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Abstract A lattice (d,k)-polytope is the convex hull of a finite set of points in dimension d whose coordinates are integers ranging between 0 and k. We consider the largest possible distance $\delta(d,k)$ between two vertices in the edge-graph of a lattice (d,k)-polytope. We show that $\delta(5,3)$ and $\delta(3,6)$ are equal to 10. This substantiates the conjecture whereby $\delta(d,k)$ is achieved by a Minkowski sum of lattice vectors.

Keywords Lattice Polytopes · Diameter · Minkowski Sums

1 Introduction

Bounding the maximal possible diameter of the edge-graph of a polyhedron as a function of its dimension d and the number n of its facets is not only a natural question of extremal discrete geometry, but it is also historically connected with the theory of simplex methods. Larman [15] gave an upper bound on this quantity that is linear as a function of n, but exponential as a function of d, which was subsequently refined by Barnette [3] and generalized by Eisenbrand, Hähnle, Razborov, and Rothvoß [9] and Labbé, Manneville, and Santos [14]. Kalai and Kleitman [11] found an upper bound that is quasi-polynomial as a function of d and n, which was subsequently refined by Todd [20] and Sukegawa [18]. Lower bounds have also been obtained by Klee and Walkup [12] and by Santos [17], disproving the Hirsch conjecture for unbounded polyhedra and for polytopes, respectively.

In the case of a lattice polytope, i.e. the convex hull of a set of points with integer coordinates, the range for the coordinates of the vertices can be used as an alternative to n. A lattice (d,k)-polytope is the convex hull of a set of points in dimension d whose coordinates are integers ranging between 0 and k. Let $\delta(d,k)$ denote the largest possible diameter of a lattice (d,k)-polytope. The case when $k=1$ was investigated by Naddef [16] who showed that $\delta(d,1)=d$, and thus that lattice $(d,1)$-polytopes satisfy the Hirsch bound. This result was generalized to $\delta(d,k)\leq kd$ by Kleinschmidt and Onn [13]. The case when $d=2$ was

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studied independently by Thiele [19], Balog and Bárány [2], and Acketa and Žunić [1]. It can also be found in Ziegler's book [21] as Exercise 4.15. In particular, $\delta(2,k)$ is known for all k. Kleinschmidt and Onn's upper bound was strengthened for $k \geq 2$ to $\delta(d,k) \leq kd - \lceil d/2 \rceil$ by Del Pia and Michini [5] with equality for $k = 2$, and then to $\delta(d,k) \leq kd - \lceil 2d/3 \rceil - (k-3)$ when $k \geq 3$ by Deza and Pournin [7]. The quantities $\delta(d,2) = \lfloor 3d/2 \rfloor, \delta(4,3) = 8$, and $\delta(3,4) = 7$ and $\delta(3,5) = 9$ were determined, respectively, in [5], [7], and [4]. Investigating the lower bound, Deza, Manoussakis, and Onn [6] build lattice (d,k)-polytopes of diameter $\lfloor (k+1)d/2 \rfloor$. These polytopes are Minkowski sums of sets of the shortest possible lattice vectors, no two of whose are collinear. In this paper, we investigate Conjecture 1 stating that $\delta(d,k)$ is achieved by such polytopes.

Conjecture 1 ([6]) For any d and k, $\delta(d,k)$ is achieved, up to translation, by a Minkowski sum of lattice vectors. In particular, when $k < 2d$, $\delta(d,k) = \lfloor (k+1)d/2 \rfloor$.

Our main contribution is the determination of $\delta(5,3)$, and $\delta(3,6)$, reported in bold in Table 1 along with the other known values of $\delta(d,k)$. The determination of $\delta(5,3)$ and $\delta(3,6)$ is detailed in Section 4.

Theorem 1 $\delta(5,3)$ *and* $\delta(3,6)$ *are equal to* 10.

	$d \backslash k$	1	2	3	4	5	6	7	8	9	…
	1	1	1	1	1	1	1	1	1	1	…
	2	2	3	4	4	5	6	6	7	8	…
d	3	3	4	6	7	9	**10**				
	4	4	6	8							
	5	5	7	**10**							
	⋮	⋮	⋮								
	d	d	$\lfloor \frac{3}{2}d \rfloor$								

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

The paper is organized as follows. Structural properties of lattice polytopes with large diameter are presented in Section 2. Those properties are used in Section 3 to generalize the computational framework introduced in [4] to determine smaller instances, allowing to prove Theorem 1. This manuscript is dedicated to the memory of Michel Deza who worked on a related question: bounding the diameter of a polytope in terms of the lattice points it contains, see [8].

2 Structural Properties of Lattice Polytopes with Large Diameter

Given two vertices u and v of a polytope P, we call $d(u,v)$ their distance in the graph of P. If F is a face of P, we further call $d(u,F) = \min\{d(u,v) : v \in F\}$. The coordinates of a vector $x \in \mathbb{R}^d$ are denoted by x_1 to x_d, and its scalar product with a vector $y \in \mathbb{R}^d$ by $x \cdot y$. We recall Lemma 1 introduced by Del Pia and Michini.

Lemma 1 ([5]) *Consider a lattice (d,k)-polytope P. If u is a vertex of P and $c \in \mathbb{R}^d$ a vector with integer coordinates, then $d(u,F) \leq c \cdot u - \gamma$ where $\gamma = \min\{c \cdot x : x \in P\}$ and $F = \{x \in P : c \cdot x = \gamma\}$.*

We consider the following $2d$ faces of P which are key objects in our computational framework. Let $\gamma_i^-(P) = \min\{x_i : x \in P\}$ and $F_i^0(P) = \{x \in P : x = \gamma_i^-(P)\}$. Similarly, let $\gamma_i^+(P) = \max\{x_i : x \in P\}$ and $F_i^k(P) = \{x \in P : x = \gamma_i^+(P)\}$. When there is no ambiguity, $F_i^0(P)$,and $F_i^k(P)$ will be simply denoted by F_i^0 and F_i^k. Considering paths from u to v going though $F_i^0(P)$ or $F_i^k(P)$, yields:

$$d(u,v) \leq \min_{i=1,\dots,d} \min\{\delta(F_i^0) + d(u,F_i^0) + d(v,F_i^0), \delta(F_i^k) + d(u,F_i^k) + d(v,F_i^k)\}. \quad (1)$$

Using inequality (1) and setting c as a basis vector or its opposite in Lemma 1 give Corollary 1.

Corollary 1 *Let u and v be two vertices of a lattice (d,k)-polytope, then*

$$d(u,v) \leq \min_{i=1,\dots,d} \min\{\delta(F_i^0) + u_i + v_i, \delta(F_i^k) + 2k - u_i - v_i\}.$$

Proposition 1 is borrowed from [10], see Corollaries 12.2 and 12.4 therein. It is used to prove Lemma 2.

Proposition 1 *Let P_1 and P_2 be two polytopes in $\mathbb{R}^d$ and $P = P_1 + P_2$ their Minkowski sum. A point $v \in P$ is a vertex of P if and only if for some $c \in \mathbb{R}^d$, $v = v_1 + v_2$, where v_1 and v_2 are vertices of P_1 and P_2, respectively such that $\{v_i\}$ is the subset of P_i wherein $c{\cdot}x$ is minimal. Moreover, if u is a vertex of P adjacent to v in the graph of P, and if u_1 and u_2 are the vertices of P_1 and P_2, respectively, such that $u = u_1 + u_2$, then for all $i \in \{1,2\}$, u_i and v_i are either equal or adjacent in the graph of P_i.*

Lemma 2 *For any lattice (d,k)-polytope Q, there exists a lattice (d,k)-polytope P of diameter at least $\delta(Q)$ satisfying $\gamma_i^-(P) = 0$ and $\gamma_i^+(P) = k$ for all $i \in \{1,\dots,d\}$.*

Proof Assume that, for some i, $\gamma_i^+(Q) - \gamma_i^-(Q) < k$. Up to translation, we can assume that $\gamma_i^-(Q) = 0$. Consider the segment $\sigma_i = \mathrm{conv}\{0, (k - \gamma_i^+(Q))e_i\}$ where e_i is the point whose all coordinates are equal to 0 except for the i-th coordinate that is equal to 1. By construction, $Q + \sigma_i$ is a lattice (d,k)-polytope such that $\gamma_i^-(Q+\sigma_i) = 0$ and $\gamma_i^+(Q+\sigma_i) = k$. Let u and v be two vertices of Q such that $d(u,v) = \delta(Q)$. By Proposition 1, there exist two vertices u' and v' of $Q + \sigma_i$ obtained as the Minkowski sums of u and v, respectively with two (possibly identical) vertices of σ_i. Moreover, for any path of length l between u' and v' in the edge-graph of $Q+\sigma_i$, there exists a path of length at most l between u and v in the edge-graph of Q. Consequently, the distance of u and v in the graph of Q is at most the distance of u' and v' in the graph of $Q+\sigma_i$. Thus, $\delta(Q) \leq \delta(Q+\sigma_i)$. If $\gamma_j^+(Q+\sigma_i) - \gamma_j^-(Q+\sigma_i) < k$ for some $j \neq i$, the above procedure can to be repeated until no such coordinate remains. □

Lemma 3 *Assume that $\delta(d,k) = \delta(d-1,k) + k - g$ for an integer g with $0 \leq g \leq k$.*

- (i) *If u and v are two vertices of a lattice (d,k)-polytope such that $d(u,v) = \delta(d,k)$, then $|u_i + v_i - k| \leq g$ for all $i \in \{1,\dots,d\}$.*
- (ii) *There exists a lattice (d,k)-polytope P of diameter $\delta(d,k)$ such that the intersection of P with each facet of the hypercube $[0,k]^d$ is, up to an affine transformation, a lattice $(d-1,k)$-polytope of diameter at least $\delta(d-1,k) - 2g$.*

Proof Setting $d(u,v) = \delta(d-1,k) + k - g$ in Corollary 1 yields:

$$\delta(d-1,k) + k - g \leq \delta(F_i^0) + (u_i + v_i) \quad \text{for all } i \in \{1,\dots,d\}, \quad (2)$$

$$\delta(d-1,k) + k - g \leq \delta(F_i^k) + 2k - (u_i + v_i) \quad \text{for all } i \in \{1,\dots,d\}. \quad (3)$$

Thus,

$$\delta(d-1,k) - \delta(F_i^0) + k - g \le u_i + v_i \quad \text{for all } i \in \{1,...,d\}, \tag{4}$$
$$\delta(F_i^k) - \delta(d-1,k) + k - g \ge u_i + v_i \quad \text{for all } i \in \{1,...,d\}. \tag{5}$$

Hence, $k-g \le u_i + v_i \le k+g$ for $i = 1,\dots,d$; that is item (i) holds. By Lemma 2 there exists a lattice (d,k)-polytope P of diameter $\delta(d-1,k)+k-g$ such that the intersection of P with each facet of the hypercube $[0,k]^d$ is nonempty. Let u and v be two vertices of P such that $d(u,v) = \delta(P)$. Inequalities (4) and (5) can be rewritten as:

$$\delta(F_i^0) \ge \delta(d-1,k) - g + k - (u_i + v_i) \quad \text{for all } i \in \{1,...,d\}, \tag{6}$$
$$\delta(F_i^k) \ge \delta(d-1,k) - g + (u_i + v_i) \quad \text{for all } i \in \{1,...,d\}. \tag{7}$$

Thus, since $k-g \le u_i+v_i \le k+g$ for all $i \in \{1,...,d\}$ by item (i), $\delta(F_i^0)$ and $\delta(F_i^k)$ are at least $\delta(d-1,k) - 2g$ for all $i \in \{1,...,d\}$; that is, item (ii) holds. □

We recall that the bounds obtained by Del Pia and Michini [5] and Deza and Pournin [7] hold in general for lattice polytopes inscribed in rectangular boxes.

Corollary 2 (Remark 4.1 in [7]) *Let $\delta(k_1,\dots,k_d)$ denote the largest possible diameter of a polytope whose vertices have their i-th coordinate in $\{0,\dots,k_i\}$ for all $i \in \{1,\dots,d\}$ and, up to relabeling, $k_1 \le k_2 \le \dots \le k_d$. The following inequalities hold:*

(i) $\delta(k_1,\dots,k_d) \le k_2 + k_3 + \dots + k_d - \lceil d/2 \rceil + 2$ *when* $k_1 \ge 2$,
(ii) $\delta(k_1,\dots,k_d) \le k_2 + k_3 + \dots + k_d - \lceil 2d/3 \rceil + 3$ *when* $k_1 \ge 3$.

Observe that the statement of Remark 4.1 in [7] contains a typographical incorrectness as k_1 and k_d were interchanged in (i) and in (ii). Conjecture 1 can also be stated for lattice polytopes inscribed in rectangular boxes; that is, $\delta(k_1,\dots,k_d)$ is at most $\lfloor (k_1 + k_2 + \dots + k_d + d)/2 \rfloor$, and is achieved, up to translation, by a Minkowski sum of lattice vectors. Note that this generalization of Conjecture 1 holds for $d = 2$ and for $(k_1,k_2,k_3) = (2,2,3)$ and $(2,3,3)$. Moreover, $\delta(k_1,k_2) = \delta(k_1,k_1)$, and $\delta(2,2,3) = \delta(2,3,3) = 5$.

3 Computational Determination of $\delta(d,k)$

3.1 Computational framework

The computational framework introduced in [4] can only determine whether $\delta(d,k)$ is equal to $\delta(d-1,k)+k$. In the terms of Lemma 3, this amounts to assume that $g = 0$. This case is significantly easier than when $g > 0$ since it can then be assumed that both $\delta(F_i^0)$ and $\delta(F_i^k)$ are equal to $\delta(d-1,k)$ and that the vertices u and v such that $d(u,v) = \delta(d,k)$ satisfy $u_i + v_i = k$ for all $i \in \{1,...,d\}$. In addition, the computations were performed for $d = 3$; that is, for instances such that the determination of all lattice $(d-1,k)$-polytopes of diameter $\delta(d-1,k)$ is computationally inexpensive compared to higher dimensions. To handle the case $g > 0$ and be able to determine all lattice $(d-1,k)$-polytopes of diameter $\delta(d-1,k)$ for $d > 3$, we introduce an enhanced algorithm exploiting the structural properties presented in Section 2. We are able to recompute previously determined values of $\delta(d,k)$ in a few seconds and obtain previously intractable values. In addition, the enhanced algorithm can be used to generate all the lattice (d,k)-polytopes maximizing the diameter. The enhanced algorithm is presented in Section 3.2 and illustrated for small instances of (d,k).

3.2 Algorithm to determine whether $\delta(d,k) = \delta(d-1,k)+k-g$

Assuming that the value for $\delta(d-1,k)$ is known, the initial upper bound used for $\delta(d,k)$ is $\delta(d-1,k)+k$. Using the necessary condition derived from the structural properties presented in Section 2, the algorithm checks whether there exists a lattice (d,k)-polytope of diameter $\delta(d-1,k)+k$. If no such polytope exists, the upper bound is updated to $\delta(d-1,k)+k-1$ and the computational framework checks whether there exists a lattice (d,k)-polytope of diameter $\delta(d-1,k)+k-1$, and so on. The lower bound is provided by the Minkowski sum of primitive lattice vectors proposed by Deza, Manoussakis, and Onn [6]. For instance, the initial upper bound for $(d,k) = (3,6)$ is $\delta(2,6)+6 = 12$ while the lower bound is 10. The algorithm first assumes that $\delta(3,6)$ is equal to 12 and determines that no lattice $(3,6)$-polytope has diameter 12. Then, assuming that $\delta(3,6)$ is equal to 11, the algorithm determines that no lattice $(3,6)$-polytope has diameter 11. Thus, we can conclude that $\delta(3,6)$ is equal to 10.

3.2.1 Input

The input of the code consists of a vector (d,k,g) and all associated pairs of vertices $\{u,v\}$ described as follows.

(i) d: the dimension,
(ii) k: the range of the coordinates; that is, $x_i \in \{0,1,\ldots,k\}$,
(iii) g: a parameter determining the diameter we wish to rule out (or achieve); i.e. we assume that $\delta(P) = \delta(d-1,k)+k-g$,
(iv) u and v: two vertices of P such that $d(u,v) = \delta(d-1,k)+k-g$.

Starting from $g=0$, computations are performed for each possible pair of vertices $\{u,v\}$ for given (d,k,g). If no lattice (d,k)-polytope of diameter $\delta(d-1,k)+k-g$ is found, g is increased by one and computations are performed for each possible pair of vertices $\{u,v\}$ for given $(d,k,g+1)$, and so forth. Thus, a critical ingredient is to reduce as much as possible the number of pairs $\{u,v\}$ that must be considered. This is achieved by noticing that some restricting conditions can be assumed without loss of generality.

First, by the symmetries of the hypercube $[0,k]^d$, we can assume that the coordinates of u satisfy:

$$u_i \le u_{i+1} \le \lfloor k/2 \rfloor \quad \text{for } i = 1,\ldots,d-1.$$

In addition, by item (i) of Lemma 3, we can assume that the coordinates of u and v satisfy:

$$k-g \le u_i + v_i \le k+g \quad \text{for } i = 1,\ldots,d.$$

Further, by the symmetries of the hypercube $[0,k]^d$ acting on the pair $\{u,v\}$ and assuming that all u are generated in the lexicographic order (denoted by $\prec$ in the following), we can further assume that the coordinates of u and v satisfy the following conditions where $\tilde{v}$ is the point consisting of the coordinates of v reordered lexicographically:

$$\begin{aligned} \{v_i \le v_{i+1} \text{ if } u_i = u_{i+1}\} \quad & \text{for } i = 1,\ldots,d-1, \\ \tilde{v} \prec (k,\ldots,k) - u \quad & \text{if } \{v_i \ge \lceil k/2 \rceil \text{ for } i = 1,\ldots,d\}. \end{aligned}$$

Finally, we can exploit the fact that the intersections of P with the facets of $[0,k]^d$ must be of sufficiently large diameter. Let $\mathscr{V}_{d,k,g}$ denote the set formed by all the vertices of all the lattice

(d,k)-polytopes P such that $\delta(P) = \delta(d,k) - g$. Let $\bar{v}_i$ denote the point in $\mathbb{R}^{d-1}$ consisting of all coordinates of v except v_i, and let $g_i^0 = g + u_i + v_i - k$ and $g_i^k = g + k - (u_i + v_i)$. The following conditions are necessary for u and v to be vertices of P:

$$\{\bar{u}_i \in \mathscr{V}_{d-1,k,g_i^0} \text{ if } u_i = 0\} \quad \text{for } i = 1,\dots,d,$$
$$\{\bar{v}_i \in \mathscr{V}_{d-1,k,g_i^k} \text{ if } v_i = k\} \quad \text{for } i = 1,\dots,d.$$

Let $\mathscr{P}_{d,k,g}$ denote the set of all points with integer coordinates belonging to the intersection of all lattice (d,k)-polytopes P such that $\delta(P) = \delta(d,k) - g$. Let $\mathscr{C}^{u,v}_{d,k,g}$ denote the convex hull of u, v, all points x such that $x_i = 0$ and $\bar{x}_i \in \mathscr{P}_{d-1,k,g_i^0}$, and all points x such that $x_i = k$ and $\bar{x}_i \in \mathscr{P}_{d-1,k,g_i^k}$. Since $\mathscr{C}^{u,v}_{d,k,g} \subset P$, the following condition is necessary for u and v to be vertices of P:

$$u \text{ and } v \text{ are vertices of } \mathscr{C}^{u,v}_{d,k,g}.$$

Let us illustrate the conditions that can be assumed for the pair $\{u,v\}$ by considering the case $(d,k,g) = (3,6,0)$. In other words, we assume that u and v are vertices of a lattice $(3,6)$-polytope P of diameter 12. Since $g = 0$, we can assume that:

$$u_1 \le u_2 \le u_3 \le 3,$$
$$u + v = (6,6,6),$$
$$\{\bar{u}_i \in \mathscr{V}_{2,6,0} \text{ if } u_i = 0\} \quad \text{for } i = 1,2,3,$$
$$u \text{ is a vertex of } \mathscr{C}^{u,v}_{3,6,0} \text{ if } u_1 \neq 0.$$

Among the 20 points u satisfying $u_1 \le u_2 \le u_3 \le 3$, the only ones such that $u_1 = 0$ and $(u_2,u_3) \in \mathscr{V}_{2,6,0}$ are $(0,0,1)$, $(0,0,2)$, $(0,0,3)$, $(0,1,1)$, and $(0,1,2)$. In addition, none is a vertex of $\mathscr{C}^{u,v}_{3,6,0}$ when $u_1 \neq 0$. Thus, since $u + v = (6,6,6)$, we need to consider only 5 pairs of vertices $\{u,v\}$. The sets $\mathscr{V}_{2,6,0}$ and $\mathscr{P}_{2,6,0}$ can be easily computed and are illustrated in Figure 1. Note that both $\mathscr{V}_{d,k,g}$ and $\mathscr{P}_{d,k,g}$ are invariant under the symmetries of $[0,k]^d$.

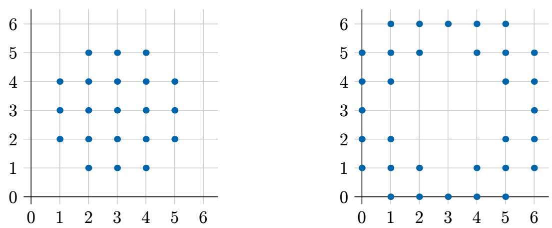

Fig. 1 The sets $\mathscr{V}_{2,6,0}$ and $\mathscr{P}_{2,6,0}$

3.2.2 Main subroutine to determine whether there exists a lattice (d,k)-polytope with vertices u and v such that $d(u,v) = \delta(d-1,k) + k - g$

Given (d,k,g), all possible pairs $\{u,v\}$ of vertices are generated. For each pair, we run the main subroutine to determine whether there exists a lattice (d,k)-polytope P with vertices u

and v such that $d(u,v) = \delta(d-1,k)+k-g$. Such polytopes P are generated by considering all possible choices for the $2d$ intersections of P with the facets of the hypercube $[0,k]^d$. This step is called the *Shelling Step*. The order in which the intersections are considered is critical to reduce the search space. It is equally critical to identify, as early as possible, paths between u and v possibly induced by the shelling process. A set of choices for the $2d$ intersections of P with the facets of the hypercube $[0,k]^d$ obtained by the shelling step is called a *shelling*. The output of the shelling step consists in the list of all the shellings generated by performing the shelling step for all possible pairs $\{u,v\}$. Shellings that are duplicate, up to the symmetries of the hypercube $[0,k]^d$, are removed. If the output of the shelling step is empty, the process stops and we can conclude that $\delta(d,k) < \delta(d-1,k)+k-g$.

If the output of the shelling step is non-empty, all possible points with integer coordinates ranging from 1 to $k-1$ are considered as potential additional vertices for each generated shelling. This step is called the *Inner Step*. Again, structural properties are critical to prune the search space. The output of the inner step consists in the list of all generated lattice (d,k)-polytopes after duplicates, up to the symmetries of the hypercube $[0,k]^d$, and lattice (d,k)-polytopes of diameter at most $\delta(d-1,k)+k-g-1$ are removed. If the output of the inner step is empty, we can conclude that $\delta(d,k) < \delta(d-1,k)+k-g$.

3.2.3 Two certificates that no lattice (d,k)-polytopes with vertices u and v such that $d(u,v) = \delta(d-1,k)+k-g$ exist

Let Γ denote the graph defined by the currently known edges and vertices of P. Γ is initially set to $\{u,v\}$. Let $d_\Gamma(x,y)$ denote the distance in Γ between two vertices x and y of P, and $d_\Gamma(x,F)$ the distance in Γ between a vertex x and the vertices of P belonging to F. We consider the following upper bounds for the distance between u or v and the intersection of P with a facet of the $[0,k]^d$, and two upper bounds for $d(u,v)$.

$$\begin{aligned}
\widetilde{d}(u,F_i^0) &= \min_{w\in\Gamma}\{d_\Gamma(u,w)+w_i\} \quad \text{for } i=1,\dots,d,\\
\widetilde{d}(u,F_i^k) &= \min_{w\in\Gamma}\{d_\Gamma(u,w)+k-w_i\} \quad \text{for } i=1,\dots,d,\\
\widetilde{d}(v,F_i^0) &= \min_{w\in\Gamma}\{d_\Gamma(v,w)+w_i\} \quad \text{for } i=1,\dots,d,\\
\widetilde{d}(v,F_i^k) &= \min_{w\in\Gamma}\{d_\Gamma(v,w)+k-w_i\} \quad \text{for } i=1,\dots,d.
\end{aligned}$$

The following quantity $d_\circ(u,v)$, where both $\delta(F_i^0)$ and $\delta(F_i^k)$ are bounded from above by $\delta(d-1,k)$, is an upper bound for $d(u,v)$ by inequality (1):

$$d_\circ(u,v) = \min_{i=1,\dots,d}\{\min\{\widetilde{d}(u,F_i^0)+\widetilde{d}(v,F_i^0)+\delta(F_i^0), \widetilde{d}(u,F_i^k)+\widetilde{d}(v,F_i^k)+\delta(F_i^k)\}\}.$$

Each time a choice for the intersection of P with a facet of the hypercube $[0,k]^d$ is considered, the value of $d_\circ(u,v)$ is updated. Similarly, since Γ is a subgraph of the edge-graph of P, $d_\Gamma(u,v)$ is another upper bound for $d(u,v)$. Thus, we consider the following nonnegative parameter γ defined as:

$$\gamma = \delta(d-1,k)+k-g-min\{d_\Gamma(u,v), d_\circ(u,v)\}.$$

Consequently, $\gamma > 0$ is a certificate that there does not exist a lattice (d,k)-polytope with vertices u and v such that $d(u,v) = \delta(d-1,k)+k-g$.

Another estimate updated along with Γ is the convex hull $\mathscr{C}^{\Gamma}_{d,k,g}$ of all vertices in Γ, all points x such that $x_i = 0$ and $\bar{x}_i \in \mathscr{P}_{d-1,k,g_i^0}$, and all points x such that $x_i = k$ and $\bar{x}_i \in \mathscr{P}_{d-1,k,g_i^k}$. Since $\mathscr{C}^{\Gamma}_{d,k,g} \subset P$, the following condition is a certificate that there does not exist a lattice (d,k)-polytopes with vertices u and v such that $d(u,v) = \delta(d-1,k)+k-g$:

$$u \text{ or } v \text{ is not a vertex of } \mathscr{C}^{\Gamma}_{d,k,g}.$$

3.2.4 Shelling Step

Given a triple (d,k,g) and a pair $\{u,v\}$, the *scores* of F_i^0 and F_i^k are $g_i^0 = g+u_i+v_i-k$ and $g_i^k = g+k-(u_i+v_i)$, respectively. The intersections with the facets of $[0,k]^d$ are ordered by their score, starting from the smaller ones. If two intersections or more have the same score, the number of currently known vertices of P belonging to the intersection is used as a tie-breaker, starting with the one containing the largest number of such vertices. As a secondary tie-breaker, an intersection containing u or v is considered before one containing neither, with "containing u" given priority over "containing v" as a further tie-breaker. If none of those rules apply, the default order is $F_1^0,\dots,F_d^0,F_1^k,\dots,F_d^k$.

Each time an intersection F_i^0, respectively F_i^k, is considered, we generate the set of lattice $(d-1,k)$-polytopes of diameter at least $\delta(d-1,k)-g_i^0$, respectively at least $\delta(d-1,k)-g_i^k$, and having $\bar{x}_i$ as vertices if x is a vertex from Γ such that $x_i = 0$, respectively such that $x_i = k$. After one such lattice $(d-1,k)$-polytope is assigned to form, up to an affine transformation, the chosen intersection with $[0,k]^d$, its vertices and edges are added to Γ. Consequently, the value of γ and $\mathscr{C}^{\Gamma}_{d,k,g}$ are updated. If u or v is not a vertex of $\mathscr{C}^{\Gamma}_{d,k,g}$, or $\gamma > 0$, the search can be pruned at this node. Typically, the very first chosen intersection with $[0,k]^d$ may yield a certificate of non-existence for the desired P. Note that all scores g_i^0 of F_i^0, respectively g_i^k of F_i^k, are updated during the shelling process. Namely, each time a choice for the intersection of P with a facet of the hypercube $[0,k]^d$ is considered, the score of a not yet considered intersection is updated to $g_i^0 = g+\widetilde{d}(u,F_i^0)+\widetilde{d}(v,F_i^0)-k$, respectively to $g_i^k = g+\widetilde{d}(u,F_i^k)+\widetilde{d}(v,F_i^k)-k$.

In order to illustrate the shelling step, we first consider the case $(d,k,g) = (3,6,0)$. As discussed in Section 3.2.1, there are 5 pairs $\{u,v\}$ to consider. Since $g = 0$, the score of any intersection with $[0,k]^d$ is zero. The only currently known vertices of P are u and v and $u_1 = 0$ for all the 5 pairs. Thus, the first considered intersection is F_1^0. Consequently, for each $\{u,v\}$, we generate the set of lattice $(2,6)$-polytopes of diameter 6 having (u_2,u_3) as a vertex. One can easily check that $\gamma > 0$ for each such choice. Thus, the shelling step terminates after considering F_1^0 for all possible pairs $\{u,v\}$ and we can conclude that $\delta(3,6) < 12$ in a matter of seconds. Another simple example is the case $(d,k,g) = (3,4,0)$ for which the output of the shelling step consists in a unique shelling where the 6 intersections with the facets of $[0,4]^3$ are, up to an affine transformation, the octagonal lattice $(2,3)$-polytope. See Figure 2 for an illustration where the edges of the shelling are shown in blue. As no point whose coordinates are $\{1,2,3\}$-valued can be added to this unique shelling as a potential vertex, the inner step is reduced to check whether the diameter of the convex hull associated to the unique shelling achieves $\delta(2,4)+4-0 = 8$. As the diameter is equal to 7, the output of the inner step is empty. Thus, we can conclude that $\delta(3,4) < 8$; that is, $\delta(3,4) = 7$.

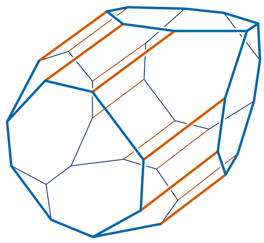

Fig. 2 The unique shelling generated for $(d,k,g) = (3,4,0)$

3.2.5 Inner Step

The input for the inner step is the output of the shelling step, assuming it is non-empty. For each shelling, the inner step considers all *inner* points p; that is, all points p such that $p_i \in \{1,\ldots,k-1\}$ for $i = 1,\ldots,d$. Let $\mathscr{C}^{\Gamma\cup p}_{d,k,g}$ denote the convex hull of p and $\mathscr{C}^{\Gamma}_{d,k,g}$. A necessary condition for p to be vertex of P is:

$$p \text{ is a vertex of } \mathscr{C}^{\Gamma\cup p}_{d,k,g}.$$

Any generated lattice (d,k)-polytope whose diameter is at most $\delta(d-1,k)+k-g-1$ is removed. Similarly any duplicate, up to the symmetries of the hypercube $[0,k]^d$, is removed. If the output of the inner step is empty, we can conclude that $\delta(d,k) < \delta(d-1,k)+k-g$. Otherwise, we can conclude that $\delta(d,k) = \delta(d-1,k)+k-g$, and the output of the inner step provides, up to the symmetries of the hypercube $[0,k]^d$, all lattice (d,k)-polytopes of diameter $\delta(d-1,k)+k-g$ whose intersection with each facet of the hypercube $[0,k]^d$ is non-empty. Further computations allow to determine all lattice (d,k)-polytopes of diameter $\delta(d-1,k)+k-g$ with an empty intersection with at least one facet of the hypercube $[0,k]^d$, as detailed in Section 3.3.

In order to illustrate the inner step, we consider the case $(d,k,g) = (3,4,2)$ and the pair $\{u,v\} = \{(0,0,0),(4,4,4)\}$. In other words, we assume that $u = (0,0,0)$ and $v = (4,4,4)$ are vertices of a lattice $(3,4)$-polytope P such that $\delta(P) = d(u,v) = 5$. Considering this pair, we first perform the shelling step. Since the scores satisfy $g^0_1 = g^0_2 = g^0_3 = g^4_1 = g^4_2 = g^4_3 = 2$, the 6 intersections of P with the facets of $[0,4]^3$ are of diameter at least 2. One can check that the shelling step output includes the shelling consisting in 6 identical, up to an affine transformation, facets forming $[0,1]^2$. Out of the 27 points whose coordinates are $\{1,2,3\}$-valued, 15 are contained in the convex hull of this shelling. Thus, the inner step must consider 12 inner points as possible vertices to be added to this shelling. One can check that, up to the symmetries of $[0,4]^3$, 214 lattice $(3,4)$-polytopes are generated and that all have diameter at most 5 including 8 achieving diameter 5. One such lattice $(3,4)$-polytope of diameter 5 is represented in Figure 3 where the 6 added vertices are show in green and the edges of the intersections with the facets of $[0,4]^3$ are shown in blue. Note that since polytopes of diameter at most $\delta(d,k-1)+k-g-1 = 4+4-2-1 = 5$ are removed, none of the 214 lattice $(3,4)$-polytopes generated by this shelling are part of the output of the inner step for $(d,k,g) = (3,4,2)$.

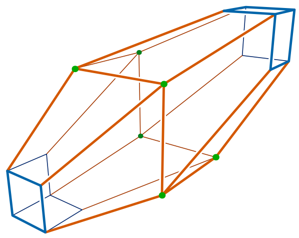

Fig. 3 A polytope considered by the inner step for $(d,k,g) = (3,4,2)$ and $\{u,v\} = \{(0,0,0),(4,4,4)\}$

3.3 Generation of all lattice (d,k)-polytopes of diameter at least $\delta(d,k-1)+k-g$

Running the algorithm for (d,k,g) allows to determine, up to the symmetries of $[0,k]^d$, the set of all lattice (d,k)-polytopes with diameter at least $\delta(d,k-1)+k-g$ whose intersection with each facet of $[0,k]^d$ is non-empty. In this section we outline how the ones with an empty intersection with at least one facet of $[0,k]^d$ can de derived from this set.

Using the notations of Lemma 2, let $I(Q)$ denote the set of coordinates i such that $\gamma_i^+(Q) - \gamma_i^-(Q) < k$. Consider a lattice (d,k)-polytope Q of diameter at least $\delta(d,k-1)+k-g$ such that $I(Q) \neq \emptyset$. For all $i \in I(Q)$, we can assume, up to translation, that $\gamma_i^-(Q) = 0$ and consider the segment $\sigma_i = \text{conv}\{0,(k-\gamma_i^+(Q))e_i\}$. Let S denote the Minkowski sum of all σ_i for $i \in I(Q)$. As shown in the proof of Lemma 2, $Q+S$ is a lattice (d,k)-polytope of diameter at least $\delta(Q)$ satisfying $I(Q+S) = \emptyset$. In other words, $Q+S$ is, up to the symmetries of $[0,k]^d$, in the output of the algorithm ran for (d,k,g). Consequently, up to translation and the symmetries of the hypercube $[0,k]^d$, the set of lattice (d,k)-polytopes Q of diameter at least $\delta(d,k-1)+k-g$ such that $I(Q) \neq \emptyset$ can be generated as follows:

(i) for each lattice (d,k)-polytope P in the output of the algorithm ran for (d,k,g), check whether $P = Q+e$ where Q is a lattice (d,k)-polytope and e a lattice segment. This can be done by checking whether the edge-graphs of P and $P+e$ are isomorphic,

(ii) for each P such that $P = Q+e$ found at step (i), determine Q and check whether $\delta(Q) \geq \delta(d,k-1)+k-g$.

As for the shelling and inner steps, the symmetries of the hypercube $[0,k]^d$ are used to remove duplicates generated within steps (i) and (ii). The set of lattice segments e considered in step (i) can be limited to a few segments whose coordinates are relatively prime and used iteratively. For an illustration, we consider the case $(d,k,g) = (3,3,1)$. As discussed in Section 4.2, the output of the algorithm consists in 9 lattice $(3,3)$-polytopes of diameter 6 whose intersection with each facet of $[0,3]^3$ is non-empty. One can check that, in order to perform step (i), it is enough to consider for e, iteratively, the 3 unit vectors and the 3 sums of 2 unit vectors. All the 9 considered lattice $(3,3)$-polytopes of diameter 6 can be written as $Q+e$. Performing step (ii), one can check that $\delta(Q) = 5$ for each such Q. Thus, there is no lattice $(3,3)$-polytope Q of diameter 6 such that $I(Q) \neq \emptyset$.

4 Proof of Theorem 1

Theorem 1 is obtained by computationally verifying that the output of the inner step is empty for $(d,k,g) = (3,6,1)$ and $(5,3,0)$. Thus, $\delta(3,6) < 11$ and $\delta(5,3) < 11$; that is,

$\delta(3,6) = \delta(5,3) = 10$. Running the algorithm for $(5,3,0)$ requires the determination of all lattice $(3,3)$-polytopes of diameter 5 or 6 and all lattice $(4,3)$-polytopes of diameter 8.

4.1 Determination of $\delta(3,6)$

As mentioned in Section 3.2.4, the output of the shelling step in empty for $(d,k,g) = (3,6,0)$ and thus we can conclude that $\delta(3,6) < 12$. Running the algorithm for $(d,k,g) = (3,6,1)$ is computationally efficient because of two key properties.

First, there are only 4 lattice $(2,6)$-polytopes of diameter 6, see Figure 4 for an illustration.

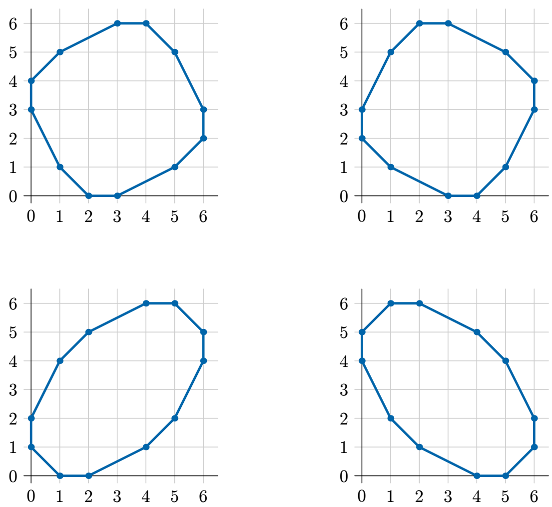

Fig. 4 All lattice $(2,6)$-polytopes of diameter 6

Second, for $d = 2$, there are only 8 lattices edges e such that $|e_1| + |e_2| \leq 2$. Thus, any lattice $(2,6)$-polytope of diameter 5 or 6 includes at least 2 edges such that $|e_1|$ or $|e_2|$ is at least 2.

Consequently, unless both u and v are inner points, the update of the scores $g_i^0 = g + \widetilde{d}(u,F_i^0) + \widetilde{d}(v,F_i^0) - k$, respectively of $g_i^k = g + \widetilde{d}(u,F_i^k) + \widetilde{d}(v,F_i^k) - k$, implies that g_i^0 or g_i^k is updated to zero for some i after the first intersection with a facet of $[0,6]^3$ is considered in the shelling step. As $g_i^0 = 0$, respectively $g_i^k = 0$, implies that $\delta(F_i^0) = 6$, respectively $\delta(F_k^0) = 6$, there are at most 4 lattice $(2,6)$-polytopes to consider for the next intersection with a facet of $[0,6]^3$, and so forth. As an illustration, consider the pair $\{u,v\} = \{(0,0,0),(6,6,6)\}$. Initially, the scores satisfy $g_1^0 = g_2^0 = g_3^0 = g_1^6 = g_2^6 = g_3^6 = 1$ and the shelling step starts by considering a lattice $(2,6)$-polytope of diameter at least 5 for F_1^0. For example, assume that F_1^0 is, up to an affine transformation, the lattice $(2,5)$-polytope obtained as the Minkowski sum of $(1,0),(2,1),(1,1),(1,2)$, and $(0,1)$. Before the next intersection with a facet of $[0,6]^3$ is considered, $\tilde{d}(u,F_2^6)$ is updated to 5 as $d(u,u') = 2$ and $u'_2 = 3$, see Figure 5 where the vertex u' is coloured black while u and v are coloured red.

The second edge on the path from u to u' satisfies $e_2 \geq 2$. Consequently, g_2^6 is updated to $g + \widetilde{d}(u, F_2^6) + \widetilde{d}(v, F_2^6) - 6 = 1 + 5 + 0 - 6 = 0$. Thus, $\delta(F_2^6) = 6$ which is impossible since $\bar{v}_2 = (6,6) \notin \mathscr{V}_{2,6,0}$; that is, there is no shelling with the current choice of F_1^0. The same holds for any choice of F_1^0 since any lattice $(2,6)$-polytope of diameter at least 5 includes at least one edge e such that $|e_1|$ or $|e_2|$ is at least 2. Consequently, there is no shelling for $\{u,v\} = \{(0,0,0),(6,6,6)\}$. Table 2 lists the 69 considered pairs $\{u,v\}$ of vertices of

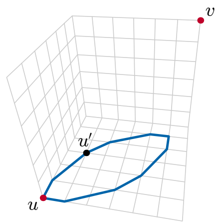

Fig. 5 Initial iteration of the shelling step for $(d,k,g) = (3,6,1)$ and $\{u,v\} = \{(0,0,0),(6,6,6)\}$

a lattice $(3,6)$-polytope P such that $d(u,v) = 11$ where P is assumed to have a non-empty intersection with each facet of $[0,6]^3$.

u	v
(0,0,0)	(6,6,6)
(0,0,1)	(5,5,4), (5,5,5), (5,5,6), (5,6,4), (5,6,5), (5,6,6), (6,6,4), (6,6,5)
(0,0,2)	(5,5,3), (5,5,4), (5,5,5), (5,6,3), (5,6,4), (5,6,5), (6,6,3), (6,6,4)
(0,0,3)	(5,5,2), (5,5,3), (5,5,4), (5,6,2), (5,6,3), (5,6,4), (6,6,2), (6,6,3)
(0,1,1)	(5,4,4), (5,4,5), (5,4,6), (5,5,5), (5,5,6), (6,4,4), (6,4,5), (6,5,5)
(0,1,2)	(5,4,3), (5,4,4), (5,4,5), (5,5,3), (5,5,4), (5,5,5), (5,6,4), (6,4,3), (6,4,4), (6,4,5), (6,5,3), (6,5,4)
(0,1,3)	(6,4,2), (6,4,3), (6,4,4), (6,5,2), (6,5,3), (6,6,2)
(0,2,2)	(6,3,4), (6,4,4)
(0,2,3)	(6,3,2), (6,3,4), (6,4,2), (6,4,3), (6,5,2)
(1,1,1)	(4,5,5), (5,5,5)
(1,1,2)	(5,5,3), (5,5,4)
(1,1,3)	(5,5,2), (5,5,3), (5,6,2), (6,6,2)
(1,2,2)	(5,4,4)
(1,2,3)	(6,5,2)
(2,2,3)	(4,5,2)

Table 2 All considered pairs $\{u,v\}$ for $(d,k,g) = (3,6,1)$

4.2 Determination of $\delta(5,3)$

The determination of $\delta(5,3)$ requires the list of all lattice $(4,3)$-polytopes of diameter 8 up to the symmetries of $[0,3]^4$. In order to obtain all lattice $(4,3)$-polytopes of diameter 8, we first determine all lattice $(4,3)$-polytopes of diameter 8 with non-empty intersection with each facet of $[0,3]^4$ by running the algorithm for $(d,k,g) = (4,3,1)$. Then, using the procedure described in Section 3.3, we can use the output of the algorithm for $(d,k,g) = (4,3,1)$

to determine all the lattice $(4,3)$-polytopes of diameter 8 with an empty intersection with at least one facet of $[0,3]^4$. Note that running the algorithm for $(d,k,g) = (4,3,1)$ requires the list of all lattice $(3,3)$-polytopes of diameter 5 or 6. This is achieved by running the algorithm for $(d,k,g) = (3,3,2)$ and using the procedure described in Section 3.3.

Table 3 lists the 6 considered pairs $\{u,v\}$ of vertices of a lattice $(3,3)$-polytope P such that $d(u,v) = 6$ where P is assumed to have a non-empty intersection with each facet of $[0,3]^3$.

u	v
(0,0,0)	(3,3,3)
(0,0,1)	(2,3,2), (2,3,3), (3,3,1), (3,3,2)
(0,1,1)	(3,2,2)

Table 3 All considered pairs $\{u,v\}$ for $(d,k,g) = (3,3,1)$

The output consists in the following 9 lattice $(3,3)$-polytopes of diameter 6, up to the symmetries of $[0,3]^3$. Using the procedure described in Section 3.3, one can check that there is no lattice $(3,3)$-polytope Q of diameter 6 with an empty intersection with at least one facet of $[0,3]^3$. In other words, any lattice $(3,3)$-polytope of diameter 6 is, up to the symmetries of $[0,3]^3$, one of the 9 polytopes depicted in Figure 6 where the edges of the intersections with the facets of $[0,3]^3$ are shown in blue. Table 4 provides the numbers $f_0(P)$ and $f_2(P)$ of vertices and facets of the 9 polytopes represented in Figure 6. The breakdown by incidence is also indicated. For example, the truncated cube P_4 has 24 vertices, all belonging to 3 facets, and 14 facets consisting in 8 triangles and 6 octagons.

Polytope	$f_0(P)$	Vertex incidence	$f_2(P)$	Facet Incidence
P_1	26	20{3}+6{4}	18	12{4}+6{6}
P_2	23	20{3}+3{4}	14	9{4}+5{6}
P_3	20	20{3}	12	6{4}+6{6}
P_4	24	24{3}	14	8{3}+6{8}
P_5	24	24{3}	14	4{3}+3{4}+4{6}+3{8}
P_6	23	22{3}+1{4}	14	4{3}+3{4}+4{6}+2{7}+1{8}
P_7	23	22{3}+1{4}	14	4{3}+3{4}+4{6}+2{7}+1{8}
P_8	22	22{3}	13	2{3}+4{4}+6{6}+1{8}
P_9	24	24{3}	14	6{4}+8{6}

Table 4 Some combinatorial properties of the lattice $(3,3)$-polytopes with maximal diameter.

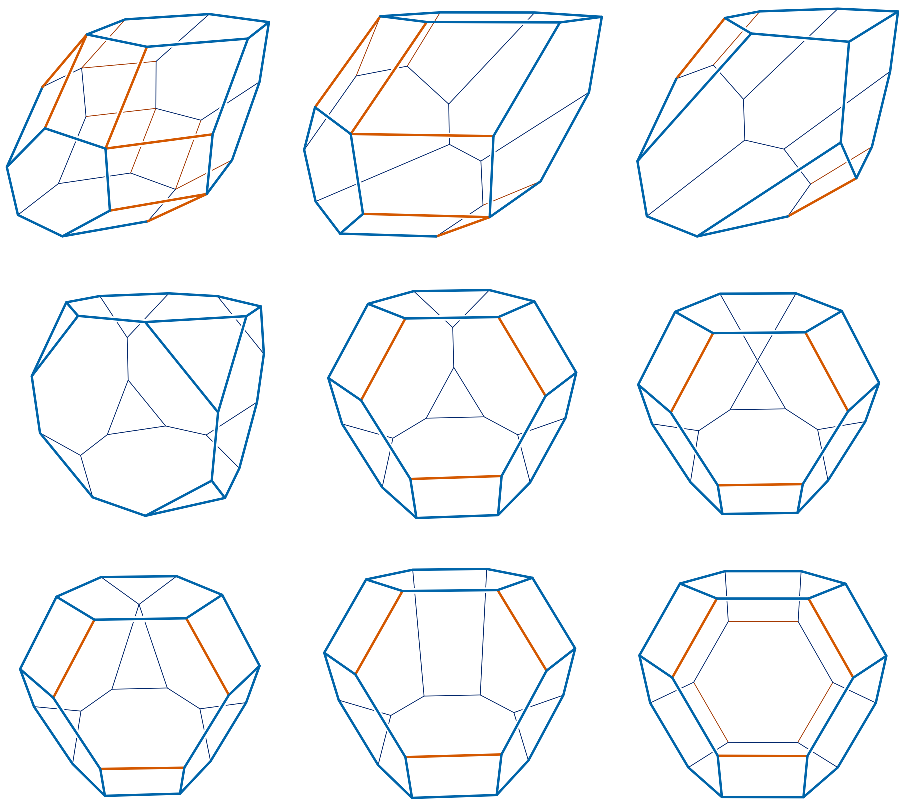

Fig. 6 All, up to the symmetries of $[0,3]^3$, lattice $(3,3)$-polytopes of diameter 6

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