Computational determination of the largest lattice polytope diameter

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A B S T R A C T

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 \([k+1]d/2\) and is achieved, up to translation, by a Minkowski sum of lattice vectors.

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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 \(\delta(d,2) = \lceil 3d/2 \rceil\). 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 \(\delta(2,k) = \frac{6}{(2\pi)^{1/2}}k^{2/3} + O(k^{1/3} \log k)\).

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 \([k+1]d/2\). Thus, they showed that \(\delta(d,k) \geq \lceil (k+1)kd/2\rceil\) 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 \(k < 2d\), \(\delta(d,k) = \lceil (k+1)kd/2\rceil\).
Table 1
The largest possible diameter \( \delta(d, k) \) of a lattice \((d, k)\)-polytope

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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 \( \tilde{x}_i \in \mathcal{P}_{d−1,k} \) for some \( 1 \leq i \leq d \). Here \( \tilde{x}_i \in \mathbb{R}^{d−1} \) 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 \(u\): \((0, 0, 0), (0, 0, 1), (0, 1, 0), (0, 1, 1), (0, 2, 0), (0, 2, 2), (1, 1, 0), (1, 1, 1), (1, 1, 2), (1, 2, 0), \) and \((1, 2, 2)\).

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 \(C_{d,k}\), 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 \(C_{3,4}\) 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 \(u + v = \{k, \ldots, k\}\). 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 \((k, \ldots, k)\), 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\(^\text{®} \) Core\(^\text{TM} \) 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 \((1, 0, 0), (0, 1, 0), (0, 0, 1), (0, 1, 1), (1, 0, 1), (1, 1, 0), (0, 1, −1), (1, 0, 0), \) and \((0, 1, 0)\) 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 \((d, d)\)-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 \( \mathcal{F}_{3,2} \) 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, \( \mathcal{F}_{3,2} = \{(1, 1, 1)\} \).

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 $[0, 2]^3$.

References