 \rfloor$ .

In Section 2, we propose a computational framework to investigate Conjecture 1 by drastically reducing the search space for lattice (d, k)-polytopes achieving a large diameter. Applying this framework to (d, k) = (3, 4) and (3, 5), we determine in Section 3 that  $\delta(3, 4) = 7$  and  $\delta(3, 5) = 9$ .

**Theorem 2.** Conjecture 1 holds for (d, k) = (3, 4) and (3, 5); that is,  $\delta(3, 4) = 7$  and  $\delta(3, 5) = 9$ , and both diameters are achieved, up to translation, by a Minkowski sum of lattice vectors.

Note that Conjecture 1 holds for all known values of  $\delta(d, k)$  given in Table 1, and hypothesizes, in particular, that  $\delta(d,3) = 2d$ . The new entries corresponding to (d,k) = (3,4) and (3,5) are entered in bold.

d $k$	1	2	3	4	5	6	7	8	9	10
1	1	1	1	1	1	1	1	1	1	1
2	2	3	4	4	5	6	6	7	8	8
3	3	4	6	7	9					
4	4	6	8							
:	:	•								
d	d	$\lfloor \frac{3d}{2} \rfloor$								

Table 1: The largest possible diameter  $\delta(d,k)$  of a lattice (d,k)-polytope

#### 2. Theoretical and Computational Framework

Since  $\delta(2,k)$  and  $\delta(d,2)$  are known, we consider in the remainder of the paper that  $d \geq 3$  and, with the exception of Section 3.2, that  $k \geq 3$ . While the number of lattice (d,k)-lattice polytopes is finite, a brute force search is typically intractable, even for small instances. Let d(u,v) denote the distance between two vertices u and v of a polytope P in the edge-graph of P. Theorem 3 considers a pair (u,v) of vertices of a lattice (d,k)-polytope such that  $d(u,v) = \delta(d,k)$ , and recalls conditions established in [6] that allow to drastically reduce the search space by exploiting integrality and convexity properties.

**Theorem 3.** For  $d \geq 3$ , let (u, v) be a pair of vertices of a lattice (d, k)polytope P such that  $d(u, v) = \delta(d, k)$ . For i = 1, ..., d, let  $F_i^0$ , respectively  $F_i^k$ , denote the intersection of P with the facet of the cube  $[0, k]^d$  corresponding to  $x_i = 0$ , respectively  $x_i = k$ . Then,  $d(u, v) \leq \delta(d - 1, k) + k$ , and the
following conditions are necessary for the inequality to hold with equality:

- (1)  $u + v = (k, k, \dots, k),$
- (2) any edge with u or v as vertex is drawn from  $\{-1,0,1\}^d$ ,
- (3) for i = 1, ..., d, both  $F_i^0$  and  $F_i^k$ , are, up to an affine transformation, lattice (d-1,k)-polytopes of diameter  $\delta(d-1,k)$ .

Thus, to show that  $\delta(d, k) < \delta(d-1, k) + k$ , it is enough to show that there is no lattice (d, k)-polytope P admitting a pair of vertices (u, v) such that  $d(u, v) = \delta(d, k)$  and the conditions (1), (2), and (3) are satisfied. Those conditions appear as items (i) and (ii) at the very end of [6] and are a

direct consequence of bounding d(u, v) by the length of path from u to v going through one the 2d faces of P formed by the points of P maximizing, or minimizing, one of the d coordinates. The computational framework to determine, given (d, k), whether  $\delta(d, k) = \delta(d - 1, k) + k$  is outlined below and illustrated for (d, k) = (3, 4) or (3, 5).

# Algorithm to determine whether $\delta(d, k) < \delta(d - 1, k) + k$

### Step 1: Initialization

Determine the set  $\mathcal{F}_{d-1,k}$  of all lattice (d-1,k)-polytopes of diameter  $\delta(d-1,k)$ . For example, for (d,k)=(3,4), the determination of all the 335 lattice (2,4)-polygons of diameter 4 is straightforward.

Determine the set  $V_{d-1,k}$  of all the vertices of all lattice (d-1,k)-polytopes of diameter  $\delta(d-1,k)$ . For example, for (d,k)=(3,4),  $V_{2,4}$  consists of all  $\{0,1,\ldots,4\}$ -valued points except (2,2).

Determine the set  $\mathcal{P}_{d-1,k}$  of all the points with integer coordinates belonging to the intersection of all lattice (d-1,k)-polytopes of diameter  $\delta(d-1,k)$ . For example, for (d,k) = (3,4),  $\mathcal{P}_{2,4} = \{(1,2),(2,1),(2,2),(2,3),(3,2)\}$ .

Determine the convex hull  $C_{d,k}$  of all the points x such that  $x_i = 0$  and  $\bar{x}_i \in \mathcal{P}_{d-1,k}$  for some  $1 \leq i \leq d$ . Here  $\bar{x}_i \in \mathbb{R}^{d-1}$  denotes the point consisting of all coordinates of x except  $x_i$ .

#### Step 2: Symmetries and other reductions

Up to the symmetries of the cube  $[0,k]^d$ , we can assume that the coordinates of u satisfy  $u_i \leq u_{i+1} \leq \lfloor k/2 \rfloor$  for  $i=1,\ldots,d-1$ . For example, for (d,k)=(3,4), the following vertices cover all possibilities for u: (0,0,0),(0,0,1),(0,0,2),(0,1,1),(0,1,2),(0,2,2),(1,1,1),(1,1,2),(1,2,2), and (2,2,2).

If  $u_1 = 0$ , we can further assume that  $\bar{u}_i \in \mathcal{V}_{d-1,k}$  for all i such that  $u_i = 0$ , as otherwise u cannot be a vertex of a lattice (d,k)-polytope P of diameter  $\delta(d-1,k) + k$  by item (3) of Theorem 3. For example, for (d,k) = (3,4), the point (0,2,2) can be removed as  $(2,2) \notin \mathcal{V}_{2,4}$ .

Similarly, if  $u_1 \neq 0$ , we can further assume that  $\bar{u}_i \notin \mathcal{P}_{d-1,k}$  for all  $i = 1, \ldots, d$  and that u is not in the interior of  $\mathcal{C}_{d,k}$ , as otherwise u is in the interior of a convex combination of points belonging to any lattice (d,k)-polytope P of diameter  $\delta(d-1,k)+k$ . For example, for (d,k)=(3,4), the points (1,1,2),(1,2,2), and (2,2,2) can be removed as (1,2) and (2,2) belong to  $\mathcal{P}_{2,4}$ , and the point (1,1,1) can be removed as (1,1,1) is in the interior of  $\mathcal{C}_{3,4}$  since (1,1,1) is a convex combination of (0,1,2),(2,0,1) and (1,2,0).

For each remaining u, we proceed to Step 3 where, by item (1) of Theorem 3, we can assume that (u,v) forms a pair of vertices satisfying  $d(u,v) = \delta(d-1,k) + k$  and  $u+v = \{k,k,\ldots,k\}$ . For example, for (d,k) = (3,4), we proceed to Step (3) for each of the 5 pairs (u,v) corresponding to u = (0,0,0), (0,0,1), (0,0,2), (0,1,1), and (0,1,2).

### Step 3: Shelling

For each of the possible pairs (u, v) determined during Step 2, the shelling step tries to embed elements of the set  $\mathcal{F}_{d-1,k}$  determined during Step 1 onto the ordered 2d intersections of P with the facets of the cube  $[0, k]^d$ . We recall that P is assumed to be a lattice (d, k)-polytope of diameter  $\delta(d-1, k) + k$ with  $d(u, v) = \delta(d-1, k) + k$ .

If  $u_1 = 0$ , only elements of the set  $\mathcal{F}_{d-1,k}$  with  $\bar{u}_1$ , respectively  $\bar{v}_1$ , as vertex are considered to be embedded into the d facets of  $[0,k]^d$  with  $(0,0,\ldots,0)$ , respectively  $(k,k,\ldots,k)$ , as vertex. For example, for (d,k) = (3,4), u = (0,0,0), and v = (4,4,4), the algorithm tries to embed 6 elements of  $\mathcal{F}_{2,4}$  into the 6 facets of  $[0,4]^3$ ; 3 with (0,0) as vertex, and 3 with (4,4) as vertex.

These embeddings must be consistent; that is, given two embeddings  $E_1$  and  $E_2$ , the intersection of  $E_1$  with the facet of  $[0,k]^d$  containing  $E_2$  should be equal to the intersection of  $E_2$  with the facet of  $[0,k]^d$  containing  $E_1$ . In addition, by item (2) of Theorem 3, if an edge of an embedding of an element of  $\mathcal{F}_{d-1,k}$  with u or v as vertex is not drawn from  $\{-1,0,1\}^d$ , this embedding can be disregarded.

Let  $\Gamma$  denote the graph defined by the vertices and edges belonging to the embeddings of elements of  $\mathcal{F}_{d-1,k}$  considered to form a shelling, and let  $d_{\Gamma}(u,v)$ 

denote the distance in  $\Gamma$  between u and v. Since  $\Gamma$  is a subgraph of the edge-graph of a lattice (d,k)-polytope P of diameter assumed to be d(u,v),  $d_{\Gamma}(u,v)$  is an upper bound for d(u,v); that is, for  $\delta(d-1,k)+k$ . Thus, if  $d_{\Gamma}(u,v)<\delta(d-1,k)+k$ , a shortcut between u and v exists and the last embedding can be disregarded.

For example, for (d, k) = (3, 5), all embeddings of 6 elements of  $\mathcal{F}_{2,5}$  forming a shelling yield a  $\Gamma$  such that  $d_{\Gamma}(u, v) < 10$ , and thus the algorithm terminates without Step 4 being executed.

## Step 4. Inner points

For each choice of 2d embeddings of elements of  $\mathcal{F}_{d-1,k}$  forming a shelling obtained during Step 3, consider the  $\{1, 2, \ldots, k-1\}$ -valued points not in the convex hull of the vertices of  $\Gamma$ ; that is, not in the convex hull of the vertices of the 2d embeddings of elements of  $\mathcal{F}_{d-1,k}$  forming a shelling.

All subsets of such points are considered as potential vertices to be added to the vertices of  $\Gamma$  via a binary tree. A convex hull and diameter computation are performed for each node of the obtained binary tree. If there is a node yielding a diameter of  $\delta(d-1,k)+k$  we can conclude that  $\delta(d,k)=\delta(d-1,k)+k$ . Otherwise, we can conclude that  $\delta(d,k)<\delta(d-1,k)+k$ .

#### 3. Computational Results and Enhancements

#### 3.1. Determination of $\delta(3,4)$ and $\delta(3,5)$

For (d, k) = (3, 4), a shelling exists for which path lengths are not decidable by the algorithm without convex hull computations. However, this shelling only achieves a diameter of 7. For (d, k) = (3, 5) the algorithm stops at Step 3, as there is no combination of 6 elements of  $\mathcal{F}_{2,5}$  which form a shelling such that  $d(u, v) = \delta(2, 5) + 5 = 10$ . Thus, no convex hull computations are required for (d, k) = (3, 5). A shortcut from u to v is typically found early during the shelling step, which leads to the algorithm terminating quickly. Run on a 2009 Intel<sup>®</sup> Core<sup>TM</sup>2 Duo 2.20GHz CPU, the algorithm is able to terminate for (d, k) = (3, 4) and (3, 5) in under a minute. Consequently,  $\delta(3, 4) < 8$  and  $\delta(3, 5) < 10$ . Since the Minkowski sum of (1, 0, 0), (0, 1, 0), (0, 0, 1), (0, 1, 1), (1, 0, 1), (1, 1, 0), and (1, 1, 1) forms

a lattice (3,4)-polytope of diameter 7, we conclude that  $\delta(3,4) = 7$ . Similarly, since  $H_1(3,2)$ ; that is the Minkowski sum of (1,0,0), (0,1,0), (0,0,1), (0,1,1), (1,0,1), (1,1,0), (0,1,-1), (1,0,-1), and <math>(1,-1,0) forms, up to translation, a lattice (3,5)-polytope of diameter 9, we conclude that  $\delta(3,5) = 9$ .

Note that  $H_1(3,2)$  is congruent to the truncated cuboctahedron; which is also called great rhombicuboctahedron, and is the Minkowski sum of an octahedron and a cuboctahedron, see Figure 1 for an illustration.

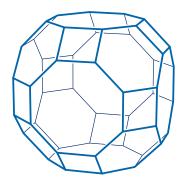


Figure 1:  $H_1(3,2)$  is congruent to the truncated cuboctahedron and maximizes the diameter among all lattice (3,5)-polytopes

Assuming that  $\delta(d-1,k)$  is known and that the set  $\mathcal{F}_{d-1,k}$  of all lattice (d-1,k)-polytopes of diameter  $\delta(d-1,k)$  can be determined, the algorithm checks whether  $\delta(d,k) = \delta(d-1,k) + k$  by performing a search over a highly constrained space. In case there exists a lattice (d,k)-polytope of diameter  $\delta(d,k) = \delta(d-1,k) + k - 1$ , the algorithm allows the determination of  $\delta(d,k)$  as being equal to  $\delta(d,k) = \delta(d-1,k) + k - 1$  or to  $\delta(d,k) = \delta(d-1,k) + k$ . The question is significantly more challenging if  $\delta(d,k) - \delta(d-1,k) < k - 1$  as the search space is much larger and additional structural properties are needed. The algorithm was enhanced in [4] to show that  $\delta(3,6)$  and  $\delta(5,3)$  are equal to 10.

# 3.2. Enumerating all lattice (3,2)-polytopes of diameter $\delta(3,2)$

The algorithm can be adapted to enumerate all lattice (d, k)-polytopes of diameter  $\delta(d, k)$ . In this section we consider the case (d, k) = (3, 2); that is,

the determination of all lattice (3, 2)-polytopes of diameter 4.

Note first that a lattice (3,2)-polytope with an empty intersection with at least one of the facet of  $[0,2]^3$  is either a hexagonal prism or a lattice (3,2)-polytope of diameter at most 3. Thus, the hexagonal prism depicted in Figure 2 in the middle of the top row is, up to the symmetries of  $[0,2]^3$ , the unique lattice (3,2)-polytope of diameter 4 with an empty intersection with at least one facet of  $[0,2]^3$ .

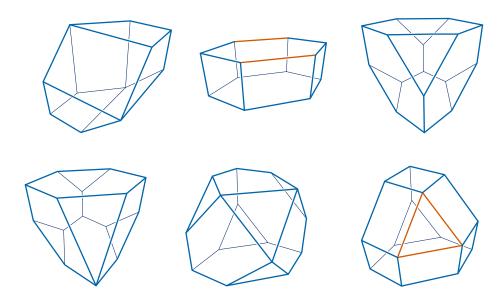


Figure 2: All, up to the symmetries of  $[0,2]^3$ , lattice (3,2)-polytopes of diameter 4 with 11, 15, or 16 vertices, or with an empty intersection with at least one facet of  $[0,2]^3$ 

For a lattice (3, 2)-polytope of diameter 4 with a nonempty intersection with each facet of  $[0, 2]^3$ , Theorem 3 can be adapted as follows. Let u and v be two vertices of a lattice (3, 2)-polytope such that d(u, v) = 4, then (u, v) must satisfy  $1 \le u_i + v_i \le 3$  for i = 1, 2, 3, and the intersection of the lattice (3, 2)-polytope with any facet of  $[0, 2]^3$  must contain at least 2 vertices. The computational results show that there are, up to the symmetries of  $[0, 2]^3$ , hundreds of lattice (3, 2)-polytopes of diameter 4 with a nonempty intersection with each facet of  $[0, 2]^3$ . The set  $\mathcal{V}_{3,2}$  of all the vertices of all the lattice (3, 2)-polytopes of diameter 4 consists of all  $\{0, 1, 2\}$ -valued points except (1, 1, 1). This point forms the intersection of all lattice (3, 2)-polytopes

of diameter 4; that is,  $\mathcal{P}_{3,2} = \{(1,1,1)\}.$ 

There are 3, up to the symmetries of  $[0,2]^3$ , lattice (3,2)-polytopes of diameter 4 with 15 vertices which are depicted in the bottom row of Figure 2 where the edges of the intersections with the facets of  $[0,2]^3$  are shown in blue. The unique, up to the symmetries of  $[0,2]^3$ , lattice (3,2)-polytope of diameter 4 with 11, respectively 16, vertices is represented leftmost, respectively rightmost, in the top row.

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