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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.

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 $\{0, 1, \ldots, k\}^d$, 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 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 $k < 2d$, $\delta(d, k) = \lfloor (k + 1)d/2 \rfloor$.*

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

$d \backslash k$	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							
$\vdots$	$\vdots$	$\vdots$								
d	d	$\lfloor \frac{3d}{2} \rfloor$								

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.

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 $i = 1,\ldots,d$, 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) *$u + v = (k,k,\ldots,k)$,*
(2) *any edge with u or v as vertex is drawn from $\{-1,0,1\}^d$,*
(3) *for $i = 1,\ldots,d$, 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 $\mathcal{V}_{d-1,k}$ of all the vertices of all lattice $(d-1,k)$-polytopes of diameter $\delta(d-1,k)$. For example, for $(d,k) = (3,4)$, $\mathcal{V}_{2,4}$ 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 $\mathcal{C}_{d,k}$ 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 Γ 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 Γ between u and v. Since Γ 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 Γ 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 Γ; 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 Γ 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,

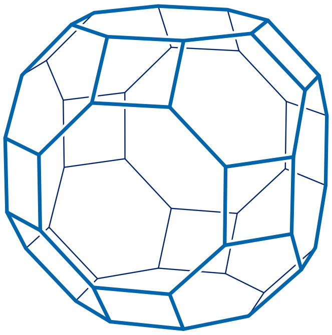

Fig. 1. $H_1(3, 2)$ is congruent to the truncated cuboctahedron and maximizes the diameter among all lattice $(3, 5)$-polytopes.

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® Core™2 Duo 2.20 GHz 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 $(1, -1, 0)$ 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 Fig. 1 for an illustration.

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 Fig. 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 $[0, 2]^3$.

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 $1 \leq u_i + v_i \leq 3$ 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 Fig. 2 where the edges of the intersections with the facets of $[0, 2]^3$ are shown in blue. For a colored representation of Fig. 2, the reader is referred to the web version of this article. 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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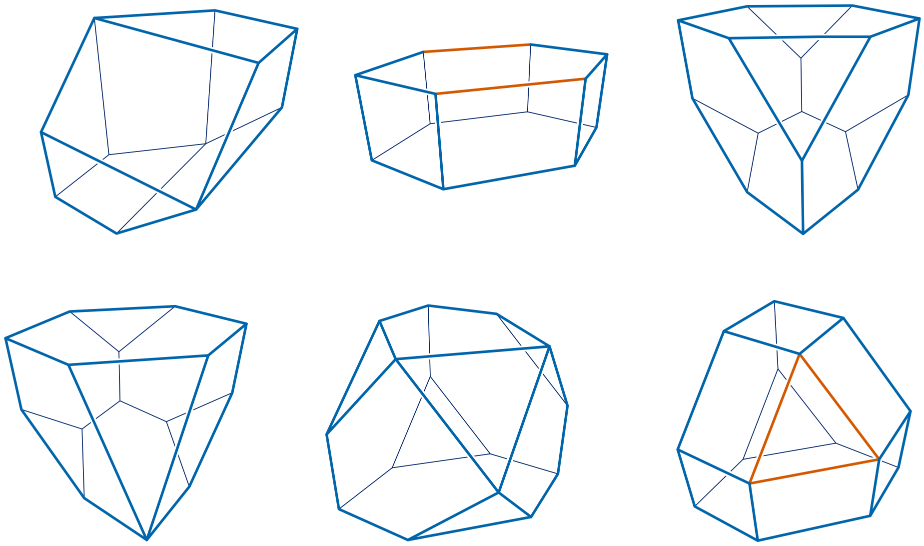

Fig. 2. All, up to the symmetries of $[0, 2]^3$, lattice $(3, 2)$-polytopes of diameter 4 with 11, 15, or 16 vertices, or with an empty intersection with at least one facet of $[0, 2]^3$.

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