DISCRETE GEOMETRY AND OPTIMIZATION APPROACHES FOR LATTICE POLYTOPES

DISCRETE GEOMETRY AND OPTIMIZATION APPROACHES FOR LATTICE POLYTOPES

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Abstract

Linear optimization aims at maximizing, or minimizing, a linear objective function over a feasible region defined by a finite number of linear constrains. For several well-studied problems such as maxcut, all the vertices of the feasible region are integral, that is, with integer-valued coordinates. The diameter of the feasible region is the diameter of the edge-graph formed by the vertices and the edges of the feasible region. This diameter is a lower bound for the worst-case behaviour for the widely used pivot-based simplex methods to solve linear optimization instances. A lattice (d,k)-polytope is the convex hull of a set of points whose coordinates are integer ranging from 0 to k. This dissertation provides new insights into the determination of the largest possible diameter $\delta(d,k)$ over all possible lattice (d,k)-polytopes. An enhanced algorithm to determine $\delta(d,k)$ is introduced to compute previously intractable instances. The key improvements are achieved by introducing a novel branching that exploits convexity and combinatorial properties, and by using a linear optimization formulation to significantly reduce the search space. In particular we determine the value for $\delta(3,7)$.

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d	:	dimension
k	:	range of integer coordinates
P	:	polytope
F	:	facet of a polytope P
$d(u,v)$	:	distance between vertices u and v in the edge-graph of P
$\delta(P)$	:	diameter of the edge-graph of the polytope P
$\delta(d,k)$	:	largest diameter achieved by a lattice (d,k)-polytope
$\gamma_i^-(P), \gamma_i^+(P)$	:	min $\{x_i : x \in P\}$, max $\{x_i : x \in P\}$
$F_i^-(P), F_i^+(P)$	:	$\{x \in P : x = \gamma_i^-(P)\}$, $\{x \in P : x = \gamma_i^+(P)\}$
$d(u,F)$	:	min $d(u,v)$ for $v \in F$
$\mathscr{F}^*_{d,k}$	:	set of lattice (d,k)-polytopes achieving $\delta(d,k)$
$\mathscr{V}_{d,k,g}$	:	set formed by all vertices of all lattice (d,k)-polytopes of diameter at least $\delta(d,k)-g$
$\mathscr{P}_{d,k,g}$	:	set of all points with integer coordinates in the intersection of all lattice (d,k)-polytopes of diameter at least $\delta(d,k)-g$
Γ	:	graph of currently known vertices and edges of P with all virtual weighted edges added.
$\mathscr{C}^{\Gamma}_{d,k,g}$	:	convex hull of all points in Γ and implicitly known points
$d_\Gamma(u,v)$	:	distance between u and v in Γ
$\widetilde{d}(u,F_i^-)$	:	upper bound $d(u,F)$
$d_\circ(u,v)$	:	upper bound for $d(u,v)$

$\delta_z(d,k)$: largest diameter of all primitive (d,k)-zonotopes

Chapter 1

Introduction

1.1 Polytopes

In this chapter we recall basic definitions and properties of polytopes. For additional properties, we refer to Ziegler [24] and references therein.

A (d,n) *convex polyhedron* P is defined by the intersection of a finite number n of half-spaces in $\mathbb{R}^d$. In other words, P can be defined as the set of solutions to a system of linear inequalities: $P = \{x \in \mathbb{R}^d : Ax \leq b\}$ where A is a d by n matrix.

A bounded convex polyhedron is called a *polytope*; that is, there exists a scalar M such that $\| x \| \leq M$ for $x \in P$. A polytope can also be defined as the convex hull of a finite set of points in $\mathbb{R}^d$. A *lattice polytope* is a polytope such that all its vertices are integer-valued. A lattice (d,k)-polytope is a polytope in dimension d whose vertices are drawn from $\{0,1,\ldots,k\}^d$.

1.2 Shortest paths in the edge-graph and diameter

Given a polytope P, its edge graph is the graph whose vertex set is the set of vertices of the P, and whose edge set is the set of edges of P. A *path* between two vertices (u,v) of P is a sequence of edges connecting u and v. A *shortest path* is a path connecting u and v consisting of the lowest possible number of edges. The number of edges of a shortest path that connects u and v is denoted by $d(u,v)$.

In terms of egde graph, the distance from a vertex $u \in P$ to a face F is defined as $d(u,F) = \min\{d(u,v) : v \in F\}$, the minimum distance between u and v over all vertices v in F.

1.3 Linear optimization and diameter of polytopes

The diameter of a polytope P is a lower bound for the worst-case number of iterations required for pivot-based linear optimization algorithms to solve the problem $\min\{c \cdot x : x \in P\}$. The main goal of this work consists in better understanding the structure of polytopes achieving large diameter. The search of a polytope is usually done by given parameters d and n, where d is the dimension and n corresponds to the number of facets, that is the number of inequalities that are facet-inducing. In this work, we use the range k for lattice polytopes.

The first part of the thesis summarizes the framework developed by Deza et al. [8] to determine the largest possible diameter $\delta(d,k)$ over all lattice (d,k)-polytopes. The second part presents a novel approach to determine a previously intractable value for $\delta(d,k)$.

1.3.1 Simplex method

Dantzig's simplex method [6] is one of the most widely used algorithms to solve linear optimization instances. It was the first practical algorithm that exploits the combinatorial properties of polyhedra. Originally introduced in 1947 by George Dantzig, the algorithm derives its name from the concept of a simplex, *i.e.* a generalization of a triangle to an arbitrary dimension. The method is pivot-based and purely combinatorial. Starting from an initial vertex, found using a surrogate formulation, the simplex method stays on the boundary of the feasible region until reaching, in a finite number of iterations, a vertex maximizing a linear function. Assuming for clarity of the exposition that every vertex of the feasible region is simple; that is, satisfies with equality exactly d inequalities, the simplex method travels from a vertex to an adjacent vertex using an edge which scalar product with the objective function is nonnegative if we are maximizing. In the dual setting, this corresponds to pivot from a simplex to an adjacent simplex sharing a face of dimension $d-1$, hence the simplex method name. The set of inequalities satisfied with equalities are associated to the basic variables and the other inequalities to the nonbasic variables.

More specifically, the simplex algorithm is applied to linear optimization instances which are in the so-called canonical form:

$$\begin{aligned}&\max\ c^T x\\ &Ax = b\\ &\text{and } x \geq 0\end{aligned}$$

where $x = (x_1, \ldots, x_d)$ are the decision variables, $c = (c_1, \ldots, c_d)$ the coefficients of the objective function, and a set of constraints defined by an $n \times d$ matrix A and $b = (b_1, \ldots, b_n)$ being the non-negative right hand side of the n inequalities.

Each constraint defines a half-space in d dimensions which is convex. The intersection of the n half-spaces forms the set of all feasible solutions which is convex as the intersection of n convex sets. If the feasible region is bounded, it is also equal to the convex hull of its vertices. Assuming the instance is feasible and bounded in the direction of the objective function, to solve the linear optimization problem is to find a feasible solution maximizing the objective function. Since the set of maximizers form a face of the feasible region, the optimal solution must occur at at least one vertex. This means that neighbouring vertices of an optimal vertex cannot have a strictly larger objective value.

The simplex algorithm can be presented in a geometrical fashion as a path traversal algorithm along the exterior of the polytope representing the set of feasible solutions, see Figure 1.1. The algorithm starts at a vertex of the polytope and checks adjacent vertices for a larger objective value. If a neighbour has a larger objective value, then the algorithms moves to that vertex according to a given pivoting rule and continues. The algorithm traverses along the exterior of the polytope, going from vertex to vertex, until it reaches a vertex with no neighbour having a better objective value.

When there are multiple neighbours with a better solution, a pivot rule is used to decide which vertex to go to. There are several choices for the pivot rule such as picking the largest value of the scalar product between the objective function and the edge, that is an analogue of a steepest gradient, or some lexicographical ordering. The chosen pivot rule can significantly affect the running time of the algorithm. While in practice the simplex algorithm is quite efficient, a worst case instance leading to an exponential number of iterations in know for nearly all existing pivoting rules. Achieving a deeper understanding of the combinatorial and geometric properties of polytopes achieving a large diameter would contribute to the quest for novel pivoting rules.

1.4 Research objectives

The first aspect to consider for finding the largest diameter of all (d,k)-polytopes, is the size of the lattice $(d-1,k)$-polytopes input set. The search space can be extremely large to examine even for small values of d and k. We first mention structural properties to explain our novel approach for determining the maximal diameter of lattice (d,k)-polytopes. Then we discuss our new linear optimization

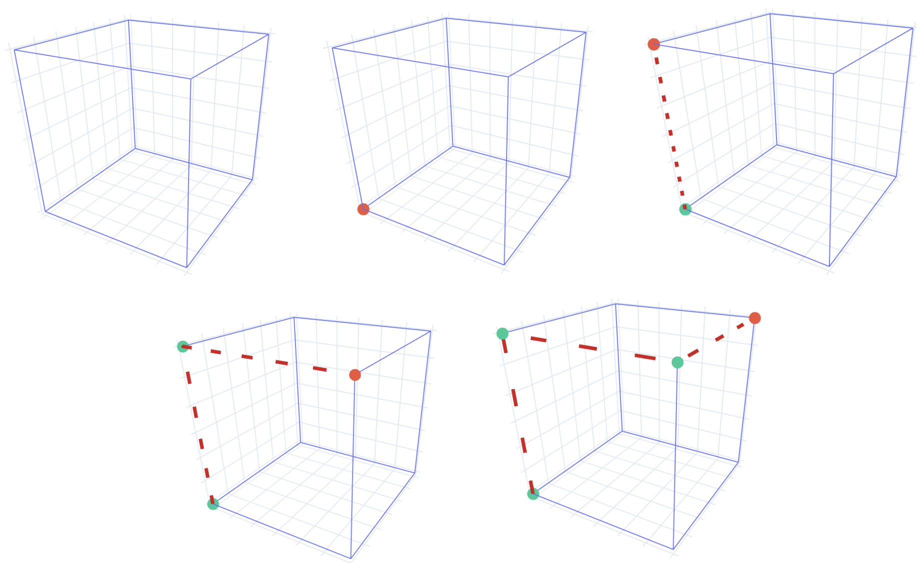

Figure 1.1: Iterations of the Simplex method, where the red point represents the current basis and the green points represent previous bases.

based on algorithm that achieve an efficient reduction of the search space. In Chapter 3 we explain an enhanced algorithm to determine $\delta(d,k)$ and a previously intractable instance is computed.

The problem is described in Section 2.1 and the structural properties of lattice (d,k)-polytopes are listed in Section 2.2. Our novel algorithm is presented in Chapter 3. This algorithm determines the largest diameter of all lattice (d,k)-polytopes. In detail we present how the search space can be efficiently examined in Sections 3.1.4 and 3.1.5. Several illustrations for $d=3$ of our linear optimization techniques used to reduce search space are shown in Section 3.1.5. Section 3.1.5 explains how the techniques illustrated in 3.1.5 can be generalized to $d=4$. Finally, we show that our novel approach is able to compute $\delta(3,7)$ in Section 3.2.

Chapter 2

Current Framework for Lattice Polytopes with Large Diameter

In this chapter we revisit the framework developed by Deza et al. [8] to compute the largest possible diameter over all lattice (d,k)-polytopes. The structural properties of lattice (d,k)-polytopes that achieve the largest possible diameter investigated by Deza et al. [8] are detailed in Section 2.2. The framework developed by Deza et al. [8] improved on the framework introduced Chadder and Deza [4]. Chadder and Deza [4] proposed an algorithm to determine whether $\delta(d,k)$ is equal to $\delta(d-1,k)+k$. The work of Deza et al. [8] exploits the structural properties showed in Section 2.2 and introduced the slack variable g. This variable is used to set the target diameter to $\delta(d-1,k)+k-g$. However, when the number of lattice $(d-1,k)$-polytopes is large, checking whether if $\delta(d,k)=\delta(d-1,k)+k-g$ becomes computationally intractable.

2.1 Introduction

In order to introduce and motivate our work, we recall the Hirsch conjecture and review the progress made on the upper and lower bounds by researchers in the second half of the 20^{th} century, and look at more recent results obtained in the past few years.

The Hirsch conjecture was formulated by Warren Hirsch in 1957 and reported in [5]. The conjecture states that for a polytope P in dimension d with n facets, $n-d$ is an upper bound for the diameter of P. The conjecture opened up a new realm of research into the diameter of polytopes with many open questions related to the diameter of polytopes and more generally to the combinatorial, geometric, and algorithmic aspects of linear optimization. Santos [20] presented a counterexample in 2012 to the Hirsch conjecture. Let $\Delta(n,d)$ be the maximal diameter of the graph of $d-$dimensional polytope P with at most n facets, for $n > d \geq 2$. Determining the behavior of $\Delta(n,d)$ has been for long time objective in this area. We observe that the number of iterations required by the simplex method in the worst case complexity, with any pivot rule, has as a lower bound, the value of $\Delta(n,d)$. Therefore, the behavior of $\Delta(n,d)$ is related to simplex method complexity. Note that the initial counterexample of Santos is of dimension 43 while further investigation lead to a counterexample of dimension 20 [18, 21].

The search for an upper bound on the largest diameter $\Delta(d,n)$ over all polytope in dimension d having n facets goes back at least to 1967 with the work of Klee and Walkup [15] and the work of Larman [17] in 1970 who provided an upper bound that was further improved by Barnette [1] to $\Delta(d,n) \leq n2^d/6$. Note that this bound, for fixed dimension d, is linear in n. In 1992, Kalai and Kleitman [14] provided a bound of $\Delta(d,n) \leq n^{\log d+2}$. This bound has since been tightened by Todd [23] and Sukegawa [22] to $\Delta(d,n) \leq (n-d)^{\log(d-1)}$. For additional results, we refer the reader to [2, 3] and references therein.

In the case of lattice (d,k)-polytopes, current work uses k as alternative to n and the value of the largest diameter $\delta(d,k)$ over all lattice (d,k)-polytopes have been investigated by Naddef [19] in 1989 who showed that $\delta(d,1) = d$, and we observe that lattice $(d,1)$-polytopes satisfy the Hirsch conjecture. A few years later, Naddef's result was generalized to any dimension by Kleinschmidt and Onn [16] who proved that $\delta(d,k) \leq kd$. Del Pia and Michini [7] were able to strengthen this upper bound to $\delta(d,k) \leq kd - \lceil d/2 \rceil$ when $k \geq 2$, and they showed that $\delta(d,2) = \lfloor 3d/2 \rfloor$. The bound was further strengthened by Deza and Pournin [10] to $\delta(d,k) \leq kd - \lceil 2d/3 \rceil - (k-3)$ when $k \geq 3$.

In 2017, Deza, Manoussakis, and Onn [9] introduced a lower bound for small k, that is achieved by a family of lattice zonotopes, referred to as primitive zonotopes. They proved that $\delta(d,k) \geq \lfloor (k+1)d/2 \rfloor$ for $k \leq 2d-1$. Furthermore, they proposed conjecture 2.1.1.

Conjecture 2.1.1. *For any d and k, $\delta(d,k)$ is achieved, up to translation, by a Minkowski sum of lattice vectors. In particular, $\delta(d,k) = \lfloor (k+1)d/2 \rfloor$ for $k \leq 2d-1$.*

Following this line of research, Chadder and Deza [4] developed a framework to show computationally that the conjecture holds for $(d,k) = (3,4)$ and $(d,k) = (3,5)$, that is, $\delta(3,4) = 7$ and $\delta(3,5) = 9$. Our research results further substantiates this conjecture. This framework was enhanced by Deza et al. [8], introducing a slack variable g.

Table 2.1 shows the latest results for the maximal diameter of lattice polytope, $\delta(d,k)$ with our contribution in bold.

Considering the largest diameter over all lattice (d,k)-zonotopes, $\delta_z(d,k)$, Deza, Pournin, and Sukegawa [11] showed that, up to an explicit multiplicative constant, $\delta_z(d,k)$ grows like $k^{d/d-1}$ when d is fixed and k goes to infinity. Since $\delta_z(d,k) \leq \delta(d,k)$, this result provides a new lower bound for $\delta(d,k)$.

						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	…
	3	3	4	6	7	9	10	**11**			
d	4	4	6	8							
	5	5	7	10							
	⋮	⋮	⋮								
	d	d	$\lfloor \frac{3}{2} d \rfloor$								

Table 2.1: Largest possible diameter $\delta(d,k)$ of a lattice (d,k)-polytope

2.2 Structural properties of lattice (d,k)-polytopes with large diameter

In this section, we recall the properties exploited by Deza et al. [8], that provide the building blocks for the new approach algorithm described in Section 3.1.

The following notation will be used throughout our work to describe how the framework was developed. Given two vertices u and v of a polytope P, let denote as $d(u,v)$ the shortest distance between u and v on the edge-graph of P. Let F be a facet of P, $d(u,F) = \min\{d(u,v) : v \in F\}$ is the shortest distance from u to any vertex $v \in F$. The diameter of the edge-graph of P is denoted by $\delta(P)$, this value corresponds to longest shortest path between any pair of vertices in the vertext set of P. 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 $x{\cdot}y$.

Lemma 2.2.1, introduced by Del Pia and Michini, is restated here. It provides an upper bound for $d(u,F)$ being u a vertex of P and F a facet of P. This lemma allows to introduce additional structural properties.

Lemma 2.2.1 ([7]). *Consider a lattice (d,k)-polytope P. If u is a vertex of P and $c \in \mathbb{R}^d$ is a vector with integer coordinates, then $d(u,F) \leq c{\cdot}u - \gamma$ where*

$\gamma = \min\{c{\cdot}x : x \in P\}$ *and* $F = \{x \in P : c{\cdot}x = \gamma\}$.

Assuming in Lemma 2.2.1 that $c = \pm c^i$ where c^i is the vector whose coordinates are all equal to 0 except for the i-th coordinate that is equal to 1, following objects are considered. Let $\gamma_i^-(P) = \min\{x_i : x \in P\}$ and $F_i^-(P) = \{x \in P : x_i = \gamma_i^-(P)\}$. Similarly, let $\gamma_i^+(P) = \max\{x_i : x \in P\}$ and $F_i^+(P) = \{x \in P : x_i = \gamma_i^+(P)\}$. $F_i^-(P)$, and $F_i^+(P)$ will be denoted by F_i^- and F_i^+, when there is no ambiguity. For paths connecting u to v that go through $F_i^-(P)$ or $F_i^+(P)$, $d(u,v)$ can be bounded as follows. Note that under some maximality conditions, F_i^- and F_i^+ can be assumed to be facets of dimension $d-1$.

$$d(u,v) \leq \min_{i=1,\ldots,d} \min\{\delta(F_i^-) + d(u,F_i^-) + d(v,F_i^-), \delta(F_i^+) + d(u,F_i^+) + d(v,F_i^+)\} \tag{2.1}$$

Setting $c = \pm c^i$, inequality (2.1) can be rewritten as Corollary 2.2.2 which is a key component to show by induction that $\delta(d,k) \leq kd$.

Corollary 2.2.2. *Let u and v be two vertices of a lattice (d,k)-polytope, then*

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

We use Proposition 2.2.3, borrowed from [12], see Corollary 12.2 and Proposition 12.4 therein, to prove Lemma 2.2.4.

Proposition 2.2.3. *Let P^1 and P^2 be two polytopes in $\mathbb{R}^d$ and $P = P^1 + P^2$ their Minkowski sum. Let $v = v^1 + v^2$, such that $v^1 \in P^1$ and $v^2 \in P^2$. Then v is a vertex of P if and only if (i) v^1 and v^2 are vertices of P^1 and P^2, respectively; and (ii) there exists an objective function $c \in \mathbb{R}^d$ that is uniquely minimized at v^1 in P^1 and at v^2 in P^2. Moreover, if u and v are adjacent vertices of P with Minkowski decompositions $u = u^1 + u^2$ and $v = v^1 + v^2$, respectively, then u^i and v^i are either adjacent vertices of P^i, or they coincide, for $i = 1,2$.*

Lemma 2.2.4. *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 $i = 1,\dots,d$.*

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 $\sigma^i = \text{conv}\{0,(k-\gamma_i^+(Q))c^i\}$ where c^i is the point whose coordinates are all 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 2.2.3, with $c = c^i$, 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 Q is at most the distance of u' and v' in $Q+\sigma^i$. 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 be repeated until no such coordinate remains. $\square$

Deza et al. [8] introduces a slack variable g to quantify the gap between the trivial upper bound, $\delta(d,k) \leq \delta(d-1,k)+k$ and a target diameter. Lemma 2.2.5 indicates how g can be used.

Lemma 2.2.5. *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 $i = 1,\dots,d$.*

(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 2.2.2 yields:

$$\delta(d-1,k)+k-g \leq \delta(F_i^-)+(u_i+v_i) \quad \text{for } i=1,\ldots,d, \tag{2.2}$$
$$\delta(d-1,k)+k-g \leq \delta(F_i^+)+2k-(u_i+v_i) \quad \text{for } i=1,\ldots,d. \tag{2.3}$$

Thus,

$$k-g \leq u_i+v_i+\delta(F_i^-)-\delta(d-1,k) \quad \text{for } i=1,\ldots,d, \tag{2.4}$$
$$k+g \geq u_i+v_i+\delta(d-1,k)-\delta(F_i^+) \quad \text{for } i=1,\ldots,d. \tag{2.5}$$

Hence, since both $\delta(F_i^-)$ and $\delta(F_i^+)$ are at most $\delta(d-1,k)$, the inequality $k-g \leq u_i+v_i \leq k+g$ holds for $i=1,\ldots,d$; that is, item (i) holds.

By Lemma 2.2.4, 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 (2.4) and (2.5) can be rewritten as:

$$\delta(F_i^-) \geq \delta(d-1,k)-g+k-(u_i+v_i) \quad \text{for } i=1,\ldots,d, \tag{2.6}$$
$$\delta(F_i^+) \geq \delta(d-1,k)-g-k+(u_i+v_i) \quad \text{for } i=1,\ldots,d. \tag{2.7}$$

Thus, since $k-g \leq u_i+v_i \leq k+g$ for $i=1,\ldots,d$ by item (i), $\delta(F_i^-)$ and $\delta(F_i^+)$ are at least $\delta(d-1,k)-2g$ for $i=1,\ldots,d$; that is, item (ii) holds. □

We recall that the bounds obtained by Del Pia and Michini [7] and Deza and Pournin [9] hold in general for lattice polytopes inscribed in rectangular boxes.

Corollary 2.2.6 (Remark 4.1 in [9])**.** *Let $\delta(k_1,\ldots,k_d)$ denote the largest possible diameter of a polytope whose vertices have their i-th coordinate in $\{0,\ldots,k_i\}$ for $i=1,\ldots,d$ and, up to relabeling, $k_1 \leq k_2 \leq \cdots \leq k_d$. The following inequalities hold:*

1. $\delta(k_1,\ldots,k_d) \leq k_2+k_3+\cdots+k_d-\lceil d/2\rceil+2$ *when* $k_1 \geq 2$*,*

2. $\delta(k_1,\ldots,k_d) \leq k_2+k_3+\cdots+k_d-\lceil 2d/3\rceil+3$ *when* $k_1 \geq 3$*.*

Observe that the statement of Remark 4.1 in [10] contains a typographical incorrectness as k_1 and k_d were interchanged in (i) and in (ii). Conjecture 2.1.1 can also be stated for lattice polytopes inscribed in rectangular boxes; that is, $\delta(k_1,\ldots,k_d)$ is at most $\lfloor (k_1+k_2+\cdots+k_d+d)/2\rfloor$, and is achieved, up to translation, by a Minkowski sum of lattice vectors. Note that this generalization of Conjecture 2.1.1 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 $\delta(2,2,3)=\delta(2,3,3)=5$.

2.3 Computational framework to determine $\delta(d,k)$

Since the hypercube $[0,k]^d$ has $(k+1)^d$ integer coordinate points, an exhaustive generation of all lattice (d,k)-polytopes would require to perform $2^{(k+1)^d}$ convex hull computations. This task is computationally intractable even for small values of d and k.

In the following sections we revisit the algorithm proposed by Deza et al. [8]. In this branch and cut approach, the algorithm starts with a pair of points (u,v) as initial node. This pair of vertices (u,v) is assume to be antipodal, that is $d(u,v)$ is equal to the target diameter. Each branch is validated to determine whether a lattice (d,k)-polytope achieving target diameter can be found. When there is no lattice (d,k)-polytope achieving target diameter, the branch is immediately pruned. The validation of each branch requires convex hull computations. Such computations are a important component and, at the same time, a bottle neck for the search space examination. For convex hull computations, the library of the double description method implemented in *C* by Komei Fukuda [13] is employed.

2.3.1 Main algorithm

The algorithm contains the following four main steps:

- Enumeration of all (u,v) pairs of vertices such that $d(u,v) = \delta(P)$.
- Shelling step.
- Inner step.
- Generation of all lattice (d,k)-polytopes with an empty intersection with at least one facet of $[0,k]^d$.

For each pair (u,v) the algorithm attempts to construct lattice (d,k)-polytopes P of maximal diameter starting with two initial vertices $\{u,v\}$. First, it tries to embed lattice $(d-1,k)$-polytopes onto the facets of the hypercube $[0,k]^d$. Thus, the size of the set of lattice $(d-1,k)$-polytopes available to embed impacts on the algorithm performance. Denote by Γ the graph containing the known vertex and edge sets. At the beginning Γ has as vertex set $\{u,v\}$ and no edges.

The idea to consider each intersection of the $[0,k]^d$ was proposed by Chadder and Deza [4], where it was checked whether $\delta(d,k)$ is equal to $\delta(d-1,k)+k$. There are lower bounds and upper bounds for the problem of finding the diameter of lattice polytopes. To target a specific value in the gap between these bounds Deza et al. [8] introduced a slack variable g. When $g = 0$ the target diameter is the upper bound. During the branch and cut procedure a target diameter is fixed as the optimal value. When an upper bound for $d(u,v)$ of the current branch is strictly less than the target diameter the branch is pruned.

In terms of Lemma 2.2.5, checking whether $\delta(d,k) = \delta(d-1,k)+k$ is equivalent to testing whether $g = 0$. Then main specificity when $g = 0$ is that F_i^- and F_i^+ must be faces that have the maximal diameter $\delta(d-1,k)$. Therefore the computation is significantly easier as the number of lattice $(d-1,k)$-polytopes that can be embedded onto F_i^- or F_i^+ is relatively small.

2.3.2 Generating all (u,v) pairs

In this section, we recall the four conditions stated by Deza et al. [8] to generate all (u,v) pairs of vertices of a lattice (d,k)-polytope that satisfy $d(u,v) = \delta(d-1,k)+k-g$. The first condition restricts the coordinates of u as follows:

$$u_i \leq u_{i+1} \leq \lfloor k/2 \rfloor \qquad \text{for } i = 1,\dots,d-1.$$

The second condition is based on the item (i) of 2.2.5. Accordingly the coordinates of u and v are restricted by the following set of inequalities:

$$k-g \leq u_i+v_i \leq k+g \qquad \text{for } i = 1,\dots,d.$$

For the third condition, let assume all u are generated in lexicographical order denoted by $\prec$. Let $\tilde{w}$ the point consisting of the coordinates of w reordered lexicographically. Then u and v can be assumed to satisfy the following conditions:

$$\begin{aligned} \{v_i \leq v_{i+1} \text{ if } u_i = u_{i+1}\} &\qquad \text{for } i = 1,\dots,d-1, \\ u \prec \tilde{w} \text{ where } w = (k,\dots,k)-v &\qquad \text{if } \{v_i \geq \lceil k/2 \rceil \text{ for } i = 1,\dots,d\}. \end{aligned}$$

The next condition exploits the fact that a set of lattice $(d-1,k)$-polytopes with sufficiently large diameter will be used during embedding process. Thus, when u or v belong to the hypercube facets, they must be vertices of at least one of the lattice $(d-1,k)$-polytopes that the algorithm is trying to embed. Let $\mathscr{V}_{d,k,g}$ be the set that contains all vertices of all the lattice (d,k)-polytopes with diameter at least $\delta(d,k)-g$ and let $\bar{v}_i$ be the point in $\mathbb{R}^{d-1}$ consisting of all coordinates of v except v_i. Then we define $g_i^- = g+u_i+v_i-k$ and $g_i^+ = g+k-(u_i+v_i)$. In order to u and v be vertices of a lattice (d,k)-polytope with diameter at least $\delta(d-1,k)+k-g$, the following conditions must hold:

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

Finally, the last condition exploits convexity and the properties of the set of all lattice $(d-1,k)$-polytopes to consider for embedding. It also provides another condition to restrict the (u,v) pairs to consider. Let $\mathscr{P}_{d,k,g}$ be the set of all the integer value coordinate points belonging to the intersection of all the lattice (d,k)-polytopes of diameter at least $\delta(d,k)-g$. Let $\mathscr{C}^{u,v}_{d,k,g}$ be the convex hull of $\{u,v\}$ and the following set:

$$\left[\bigcup_{i=1}^{d}\{x \in \mathbb{R}^d : x_i = 0 \text{ and } \bar{x}_i \in \mathscr{P}_{d-1,k,g_i^-}\}\right] \cup \left[\bigcup_{i=1}^{d}\{x \in \mathbb{R}^d : x_i = k \text{ and } \bar{x}_i \in \mathscr{P}_{d-1,k,g_i^+}\}\right].$$

The following condition must be met for u and v to be vertices of a lattice (d,k)-polytope with diameter at least $\delta(d-1,k)+k-g$:

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

2.3.3 Shelling step

In the shelling step, for a given pair (u,v), the algorithm tries to embed a set of lattice $(d-1,k)$-polytopes with sufficiently large diameter onto the $2d$ intersections of P with the facets of the hypercube $[0,k]^d$. For each resulting shelling the inner step is performed. During the inner step all subsets of inner points in $\{1,2,\ldots,k-1\}^d$ are considered to be added as vertices of P.

The input of the shelling step is a triple (d,k,g) and a pair (u,v) of initial vertices. The target diameter is defined by $d(u,v) = \delta(d-1,k)+k-g$. Only $0,1,\ldots,k$-

valued coordinate vertices are considered and g is the slack variable.

Section 2.3.3 presents the ordering criteria to select next hypercube facet for intersecting. Recalling the branch and cut approach presented by Deza et al. [8], the shelling step attempts to build skeletons or shellings of lattice (d,k)-polytopes embedding lattice $(d-1,k)$-polytopes onto the $2d$ hypercube facets, one at the time. Let assume that we have selected the next facet F_i^- or F_i^+ to embed. Then a set of all consistent lattice $(d-1,k)$-polytopes of diameter at least $\delta(d-1,k)-g_i^-$ or $\delta(d-1,k)-g_i^+$ respectively are listed. Consistency implies that if before embedding we know that:

- Some vertices belong to the next hypercube facet to embed.
- Some points can not be considered as vertices in the next hypercube facet to embed.

Then iteratively each lattice $(d-1,k)$-polytope is evaluated using the two certificates detailed in Section 2.3.3. If a lattice $(d-1,k)$-polytope meets the conditions, a branch is created. Otherwise the current node is pruned.

When a lattice $(d-1,k)$-polytope is considered, its vertices and edges are added to Γ. The values of γ, $\mathscr{C}^{\Gamma}_{d,k,g}$ and gap scores of non-embedded yet hypercube facets in the shelling are updated. The gap scores g_i^-, and g_i^+, are updated accordingly to $g_i^- = g + \widetilde{d}(u,F_i^-) + \widetilde{d}(v,F_i^-) - k$ and $g_i^+ = g + \widetilde{d}(u,F_i^+) + \widetilde{d}(v,F_i^+) - k$. If either Certificates 1 or 2 of non-existence is fulfilled, then the current node can be pruned and the search continues checking to the next candidate for the selected intersection.

The output of the shelling step is a set of skeletons or shellings. Because the vertices of the shelling could not be enough to define a lattice (d,k)-polytope such as $d(u,v) = \delta(d-1,k)+k-g$. One more step may be required to perform. This further step is called the inner step. Essentially, this step considers the inner points of the hypercube for completing the construction of polytope P with maximal diameter. Each skeleton could be completed adding further vertices in order to build a lattice (d,k)-polytope that achieves target diameter $d(u,v) = \delta(d-1,k) + k - g$.

Key ideas to reduce the search space

The algorithm starts with only u and v as vertices. Then one of the facets of the $[0,k]^d$ is selected to be embedded as the first intersection with P. For each non-embedded hypercube facet, the available number of lattice $(d-1,k)$-polytopes to intersect depends on the information that we currently know. Therefore different ordering sequences will impact in the required computational time for the examination of search space. We are interested in an embedding sequence such as the output of the shelling step can be obtained as efficiently as possible.

To estimate which facets of the hypercube correspond to the lowest number of lattice $(d-1,k)$-polytopes available to intersect we use the gap parameters g_i^- and g_i^+. Such gap parameters are calculated as follows:

$$g_i^- = g + u_i + v_i - k$$
$$g_i^+ = g + k - (u_i + v_i)$$

A lower score is assume to yield a lower number of lattice $(d-1,k)$-polytopes. Thus, for the next intersection with hypercube we are interested in the lowest possible gap score. Typically we select the score equal to zero. If there are non-embedded intersections with the same lowest score, the number of known vertices in the corresponding intersections is considered as tie breaker. Finally if a tie persists, the algorithm uses a default order. The following tie breaker criteria are employed by the framework developed by Deza et al. [8] in the order:

1. The lowest facet gap parameter, g_i^- or g_i^+.
2. The number of known vertices in F_i^- or F_i^+.
3. Finally, the default order of $F_1^-, ..., F_d^-, F_1^+, ..., F_d^+$.

We recall Certificates 1 and 2 introduced by Deza et al. [8] that show no lattice (d,k)-polytope with vertices u and v can exist such that $d(u,v) = \delta(d-1,k)+k-g$.

Certificate 1: Shortest path in shelling is less than $\delta(d-1,k)+k-g$

During the shelling step the algorithm starts the construction of a lattice (d,k)-polytope P with only two vertices $\{u,v\}$. The algorithm continues to embed a lattice $(d-1,k)$-polytope onto a facet of $[0,k]^d$. It is important to determine with the lowest possible number of embeddings whether the current shelling potentially can be or not part of lattice (d,k)-polytopes that achieve the target diameter. Given an intersection F_i^- or F_i^+ of P with the hypercube, Certificate 1 consists of an upper bound calculated as the sum of following three terms:

- The minimum distance from u to any vertex of any F_i^- or F_i^+.
- $\delta(F_i^-)$ or $\delta(F_i^+)$.
- The minimum distance from v to any vertex of any F_i^- or F_i^+.

Note that u or v are not always connected via Γ with vertices in F_i^- or F_i^+. The following values are upper bounds for the distance in Γ between u or v and the intersection of P with a facet of the hypercube $[0,k]^d$:

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

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

We observe that the distance from a vertex to an intersection of P with the hypercube can not exceed the minimum of the value of the coordinate in said dimension, u_i or v_i, and $k - u_i$ or $k - v_i$. Define $d_\circ(u,v)$ as follows:

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

Where $d_\circ(u,v)$ is an upper bound for $d(u,v)$ defined by inequality (2.1). When the diameters $\delta(F_i^-)$ and $\delta(F_i^+)$ are not known yet, we use the corresponding upper bound $\delta(d-1,k)$.

Every time a lattice $(d-1,k)$-polytope is successfully embedded onto a facet of $[0,k]^d$, Γ is updated by adding new vertices an edges of the lattice $(d-1,k)$-polytope. Γ can be considered a sub-graph of the edge-graph of the final polytope P. Therefore $d_\Gamma(u,v)$ also represents an upper bound for $d(u,v)$. Given the target diameter $\delta(d-1,k) + k - g$ and two upper bounds for $d(u,v)$, we are able to determine efficiently if the current subgraph of the edge-graph corresponds to a shelling that potentially could become in a lattice (d,k)-polytope P of maximal diameter. Define the following parameter γ:

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

When $\gamma > 0$ we conclude that from the current node the search space tree, no lattice (d,k)-polytope such that $d(u,v) = \delta(d-1,k) + k - g$ can be constructed.

Certificate 2: u **or** v **is not a vertex of** $\mathscr{C}^{\Gamma}_{d,k,g}$

If the vertices u or v are inner points of $[0,k]^d$, the algorithm must check whether u and v remain as vertices of polytope P during the shelling step. Let $\mathscr{P}_{d,k,g}$ be the set of all integer points that belong to the intersection of all lattice (d,k)-polytopes of diameter at least $\delta(d,k)-g$. The set $\mathscr{P}_{d,k,g}$ and the current vertex set of Γ make possible to establish a condition for determining whether the current shelling can be pruned. Denote by $\mathscr{C}^{\Gamma}_{d,k,g}$ the convex hull of the vertex set of Γ and the following set of points:

$$\left[\bigcup_{i=1}^{d}\{x\in\mathbb{R}^d : x_i = 0 \text{ and } \bar{x}_i \in \mathscr{P}_{d-1,k,g_i^-}\}\right] \cup \left[\bigcup_{i=1}^{d}\{x\in\mathbb{R}^d : x_i = k \text{ and } \bar{x}_i \in \mathscr{P}_{d-1,k,g_i^+}\}\right].$$

The current shelling is removed from consideration if:

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

2.3.4 Inner step

The inner step takes as input a set of shellings or skeletons in order to find lattice (d,k)-polytopes that achieve diameter $\delta(d-1,k)+k-g$. For each shelling, the following points p are considered:

- $p_i \in \{1,...,k-1\}$ for $i = 1,\dots,d$.
- $p \notin$ vertex set of Γ.
- p is a vertex of convex hull of vertices in $\Gamma \cup p$.

During the inner step, Deza et al. [8] considered all subsets of points satisfying conditions above to attempt constructing lattices (d,k)-polytopes achieving target diameter. Even for a small number of inner points of $[0,k]^d$, performing convex hull computations for all possible subsets makes the search computationally intractable.

The generated lattice (d,k)-polytopes whose diameter is less or equal $\delta(d-1,k)+k-g-1$ as well as duplicates, up to the symmetries of the hypercube $[0,k]^d$, are removed. When the inner step output is empty, we conclude that $\delta(d,k) < \delta(d-1,k)+k-g$. If it is non-empty, the inner step provides, up to the symmetries of the hypercube $[0,k]^d$, all lattice (d,k)-polytopes of diameter $\delta(d-1,k)+k-g$ having non-empty intersection with the $2d$ facets $[0,k]^d$. Additional computations are required to find, if possible, all lattice (d,k)-polytopes of diameter $\delta(d-1,k)+k-g$ with at least one empty intersection with facet of $[0,k]^d$. This will be detailed in Section 2.3.5.

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

In this section, we recall from the work of Deza et al. [8], how the lattice (d,k)-polytopes with an empty intersection with at least one facet of $[0,k]^d$ can be derived from the output of shelling step.

The main idea behind generating all lattice (d,k)-polytopes with diameter at least $\delta(d-1,k)+k-g$ whose intersection with one of the facets of $[0,k]^d$ is empty is to use the idea from Lemma 2.2.4. We will attempt to expand the polytope in a direction, s, to check the possibility of contracting P in the direction of $-s$. If a possible contraction exists, we can then check the diameter of the resulting polytope to see if a new valid polytope of diameter at least $\delta(d-1,k)+k-g$ with an empty intersection with one of the facets of $[0,k]^d$.

Let $I(Q)$ denote the set of the coordinates i such that $\gamma_i^+(Q)-\gamma_i^-(Q) < k$. Consider a lattice (d,k)-polytope Q of diameter at least $\delta(d-1,k)+k-g$ 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 $\sigma^i = \mathrm{conv}\{0,(k-\gamma_i^+(Q))c^i\}$. Let S denote the Minkowski sum of all σ^i for $i \in I(Q)$. As shown in the proof of Lemma 2.2.4, $Q+S$ 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). Note that setting $P^1=Q$ and $P^2=[0,s]$ where $s_i\geq 0$ for all i in Proposition 2.2.3 gives Remark 2.3.1.

Remark 2.3.1. *Consider a segment $\sigma=[0,s]$; a point v' is a vertex of $Q+\sigma$ if and only if there exists an objective function $c\in\mathbb{R}^d$ that is uniquely minimized at v in Q and (i) $v'=v$ and c is uniquely minimized at 0 in σ, or (ii) $v'=v+s$ and c is uniquely minimized at s in σ. Moreover, if u' and v' are adjacent vertices of $Q+\sigma$, then either (u',v') is equal to (u,v) or to $(u+s,v+s)$ where u and v are adjacent vertices of Q, or it is equal to $(u,u+s)$ where u is a vertex of Q.*

Consequently, up to translation and up to the symmetries of the hypercube $[0,k]^d$, the set of the lattice (d,k)-polytopes Q of diameter at least $\delta(d-1,k)+k-g$ such that $I(Q)\neq\emptyset$ can be generated as follows:

1. for each lattice (d,k)-polytope P in the output of the algorithm for (d,k,g), check whether $P=Q+\sigma$ where Q is a lattice (d,k)-polytope and σ a lattice segment. By Remark 2.3.1, this can be done by checking whether P and $P+\sigma$ have the same number of vertices.

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

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 σ considered in step (i) can be limited to a few segments whose coordinates are relatively prime and used iteratively. One can check that, in order to perform step (i) for $d=3$, it is enough to consider for σ, iteratively, the 3 unit vectors and the 3 sums of 2 unit vectors.

Chapter 3

Enhanced Framework for Lattice Polytopes with Large Diameter

In this chapter we present a novel approach to determine the largest possible diameter over all lattice (d,k)-polytopes, denoted by $\delta(d,k)$. From a theoretical perspective, the framework developed by Deza et al. [8] can determine $\delta(d,k)$. However, in practice when the number of lattice $(d-1,k)$-polytopes is large, the problem to determine whether $\delta(d,k)$ is equal to $\delta(d-,k)+k-g$ becomes quickly intractable. In Section 3.1, we explain an linear optimization based algorithm to determine $\delta(d,k)$, focusing on the case when $d=3$ and $d=4$. In addition, new ideas to reduce the search space are introduced. Finally, we present in Section 3.2 a new, previously intractable, entry $\delta(3,7)$ and summarize the key challenges. Given a shelling, the main contribution of this new approach allows the new algorithm to determine early on whether a shelling can be removed. Thus, a significantly lower number of embeddings is required in comparison with the framework developed by Deza et al. [8]. For some (u,v) pairs the search space reduction is in the order of thousands of times.

3.1 Enhanced algorithm to determine $\delta(d,k)$

In this section, we formally describe our new approach based framework to determine $\delta(d,k)$. We introduce three types of improvements to the framework developed by Deza et al. [8]:

- The first improvement is a simple combinatorial property that was overlooked in the work of Deza et al. [8]. For k even, a new condition is added to the pair (u,v) generation process. Consequently, fewer (u,v) pairs are considered as input of shelling step. In Subsection 3.1.2, this condition is introduced and illustrated for $(d,k,g) = (3,4,1)$. While it is not used for $(d,k) = (3,7)$, this property is considered for $(d,k) = (4,4)$ which is currently under computation.

- The second improvement consists of efficient convexity based branching. For u or v strictly inner points of the hypercube additional edges can be added to Γ. These edges allow to connect u or v with F_i^- or F_i^+ respectively, leading to decrease the gap scores with a lower number of embedding in comparison with the framework developed Deza et al. [8]. Furthermore, there are points on the facets of the hypercube that can not be vertices of polytope P. These points can be removed from consideration before starting shelling process, decreasing the number of lattice $(d-1,k)$-polytopes to list for each facet of the $[0,k]^d$.

- The last improvement is a linear optimization-based addition of edges not belonging to any F_i^- or F_i^+. During the shelling step new edges of P and weighted virtual edges are added to Γ, increasing the likelihood of discovering new paths connecting u and v with a lower number of embeddings, in comparison with the framework developed by Deza et al. [8]. These edges plays a key role in the pruning. They can be seen as diagonal,that is, connecting vertices in dimension d instead of within a $(d-1)$ dimensional space. Given a shelling or skeleton that corresponds to a lattice (d,k)-

polytope P, the problem $\min\{c \cdot x : x \in P\}$ and integrality conditions make possible to identify additional faces in the shelling. Consequently new edges from the edge graphf of P can be added to Γ. Moreover, we will show how weighted virtual edges can be added to Γ. The improvements to shelling step are detailed in the subsection 3.1.5.

3.1.1 Limitations of the framework developed by Deza et al. [8]

The algorithm developed by Deza et al. [8] is unable to determine the shelling step output when the number of lattice $(d-1,k)$-polytopes is large. As illustration, in dimension $d=3$, the maximum value of k that can be verified by using mentioned algorithm is 6. For example for $(d,k)=(3,7)$ the framework developed by Deza et al. [8] would require thousands times more effort than $(d,k)=(3,6)$.

In this subsection, we list the two main reasons why under this scenario the algorithm developed by Deza et al. [8] can not determine whether lattice (d,k)-polytopes with large diameter exists:

- Convex hull computations are a key component of the algorithm. They are required during the shelling and inner steps. Significant number of lattice $(d-1,k)$-polytopes, requires a large number of executions of convex hull computation. These convex hull computations significantly slow down the algorithm. Therefore it is important to find an alternative and efficient strategies to verify convexity during the exploration of the search space.
- The previous version of the shelling step generates shellings of lattice (d,k)-polytopes with diameter lower than the target diameter. These partial shellings should be pruned early as they never lead to (d,k)-polytopes achieving the target diameter. The framework developed by Deza et al. [8] is able to determine whether those shellings can be part of lattice (d,k)-polytopes that achieve target diameter only after the inner step. We will illustrate in Section 3.1.5 that such shellings can be removed before completing the $2d$ embeddings onto the facets of the $[0,k]^d$ by our novel framework. Furthermore,

unnecessary shellings lead to unnecessary executions of the inner step.

These limitations suggests the idea of finding an alternative approach to verify the convexity condition at every attempt to add vertices during shelling and inner steps. In the shelling step and under specific conditions, exploiting convexity and integrality of the problem $\min\{c \cdot x : x \in P\}$ we can identify additional faces of P. Additional faces allow to add new edges to Γ. Furthermore, there are other cases where adding weighted virtual edges to Γ is possible. As a result, new paths from u to v, previously undiscovered until the end of inner step, can be identified in our new approach of the shelling step. Thus upper bounds for $d(u,v)$ can be achieved early on in the shelling step in comparison with the framework developed by Deza et al. [8]. This yields a reduction of processing times and the size of the shelling step output. The linear optimization formulation $\min\{c \cdot x : x \in P\}$ also allows us to identify critical inner points of the hypercube to be used as branching criteria.

This new approach creates a new order criteria to select the next facet of the $[0,k]^d$ for intersecting. The useful fact that during the shelling step we can connect through Γ previously disconnected intersections of P with the hypercube, allows us to introduce a new order embedding criteria. In the work of Deza et al. [8], the number of currently known vertices of P that belong to the next candidate intersections was used as the main criterion to select next facet of the $[0,k]^d$ to intersect. This was a reasonable choice when the mentioned algorithm is trying to build paths from u to v, and adjacent embeddings having empty intersections remain disconnected in Γ during construction of shellings.

The most challenging scenario for the framework developed by Deza et al. [8] corresponds to the case when k is large and vertices u or v are inner points of the hypercube. For a large value of k there is a significant number of (u,v) pairs of inner points to consider. This is one of the reasons why $\delta(3,7)$ was intractable. The following changes are proposed for this entry:

- Prior to starting the shelling step some integer value coordinate points in the facets of hypercube can be removed from consideration. By convexity this leads to list a lower number of lattice $(d-1,k)$-polytopes as candidates for each embedding onto the $2d$ intersection of P with the hypercube.

- If $u_i = 1$ for some i, then we know that an edge $[u,w]$ exists for $w \in F_i^-$. We will branch on the possible choices for w. Similarly, if $v_i = k-1$ for some i, we will branch for $w \in F_i^+$.

- Finally, in the inner step an efficient examination of subsets of inner points of the hypercube is added. This avoid unnecessary examinations of subsets of points as candidates to be vertices of the polytope P. A branching process is also included to exploit the upper bound certificates for determining if a current construction can be or not a polytope P that achieves the target diameter. Convex hull computations are performed as last resort to verify potential vertices of polytope P.

These improvements make a significant impact in the search space tree growing process. Basically the new algorithm prunes early on shellings that were considered by the framework developed by Deza et al. [8] as potential skeletons of lattice (d,k)-polytopes with large diameter. Therefore the inner step was processing shellings that correspond to lattice (d,k)-polytopes that can not achieve maximal diameter.

During the exploration of strategies to reduce as much as possible the size of search space tree, we identified a new condition for k even during generations of all (u,v) pairs, that can be used for $(d,k) = (4,4)$. We start the study of the mentioned improvements, by illustrating this extra condition for the pair generation process in Section 3.1.2.

3.1.2 Extra condition for generation of all (u, v) pairs

The shelling step is performed for every pair (u, v). Therefore, it is crucial to remove redundant pairs prior to its execution. We add the following new condition on v for k even:

$$v_i \geq k/2 \qquad \text{if } u_i = k/2$$

As illustration, Table 3.1 shows coloured in red the (u, v) pairs for $(d, k, g) =$

u	v
$(0,0,0)$	$(3,3,3)$, $(3,3,4)$, $(3,4,4)$, $(4,4,4)$
$(0,0,1)$	$(3,3,2)$, $(3,3,3)$, $(3,3,4)$, $(3,4,2)$, $(3,4,3)$, $(3,4,4)$, $(4,4,2)$, $(4,4,3)$
$(0,0,2)$	$(3,3,2)$, $(3,3,3)$, $(3,4,2)$, $(3,4,3)$, $(4,4,2)$
	$(3,3,1)$, $(3,4,1)$, $(4,4,1)$
$(0,1,1)$	$(3,2,2)$, $(3,2,3)$, $(3,2,4)$, $(3,3,3)$, $(3,3,4)$, $(4,2,2)$, $(4,2,3)$, $(4,3,3)$
$(0,1,2)$	$(3,2,2)$, $(3,2,3)$, $(3,3,2)$, $(3,3,3)$, $(3,4,2)$, $(4,2,2)$, $(4,2,3)$, $(4,3,2)$
	$(3,2,1)$, $(3,3,1)$, $(3,4,1)$, $(4,2,1)$, $(4,3,1)$, $(4,4,1)$
$(0,2,2)$	$(4,2,2)$, $(4,1,1)$, $(4,1,2)$, $(4,1,3)$
$(1,1,1)$	$(2,2,2)$, $(2,2,3)$, $(2,3,3)$, $(3,3,3)$
$(1,1,2)$	$(2,2,2)$, $(2,2,3)$, $(2,3,2)$, $(2,3,3)$, $(3,3,2)$
	$(2,2,1)$, $(2,3,1)$, $(2,4,1)$, $(3,3,1)$, $(3,4,1)$, $(4,4,1)$
$(1,2,2)$	$(2,2,2)$, $(2,2,3)$, $(3,2,2)$, $(2,1,1)$, $(2,1,2)$, $(2,1,3)$, $(3,1,1)$, $(3,1,2)$
	$(3,1,3)$, $(4,1,1)$, $(4,1,2)$, $(4,1,3)$
$(2,2,2)$	$(1,1,3)$, $(1,2,3)$

Table 3.1: All pairs (u, v) pairs for $(d, k, g) = (3, 4, 1)$

$(3, 4, 1)$ that are removed based on the new condition for k even. Consequently, 25 out of 71 original pairs are removed, representing a considerable reduction of pairs to consider.

3.1.3 (u, v) as inner points of the hypercube

In this subsection, we present how u or v can be connected in Γ with current embeddings. When u or v are inner points of $[0, k]^d$ and have at least one coordinate equal to 1 or $k-1$, it is possible to connect these vertices via Γ to F_i^- or F_i^+ respectively. Given a shelling and without loss of generality, assume:

- F_i^- is the next intersection to embed.
- $u_i = 1$.
- w is a vertex in F_i^-.

We know there is at least one edge connecting u with F_i^-, in the edge graph of P. Considering that convex hull computations should be performed only when it is strictly necessary, the upper bounds for $d(u,v)$ are used to discard potential edges between u and F_i^-. For each vertex w of F_i^- a branch is created. Each branch includes corresponding edge $[u,w]$ in Γ and up to two conditions are verified:

- The upper bounds given by distances via Γ are updated to determine whether the branch can be pruned or not.
- If a branch satisfies the upper bound certificates, the algorithm determines whether the edge $[u,w]$ is valid by convexity.

For the second condition let the point $q = \frac{u}{2k} + (1-\frac{1}{2k})w$. Denote by S the set formed by the vertex set of Γ and the following set:

$$\left[\bigcup_{i=1}^{d}\{x \in \mathbb{R}^d : x_i = 0 \text{ and } \bar{x}_i \in \mathscr{P}_{d-1,k,g_i^-}\}\right] \cup \left[\bigcup_{i=1}^{d}\{x \in \mathbb{R}^d : x_i = k \text{ and } \bar{x}_i \in \mathscr{P}_{d-1,k,g_i^+}\}\right].$$

A necessary condition such as there is an edge $[u,w]$ in P, is

$$q \text{ is a vertex of } S \cup \{q\} \setminus \{u\}.$$

Note that if there is no edge satisfying the upper bound verifications, the shelling is pruned from the search space tree.

The illustrations in Figures 3.1 and 3.2 show for the triple $(d,k,g) = (3,7,1)$ and target diameter $\delta(2,7)+7-1 = 12$ how elements of a shelling can be connected

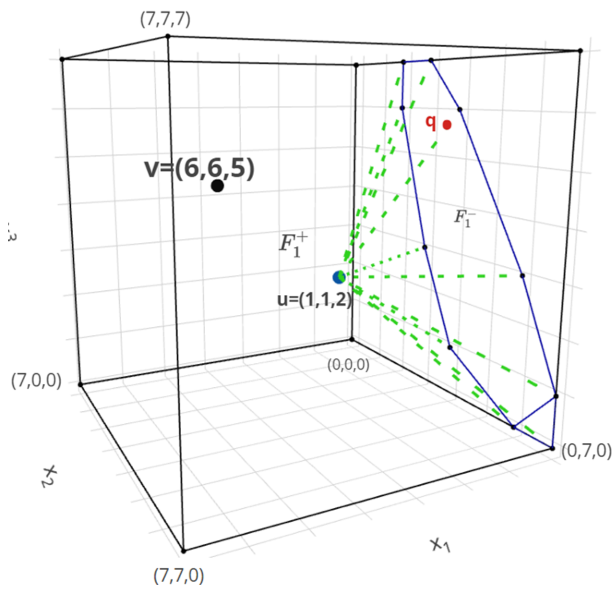

Figure 3.1: Shelling pruned after the first embedding onto F_1^- for $(u,v) = ((1,1,2),(6,6,5))$.

through new paths. Figure 3.1 illustrates how a shelling is removed without performing convex hull computations being u and v inner points of the cube.

Given a shelling, for each vertex w in F_1^- a new branch is created. The Γ graph of each branch has as vertex and edge sets, the corresponding sets of the shelling. Then edge $[u,w]$ is added to Γ and the upper bounds for $d(u,v)$ are updated. If for all edges $[u,w]$, the target diameter can not be achieved, as illustrated at Figure 3.1, the lattice $(d-1,k)$-polygon that the algorithm is trying to embed onto F_1^- is not considered and all new branches are pruned. Prior to any convex hull computation, Γ graph and upper bounds are updated to check whether a node can be pruned.

Otherwise if at least one vertex w satisfies the certificates, corresponding branches are not pruned. We remark that any verification using Γ is computationally more efficient than convex hull computations.

Figure 3.2 shows an example where the first embedding onto F_1^- met the certificates. To determine whether $[u,(0,3,1)]$ can be added to Γ or not, the algorithm verifies if the point q is a vertex of $S \cup \{q\} \setminus \{u\}$. In this case, the construction satisfies the upper bound certificates and it is considered for further attempts of embedding. We will call real edges, those edges of the edge graph of a lattice (d,k)-polytope P that are discovered before the completion of inner step. Only the real edge $[(1,1,2),(0,3,1)]$, coloured in green, satisfies convexity and the upper bound certificates.

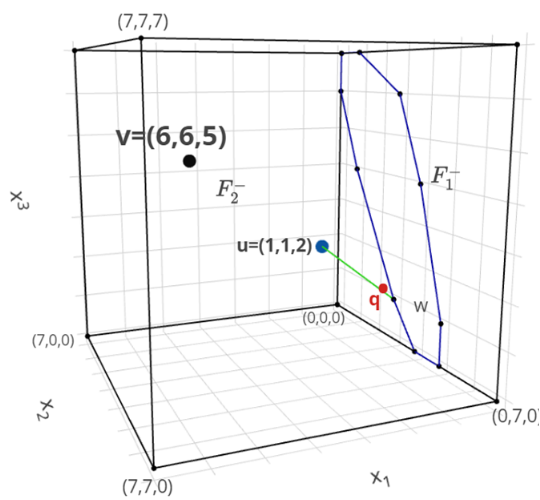

Figure 3.2: A real edge is added for connecting the inner vertex u with F_1^- for $(u,v) = ((1,1,2),(6,6,5))$. The partial shelling meets the upper bound certificates.

3.1.4 New approaches to reduce the search space

The algorithm during the shelling step attempts to sequentially embed lattice $(d-1,k)$-polytopes onto the facets of the $[0,k]^d$. Thus a large number of lattice $(d-1,k)$-polytopes implies that determining whether the shelling step output is empty or not can be computationally intractable. For each non-embedded facet of the hypercube there are a number of lattice $(d-1,k)$-polytopes available to intersect, that can vary depending on available information. Given a shelling and the next facet of the $[0,k]^d$ to embed F, this information consists of:

- The number of known vertices in F.
- The number of points that cannot be considered as vertices, either by convexity or determined by previous embeddings.
- Gap scores g_i^+ or g_i^-.

In fact, different sequence orderings impact on the computational time required for the search space examination. We want to follow an embedding sequence such that shelling step output can be obtained as efficient as possible. Hence it is important to follow a strategy that allows us:

(i) To select a facet of the $[0,k]^d$ with the lowest possible number of lattice $(d-1,k)$-polytopes available to intersect.

(ii) To select a facet of the $[0,k]^d$ such that u and v can be connected via Γ or the upper bounds can be updated with the lowest possible number of embeddings. This determines whether the node satisfies the upper bound certificates or it can be pruned.

To identify the facet of the hypercube corresponding to the lowest number of lattice $(d-1,k)$-polytopes available to intersect, Deza et al. [8] proposed the gap parameters g_i^- and g_i^+, calculated as follows:

$$g_i^- = g + u_i + v_i - k$$
$$g_i^+ = g + k - (u_i + v_i)$$

A lower score is associated with a lower number of lattice $(d-1,k)$-polytopes. It is common to have the same g_i^- and g_i^+ scores for different candidate intersections. Thus a tie-breaker criteria should be defined to select the most suitable facet of the $[0,k]^d$ for embedding. We propose the following order criteria:

1. The facet gap parameters, g_i^- and g_i^+, for $i = 1,...,d$. A gap score equal to zero is the highest priority.

2. The number edges of F_i^- or F_i^+, that do not contain vertices of P. It is important to prioritize a facet of the $[0,k]^d$ restricted to a lower number of integer value coordinate points.
3. $\text{argmin}\{\min_{i=1,\ldots,d}\{u_i, k-v_i\}\}$. For example if $u = (1,1,2)$, then F_1^- or F_2^- have a higher priority than F_3^- due to edges that could be added to Γ as presented in subsection 3.1.3.
4. The number of currently known vertices of P belonging to the intersections F_i^- or F_i^+, with more points contained being higher priority. A higher number of points reduces number of lattice $(d-1,k)$-polytopes being more likely to discover paths from u to v.
5. Finally, the default order of $F_1^-,\ldots,F_d^-,F_1^+,\ldots,F_d^+$.

When both vertices u and v have at least one coordinate equal to 0 or k, it is not necessary to verify whether they are vertices of the set $\mathscr{C}_{d,k,g}^{u,v}$. Therefore Certificate 2 can be omitted in this case. On the other hand, when vertices u or v are inner points to the hypercube, this condition must be verified as we continue intersecting with the hypercube faces.

Let assume that u or v are inner points of the hypercube. In this case, Certificate 2 should be checked. But, the large number of convex hull computations to perform leads to an intractable search space. A preprocessing step that allows us to reduce the search space is added. The following verification is proposed for each point p with at least one coordinate equal to 0 or k. Let p a point with at least one coordinate equal to 0 or k and let $S_{d,k,g}^{u,v,p}$ denote the convex hull of u, v, p and the following set:

$$\left[\bigcup_{i=1}^{d}\{x\in\mathbb{R}^d : x_i = 0 \text{ and } \bar{x}_i \in \mathscr{P}_{d-1,k,g_i^-}\}\right] \cup \left[\bigcup_{i=1}^{d}\{x\in\mathbb{R}^d : x_i = k \text{ and } \bar{x}_i \in \mathscr{P}_{d-1,k,g_i^+}\}\right].$$

Given the pair of vertices (u,v), the following condition is necessary for p to be a potential vertex of a lattice (d,k)-polytope such as $d(u,v) = \delta(d-1,k)+k-g$:

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

Thus we can remove points p for which the previous condition is not satisfied, reducing the computational time. In this chapter, we determine $\delta(3,7)$. To illustrate the size of search space and the impact of selection criteria of the following facet of the $[0,k]^d$ to intersect, Table 3.2 shows the number of lattice $(2,7)$-polygons of diameter 5 or 6. If we know that $(0,1)$ and $(0,2)$ must be vertices in the next intersection, fewer lattice $(2,7)$-polygons are considered for embedding as presented in Table 3.3. Finally Table 3.4 presents the polygons without points $(0,*)$ or $(*,7)$ as vertices.

Diameter	Polygons
5	801 986
6	2 660

Table 3.2: Number of lattice $(2,7)$-polygons with diameter 5 or 6.

Diameter	Polygons
5	52 308
6	167

Table 3.3: Number of lattice $(2,7)$-polygons with diameter 5 or 6 such that $(0,1)$ and $(0,2)$ are both vertices.

Diameter	Polygons
5	11 472
6	4

Table 3.4: Number of lattice $(2,7)$-polygons with diameter 5 or 6 such that neither $(0,*)$ or $(*,7)$ are vertices.

Identifying paths between u and v with the lowest possible number of embeddings is critical to reduce the processing time. In the present work, we explain several results that allow us to identify additional faces. Previously the work of Deza et al. [8], after completing the $2d$ embeddings, during the inner step all edges belonging to Γ were added. Now, we propose to add additional edges, during the shelling step, tightening upper bounds from early stages.

When an upper bound for $d(u,v)$ is strictly lower than $\delta(d-1,k)+k-g$, there cannot exist a candidate in the current branch capable of achieving the target diameter. Finally in subsection 3.1.4, a new certificate is introduced, consisting of a new upper bound for $d(u,v)$.

Certificate 3: Upper bound for $d_(u,v)$

The following are upper bounds for the distance between u and v, $d(u,v)$:

$$d_1(u,v) = \min_{i=1,\dots,d}\{\min\{\widetilde{d}(v,F_i^-) + \max_{w\in F_i^-}\{d_\Gamma(u,w)\}, \widetilde{d}(v,F_i^+) + \max_{w\in F_i^+}\{d_\Gamma(u,w)\}\}\}$$

$$d_2(u,v) = \min_{i=1,\dots,d}\{\min\{\widetilde{d}(u,F_i^-) + \max_{w\in F_i^-}\{d_\Gamma(v,w)\}, \widetilde{d}(u,F_i^+) + \max_{w\in F_i^+}\{d_\Gamma(v,w)\}\}\}$$

These upper bounds provide a new alternative when $d(u,v)$ is undetermined or current upper bounds do not allow to conclude whether shelling can be pruned. When there is not a path from u to v in Γ, $d(u,v)$ is considered as undetermined. These upper bounds are useful when one of u and v are disconnected in Γ by real edges. As illustration, let $d=3$, $u=(0,1,2)$ and $v=(6,5,5)$, and two intersections with the cube $[0,k]^3$ have been selected: F_1^- and F_2^+ such that $F_1^- \cap F_2^+$ is not empty. Consequently there is a path from u to every vertex $w \in F_2^+$, and $d_1(u,v)$ can be updated. The values of $d_1(u,v)$ and $d_2(u,v)$ are updated every time a choice for the intersection with a facet of the hypercube $[0,k]^d$ is selected. Thus we define the following non-negative integer parameter η:

$$\eta = \delta(d-1,k)+k-g-\min\{d_1(u,v),d_2(u,v)\}.$$

Therefore similar to Certificate 1, $\eta > 0$ is a certificate that no lattice (d,k)-polytope with vertices u and v such that $d(u,v) = \delta(d-1,k)+k-g$ exists.

3.1.5 Enhanced shelling step

In this subsection, the enhancements of shelling step are explained. First, findings for dimension 3 are presented, followed by their generalization to dimension 4 and higher. Given a lattice (d,k)-polytope P that achieves target diameter, convexity and integrality of the formulation $\min\{c \cdot x : x \in P\}$ are exploited to identify additional faces of P during the embedding process.

Let suppose the algorithm is trying to embed the second intersection with the cube $[0,k]^3$. Under certain conditions, it is possible to identify additional faces in P, that is additional edges in Γ. These edges make possible to connect u and v or tightening the upper bounds defined by Certificates 1 and 3 with a lower number of embeddings in comparison with the the algorithm developed by Deza et al. [8].

Without loss of generality, assume that the partial shelling consists of F_1^-, F_2^- and F_3^-. And illustrate the Lemma 3.1.1 by considering the minimization problem $\min\{ix_1 + x_2 : x \in P\}$ to add information from additional discovered faces during the construction of a lattice $(3,k)$-polytope P of large diameter.

Lemma 3.1.1. *Assume that, up to the symmetry of the cube* $[0,k]^3$*:*

(i) $v^+ = (1,0,v_3^+)$ *and* $v^- = (1,0,v_3^-)$ *are vertices of P for some* $(v_3^+, v_3^-) \in \{0,1,\ldots,k\}^2$ *where* $v_3^+ \geq v_3^-$.

(ii) $w^+ = (0,w_2^+,w_3^+), w^- = (0,w_2^-,w_3^-)$ *are vertices of P for some* $(w_2^+,w_3^+,w_3^-) \in \{0,1,\ldots,k\}^3$ *where* $w_2^+ = w_2^-$ *and* $w_3^+ \geq w_3^-$.

(iii) $x = (0,0,x_3)$ *is not a vertex for any* $x_3 \in \{0,1,\ldots,k\}$.

(iv) $x = (0,x_2,x_3)$ *is not a vertex for any* $(x_2,x_3) \in \{0,1,\ldots,k\}^2$ *and* $x_2 < w_2^+$.

Then, (v_3^+, w_3^+) *and* (v_3^-, w_3^-) *form edges of P and* $d(v_3^+, w_3^+) = d(v_3^-, w_3^-) = 1$.

Proof. Consider $\alpha = \min\{w_2^+ x_1 + x_2 : x \in P\}$. Note that $\alpha = w_2^+$ by items (iii), (iv) and the integrality of the coordinates of P. Thus $\mathrm{argmin}\{w_2^+ x_1 + x_2 : x \in P\}$ forms a face f of P. To identify the vertices of f, we observe that v^+, w^+, v^-, w^- are the only $\{0,1,2,...,k\}$ value vertices of P satisfying $w_2^+ x_1 + x_2 = w_2^+$. Since no more than two vertices can belong to the same line, (v_3^+, w_3^+) and (v_3^-, w_3^-) form edges of P and $d(v_3^+, w_3^+) = d(v_3^-, w_3^-) = 1$. $\square$

Note that in Lemma 3.1.1 the face f can be a line, triangle or a rectangle. In the framework developed by Deza et al. [8], for 2 adjacent embeddings with empty intersection, only Certificate 1 was updated. Now Lemmas 3.1.1 and 3.1.2 make it possible to connect embeddings under the mentioned conditions and Certificate 3 is included as an additional upper bound for $d(u,v)$ to determine whether current partial shelling can be pruned or not. As a remark, having more paths on Γ from u or v to F_i^- or F_i^+, respectively, is more likely to decrease gap parameters. Lower g_i scores of non embedded facets of the cube $[0,k]^3$, reduce the number of lattice $(2,k)$-polygons to list for next intersections of P with the cube $[0,k]^3$.

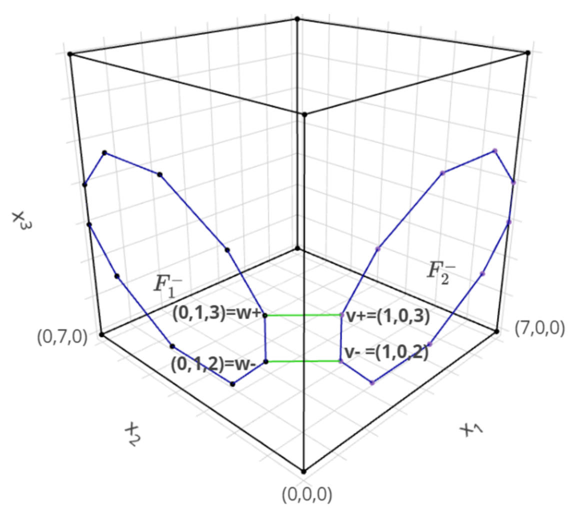

Figure 3.3: Facet of P with vertices $\{v^+, v^-, w^+, w^-\} = \mathrm{argmin}\{x_1 + x_2 : x \in P\}$ is identified by Lemma 3.1.1, where $v^+ = (1,0,3)$, $v^- = (1,0,2)$, $w^+ = (0,1,3)$ and $w^- = (0,1,2)$.

Lemma 3.1.2. *Assume that, up to the symmetries of the cube* $[0,k]^3$*:*

(i) $v^+ = (2,0,v_3^+), v^- = (2,0,v_3^-)$ *are vertices of* P *for some* $(v_3^+, v_3^-) \in \{0,1,\dots,k\}^2$ *where* $v_3^+ \geq v_3^-$.

(ii) $w^+ = (0,2,w_3^+), w^- = (0,2,w_3^-)$ *are vertices of* P *for some* $(w_3^+, w_3^-) \in \{0,1,\dots,k\}^2$ *where* $w_3^+ \geq w_3^-$.

(iii) $x = (0,0,x_3)$ *is not a vertex for any* $x_3 \in \{0,1,\dots,k\}$.

(iv) $x = (x_1,x_2,x_3)$ *is not a vertex for any* $(x_1,x_2,x_3) \in \{0,1,\dots,k\}^3$ *and* $x_1 + x_2 = 1$.

Then $d(v_3^+, w_3^+) \leq 2$ *and* $d(v_3^-, w_3^-) =\leq 2$.

Proof. Consider $\alpha = \min\{x_1 + x_2 : x \in P\}$. Note that $\alpha = 2$ by items (iii) and (iv) and the integrality of the coordinates of vertices of P. We observe $\{v^+, v^-, w^+, w^-\} \subseteq f = \operatorname{argmin}\{x_1 + x_2 : x \in P\}$ and at most 3 points $x = (1,1,x_3)$ for some $(x_3) \in \{0,1,\dots,k\}$ can be also vertices of f. Therefore the weighted virtual edges $[v^+, w^+]$ and $[v^-, w^-]$ of length 2 are added to Γ. □

Lemma 3.1.2 considers inner points of the cube $[0,k]^3$ to add weighted virtual edges to Γ, make it possible to remove partial shellings before the inner step.

Lemma 3.1.3. *Assume that, up to the symmetry of the cube* $[0,k]^3$*:*

(i) $(0,0,0)$ *is not a vertex of* P.

(ii) F_3^- *a non-embedded facet of the cube* $[0,k]^3$.

(iii) $x = (c_1,0,0)$ *is a vertex of* P *for some* $c_1 \in \{1,2,3,4\}$.

(iv) $w = (0,c_2,0)$ *is a vertex of* P *for some* $c_2 \in \{1,\dots,k\}$.

Define vector $c = (c_1,c_2)$*, we determine the following values for* $d(x,w)$

(i) *If* $c = (1,c_2)$*,* $d(x,w) = 1$.

(ii) *If* $c = (2,c_2)$*,* $d(x,w) \leq 2$.

(iii) *If* $c = (3,c_2)$*,* $d(x,w) \leq 2$.

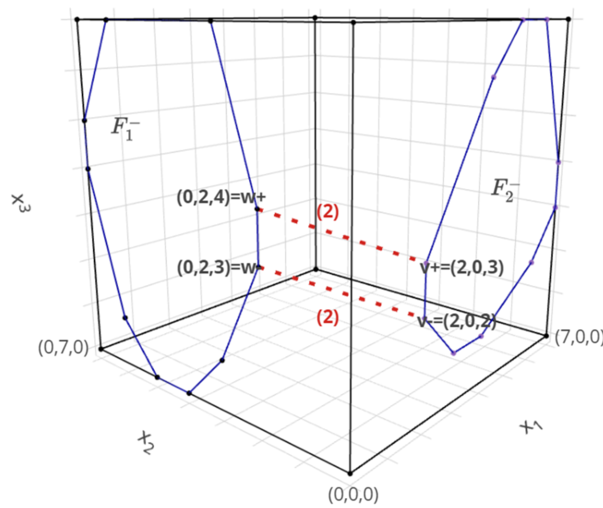

Figure 3.4: Weighted virtual edges $[v^+, w^+]$ and $[v^-, w^-]$ of length 2, coloured in red, are added to Γ by Lemma 3.1.2, where $v^+ = (2,0,3)$, $v^- = (2,0,2)$, $w^+ = (0,2,4)$ and $w^- = (0,2,3)$.

(iv) *If* $c = (4, c_2)$*,* $d(x, w) \leq 3$*.*

Proof. Consider $\alpha = \min\{c_1x_1 + c_2x_2 : x \in P\}$. For each case, by the integrality of the coordinates of vertices of P, we can see that a path with at most $1, 2$ or 3 edges respectively can connect x with w via Γ. □

Lemmas 3.1.3 and 3.1.4 present the conditions to add weighted virtual edges in order to connect vertices through non-embedded facets of the cube $[0, k]^3$. In the illustrations, weighted virtual edges are labelled with the corresponding weight. If the node is pruned after adding weighted virtual edges induced by Lemmas 3.1.3 and 3.1.4, we are avoiding to list all lattice $(2, k)$-polygons available to embedding on the corresponding facets of the cube.

Lemma 3.1.4. *Assume that, up to the symmetries of the cube* $[0, k]^3$*:*

(i) $v^- = (0, 1, v_3^-)$ *is a vertex of* P *for some* $v_3^- \in \{0, 1, \ldots, k\}$*, and* $(0, 1, x_3)$ *is not a vertex of* P *for any* $x_3 < v_3^-$*.*

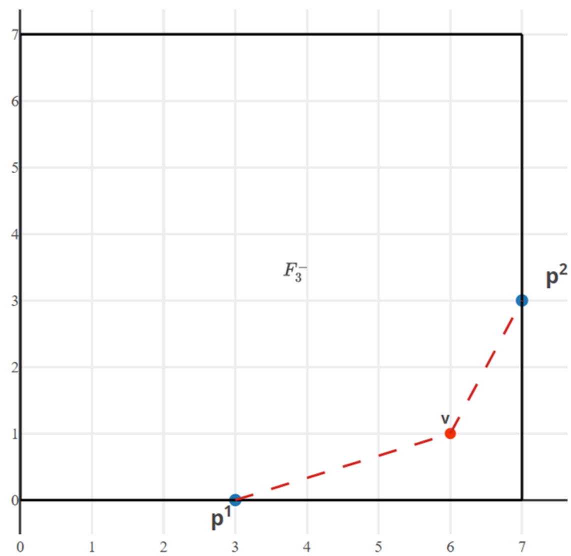

Figure 3.5: Weighted virtual edge $[p^1, p^2]$, coloured in red, of length 2 is is added to Γ. $p^1 = (3,0,0)$ and $p^2 = (7,3,0)$.

(ii) $w = (w_1, 0, 0)$ *is a vertex of* P *for some* $w_1 \in \{0, 1, \ldots, k\}$

(iii) $x = (0, 0, x_3)$ *is not a vertex of* P *for any* $x_3 \in \{0, 1, \ldots, k\}$

Then $d(v^-, w) \leq w_1$.

Proof. Note that the vertex v^- corresponds to the vertex v^- used in the proof of Lemma 3.1.1. Similarly, items (ii) and (iii) yield a vertex $w^- = (w_1^-, 0, w_3^-)$ such that $(w_1^-, 0, x_3)$ is not a vertex of P for $x_3 < w_3^-$. By Lemma 3.1.1, $d(v^-, w^-) = 1$. Note that w^- and w both belong to the face f of P of dimension at most 2 defined by $f = \text{argmin}\{c^T x : x \in P\}$ where $c = (0, 1, \ldots, 1, 0)$. Thus $d(w^-, w) \leq w_1 - w_1^-$. Since $d(v^-, w) \leq d(v, w^-) + d(w^-, w)$, $d(v^-, w) \leq w_1$ if $w_1 \neq w_1^-$ and $d(v^-, w) = 1$ if $w_1 = w_1^-$ as this occurs only if $w^- = w$. $\square$

Lemma 3.1.5. *Assume that* 3 *intersections of* P *with the cube* $[0, k]^3$ *such that the* 3 *supporting hyperplanes share a common vertex are known, up to symmetry without loss of generality* F_i^- *for* $i = 1, 2$ *and* 3. *Let* $\alpha = \min\{x_1 + x_2 + x_3 : x \in P\}$

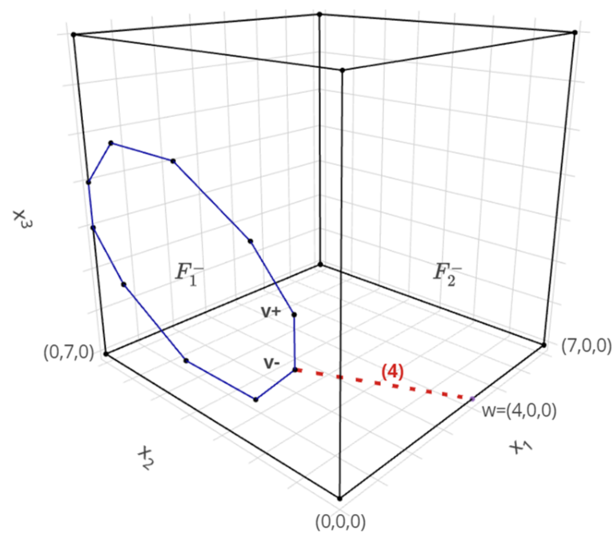

Figure 3.6: Weighted virtual edge $[v^-, w]$ of length 4 is added to Γ By Lemma 3.1.4. Points $v^- = (0,1,2)$ and $w = (4,0,0)$ are vertices.

and $f = argmin\{x_1 + x_2 + x_3 : x \in P\}$. *Thus,*

(i) *If* $\alpha = 2$ *and* f *contains at least* 3 *vertices,* f *is a face of* P.

(ii) *If* $\alpha = 3$, f *contains at least* 3 *vertices and* $(1,1,1)$ *is not a vertex of convex hull of* $\{(1,1,1)\} \cup P$ *then vertices in* f *form a face of* P.

(iii) *If* $\alpha = 3$, f *contains at least* 2 *vertices and* $(1,1,1)$ *is a vertex of convex hull of* $\{(1,1,1)\} \cup P$ *then vertices in* f *form a face of* P.

Proof. Consider the problem $\alpha = \min\{x_1 + x_2 + x_3 : x \in P\}$. By integrality of coordinates of the vertices of P and conditions expressed in items (i), (ii), (iii). We observe $\text{argmin}\{x_1 + x_2 + x_3 : x \in P\}$ forms a face f of P.

□

Previous findings allow to identify new paths from u to v when trying to embed three adjacent facets of P to a corner of the cube. Lemma 3.1.5 exploits the problem $\min\{x_1 + x_2 + x_3 : x \in P\}$ at an empty corner and new edges can be added to

Γ.

The results in this section allow to find new paths through Γ that potentially can connect u and v, tightening upper bounds and decreasing gap scores. Thus, more alternatives are available to conclude whether the current shelling can be pruned. Resultant shellings most likely adopt two patterns. First, given $x \in P$ a corner of hypercube $[0,k]^d$, $(k,\dots,k)$–x will be also a vertex of P. Second, embeddings onto the facets of the $[0,k]^d$s will be relatively centred and far from edges of the facets of the $[0,k]^d$, avoiding edges can be added during shelling step. Given the convex hull computations to perform during inner step, decreasing the number of duplicate shellings up to symmetry impact on the execution time of the algorithm.

In the work of Deza et al. [8], during the shelling step, only the $2d$ intersections with then facets of the $[0,k]^d$ were considered as facets of polytope P. This is equivalent to use hyperplanes with normal vectors c parallel to coordinate axis for identifying facets of polytope P. Our novel approach considers different vectors c from the problem $\min\{c \cdot x : x \in P\}$, to identify existing facets of P, or adding weighted virtual edges. Hereinafter denote by g^+ and g^- the vectors whose coordinates are the scores g_i^- and g_i^- respectively.

Shelling step illustrations for $d = 3$

The new framework can efficiently process previously intractable instances. In this subsection we present several illustrations of our new approach and how most of the shelling can be pruned with at most two embedding onto facets of the cube. We consider the triple $(d,k,g) = (3,7,1)$ and its corresponding target diameter $\delta(2,7) + 7 - 1 = 12$. For this input the most challenging pair to process was $(u,v) = ((1,1,2),(6,6,5))$. Right from the start for the framework developed by Deza et al. [8], this pair is intractable due to three reasons:

- The large number of lattice $(2,7)$-polygons to consider for embedding onto each facet of the $[0,k]^d$.

- Vertices $u=(1,1,2)$ and $v=(6,6,5)$ are inner points of the cube $[0,7]^3$. The gap vector scores g^+ and g^- do not change during shelling step due to these vertices remain disconnected via Γ in the algorithm developed by Deza et al. [8]. In the mentioned algorithm the use of Certificate 2 , which involves convex hull computations, would have reduced the search space. However, in an extremely slow computational time. As result the determination of the shelling step output was an impossible task.

- The algorithm developed by Deza et al. [8] does not consider the case when the edges of the cube do not contain vertices of P during shelling step. As a result, the upper bounds for $d(u,v)$ are not tightened with 2 or 3 embeddings. This yields an intractable growing of the search space tree from the first 2 embeddings.

In this subsection the weighted virtual edges are shown as red dotted segments to differentiate from edges of P. The real edges are coloured in green. For the next example, Figure 3.7 illustrates Lemmas 3.1.1 and 3.1.3. These Lemmas allow to identify edges of P when trying to embed onto F_2^+. Identified edges of additional faces are added to Γ.

Note that the plane $-2x_1+x_2=5$ contains a face of P. This face has the following vertices: $\{(0,5,0),(0,5,1),(1,7,3),(1,7,4)\}$ and additional edges are added to Γ. Additional edges $[(0,5,0),(1,7,3)]$ and $[(0,5,1),(1,7,4)]$ allow a new path in Γ from u to F_2^+. Furthermore Lemma 3.1.1 states the conditions for adding weighted virtual edge $[(0,5,0),(3,7,0)]$ of length 2 to Γ. Then, upper bound is calculated as follows:

$$d(u,v) \leq \widetilde{d}(u,F_2^+) + \widetilde{d}(v,F_2^+) + \delta(F_2^+) = 11$$

Given that $d(u,v)=11$, the second polygon can not be embedded onto F_2^+ and partial shelling is pruned.

The following case considers the triple $(d,k,g)=(3,4,1)$ that corresponds to a

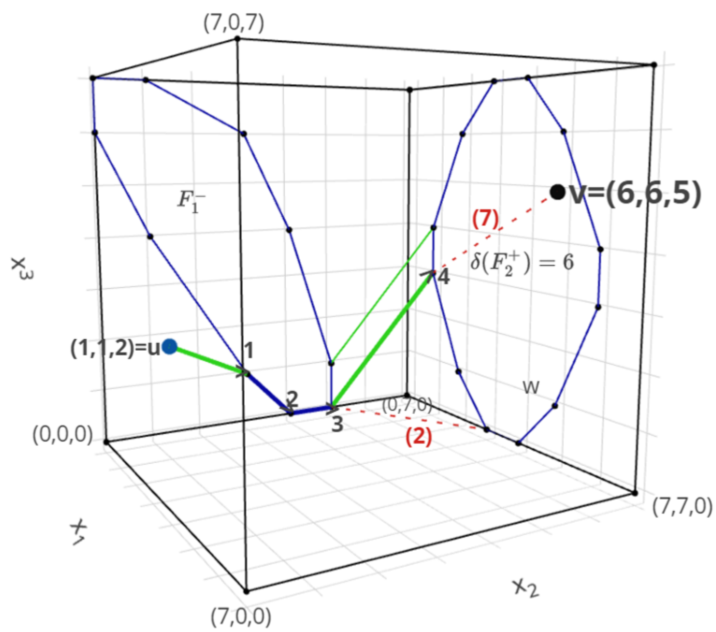

Figure 3.7: Weighted virtual edge and real edges are added to Γ for $(u,v) = ((1,1,2),(6,6,5))$. Shelling pruned after two embeddings due to $d(u,v) \leq \widetilde{d}(u,F_2^+) + \widetilde{d}(v,F_2^+) + \delta(F_2^+) = 11$.

maximal diameter of 7. Figure 3.8 illustrates how the algorithm removes a partial shelling by Lemma 3.1.5 when it is trying to embed 3 adjacent facets to the corner $(0,4,0)$. Note that the plane $-x_1 + x_2 - x_3 = 2$ contains the following three vertices $\{(0,3,1),(0,3,1),(1,4,1)\}$ which form the facet $\operatorname{argmin}\{-x_1 + x_2 - x_3 : x \in P\}$. Therefore the edge $[(0,2,0),(1,4,1)]$ is added to Γ and $d(u,v) = 6$.

In general as result of adding additional edges upper bounds for $d(u,v)$ are decreased early on in the shelling process in comparison with the framework developed by Deza et al. [8]. It is likely to discover new paths from u to v in Γ. Consequently, we could conclude that $d(u,v) < \delta(u,v) + k - g$ and partial shellings can be pruned with a lower number of embedding as mentioned before. Preventing the search tree from growing in an intractable manner. For this reason, fewer lattice $(2,k)$-polygons are considered for the next embeddings.

It is important to detail how Lemma 3.1.5 is included during shelling step to add

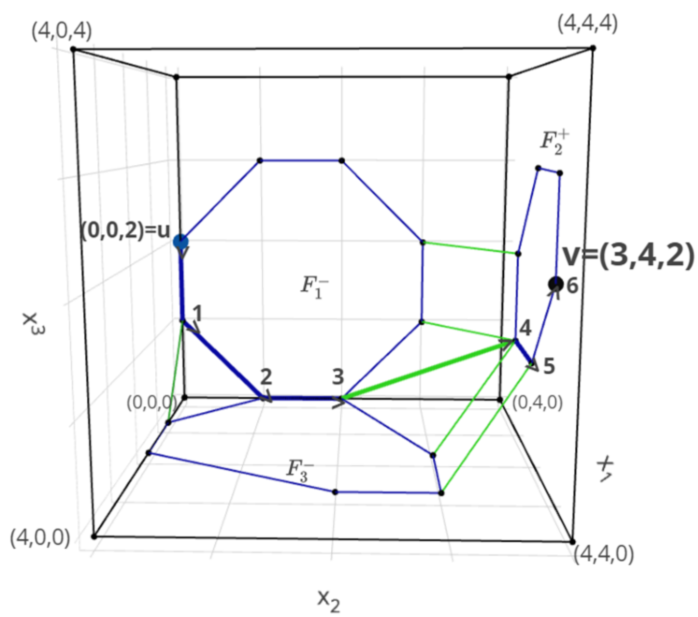

Figure 3.8: Shelling pruned after 3 embeddings: F_1^-, F_2^+ and F_3^- for $(u,v) = ((0,0,2),(3,4,2))$. The edge $[(0,2,0),(1,4,1)]$ is added to Γ by Lemma 3.1.5 allowing $d(u,v) = 6$.

additional edges. Denote by P a lattice $(3,7)$-polytope and assume the following conditions:

- Non-empty intersections F_1^-, F_2^- and F_3^-.
- $F_1^- \cap F_2^- \cap F_3^- = \emptyset$.

Let $\alpha = \min\{x_1 + x_2 + x_3 : x \in P\}$ and $f = \operatorname{argmin}\{x_1 + x_2 + x_3 : x \in P\}$. Next we detail how Lemma 3.1.5 is used during implementation. Note that case when $\alpha = 1$ is already considered in Lemma 3.1.3.

$\alpha = 2$ and f contains at least three vertices

When f contains 3 or 4 vertices, edges of corresponding facet can be added without calling a convex hull subroutine. We notice that f can contain at most 4 vertices, as observed in Figure 3.9.

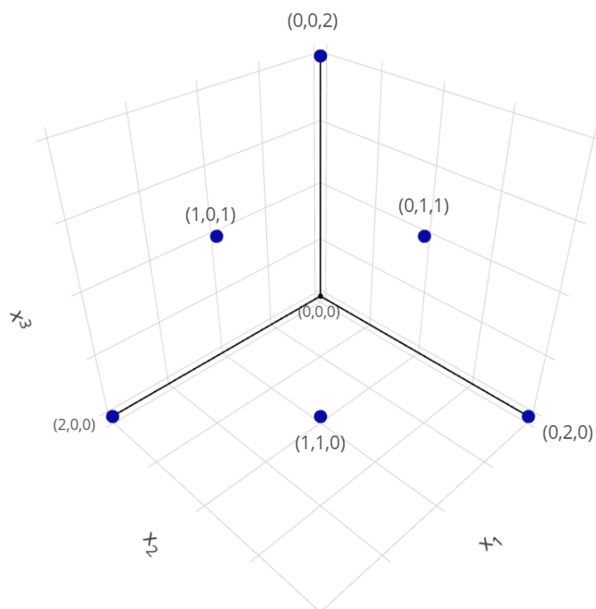

Figure 3.9: All non-negative integer value points that belong to the plane $x_1 + x_2 + x_3 = 2$.

$\alpha = 3$ and f contains at least two vertices

In this case, note that the inner point of the cube $[0,k]^3$, $(1,1,1)$ belongs to the plane $x_1 + x_2 + x_3 = 3$. In Figure 3.10 we can observe that if plane $x_1 + x_2 + x_3 = 3$ contains 4 points of the current shelling, $(1,1,1)$ can not be a vertex. We branch into 2 cases depending on whether $(1,1,1)$ is a vertex or not:

- First, if f contains at least 4 vertices of shelling, we know that $(1,1,1)$ can not be a vertex and the new facet is identified.
- Second, assume f contains 3 vertices and let v^1, v^2, v^3 vertices in f, we consider two sub-cases whether $(1,1,1)$ is vertex or not of the convex hull of the set of points $\{v^1, v^2, v^3, (1,1,1)\}$.
  - First sub-case, $(1,1,1)$ is a vertex of the convex hull of the set of points $\{v^1, v^2, v^3, (1,1,1)\}$. Then the edges in common among triangle $\{v^1, v^2, v^3\}$ and edges of $\{v^1, v^2, v^3, (1,1,1)\}$ are added to Γ.

- Second sub-case, $(1,1,1)$ is not a vertex of the convex hull of the set of points $\{v^1, v^2, v^3, (1,1,1)\}$. Then edges of the triangle are added to Γ.

Under the conditions of Lemma 3.1.5 different vectors from $c = (1,1,1)$ are considered. As result following two cases are included in the algorithm to systematically add edges to Γ.

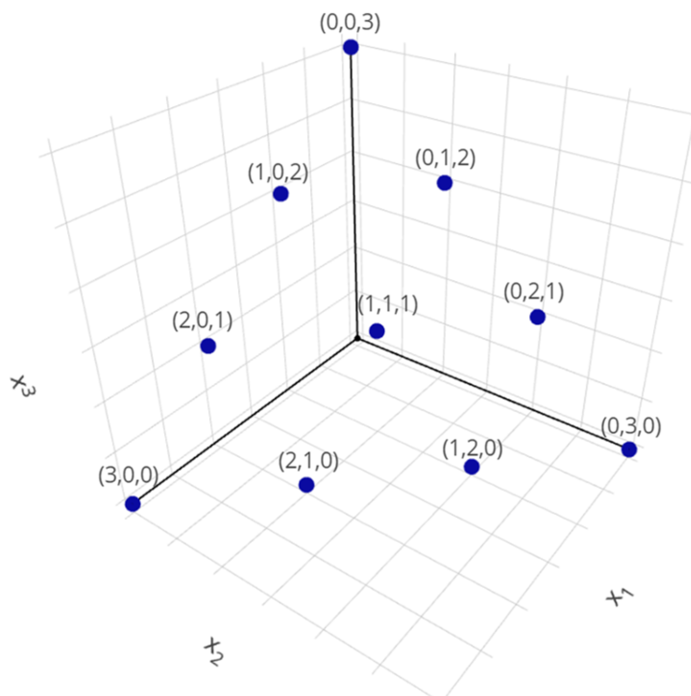

Figure 3.10: All non-negative integer value points that belong to the plane $x_1 + x_2 + x_3 = 3$.

$\alpha = 2$ and f contains one or two vertices

If the plane $x_1 + x_2 + x_3 = 2$ contains 1 or 2 vertices, the vertices in $x_1 + x_2 + x_3 = 3$ are considered to identify new faces of P and add new edges to Γ.

$\alpha = 4$ and f contains at least two vertices

In this case, the algorithm considers two cases, whether $(1,1,1)$ is vertex or not of the shelling:

- If $(1,1,1)$ is not a vertex, new edges from f are added to Γ.
- If $(1,1,1)$ is a vertex, vertices that belong to the plane $x_1+x_2+x_3=4$ are used to identify new faces and add additional edges to Γ.

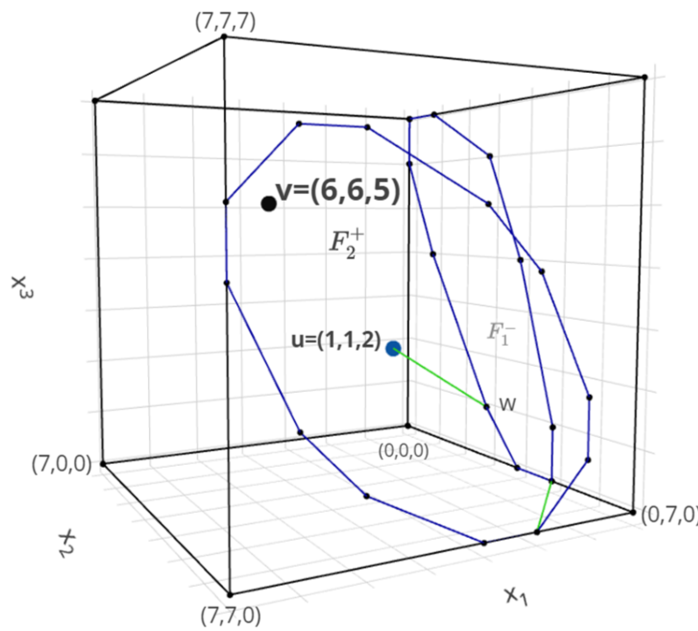

Figure 3.11: Shelling pruned by Certificates 2 and 3 after two embeddings F_1^- and F_2^+. Points $(u,v)=((1,1,2),(6,6,5))$ and $w=(0,3,1)$ are vertices of the shelling.

The order in which the results of the previous section are considered has an impact on the processing time of the algorithm. Figure 3.11 shows a partial shelling with two embeddings which are removed due to Certificates 2 and 3. Once the additional edges that do not require convex computations are added to Γ, upper bounds are updated. Only if the node satisfies the upper bound certificates, convex hull computations are performed to determine if additional edges can be added to decide whether the node can be pruned or not.

u	Search space reduction
$(1,1,1)$	25%
$(1,1,2)$	81%
$(1,1,3)$	89%
$(1,2,2)$	98%

Table 3.5: Space reduction out of 804 646 available polygons for the first embedding after integer points are removed from the facets of $[0,7]^3$.

Among the strategies to reduce search space, removing points from the facets of the cube is quite useful. For this reason, this strategy is used before starting the embedding process. Once points in the facet of the cube that can not be vertices of P are removed for $(d,k,g) = (3,7,1)$, the search space is reduced. Table 3.5 shows the percentage of polygons from the set of lattice $(2,7)$-polytopes that are considered for the first embedding after removing the points that cannot be vertices of the polytope. As the coordinates of vertex u become larger, a smaller percentage of lattice $(2,7)$-polytopes will be considered.

According to Table 3.5, it could be counter-intuitive that the pair $(u,v) = ((1,1,2), (6,6,5))$ is the hardest to determine the shelling step output considering that the pair $(u,v) = ((1,1,1),(6,6,6))$ has larger search space. The reason is that $(1,1,1)$ and $(6,6,6)$ can be connected to the 3 corresponding intersections of the cube $[0,7]^3$. For the pair $(u,v) = ((1,1,2),(6,6,5))$, considering the first two embeddings F_1^- and F_2^- the search space was reduced approximately 35 000 times in comparison to the framework developed by Deza et al. [8].

Finally, let consider the case when an edge of $[0,k]^3$ contains vertices of P. Figure 3.12 shows two embeddings F_1^- and F_2^+ having $(0,7,4)$ and $(0,7,5)$ as intersection. Conditions of Lemma 3.1.4 are met, thus the weighted virtual edges $[(0,5,6),(3,7,7)]$ and $[(0,2,0),(2,7,1)]$ of length 3 and 5 respectively, are added to Γ. These weighted virtual edges are coloured in red in Figure 3.12.

After adding these weighted virtual edges, the partial shelling presented in Figure 3.12 is not pruned yet due to $d(u,v) = \delta(2,7) + 7 - 1 = 12$. Taking one of

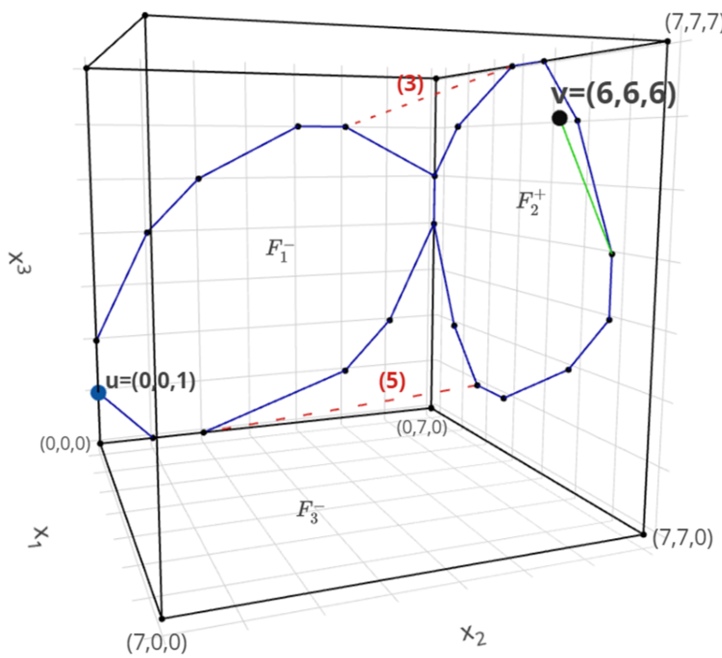

Figure 3.12: Shelling met the certificates after two embeddings for $(u,v) = ((0,0,1),(6,6,6))$. Weighted virtual edges $[(0,5,6),(3,7,7)]$ and $[(0,2,0),(2,7,1)]$ are added by Lemma 3.1.4.

the vertices in the intersection between F_1^- and F_2^+, $(0,7,4)$ and its two adjacent vertices $(0,6,2)$ and $(0,7,4)$, the plane $2x_1 - 2x_2 + x_3 = -10$ can be defined. This plane is used to branch the current partial shelling into two cases. Each branch is analyzed, concluding whether target diameter is achieved or not. From the search space, only one point can be a vertex, $(1,6,0)$, so there are 2 cases to check:

(i) Figure 3.13 illustrates when $(1,6,0)$ is assumed to be vertex. The real edges $[(1,6,0),(2,7,1)]$ and $[(1,6,0),(0,2,0)]$ respectively are added to Γ by Lemmas 3.1.1 and 3.1.3. These two edges are coloured in green. A path of length 9 is identified, thus the branch is removed from the search space tree.

(ii) For the second case Figure 3.14 shows that the additional edge $[(0,6,2),(1,7,2)]$ is added to Γ due to the plane $2x_1 - 2x_2 + x_3 = -10$ containing a facet of P. These real edge is coloured in green. A path of length 11 is labelled, thus the branch is removed from the tree.

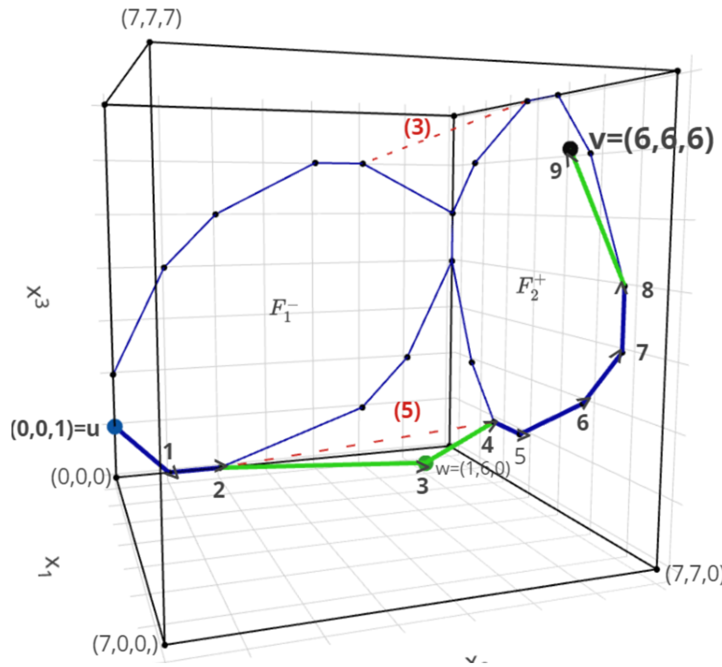

Figure 3.13: Shelling pruned as $d(u,v) = 9$ for $(u,v) = ((0,0,1),(6,6,6))$. The point $w = (1,6,0)$ is assumed to be vertex. Virtual weighted edge $[(0,2,0),(2,7,1)]$ of length 5 is added to Γ.

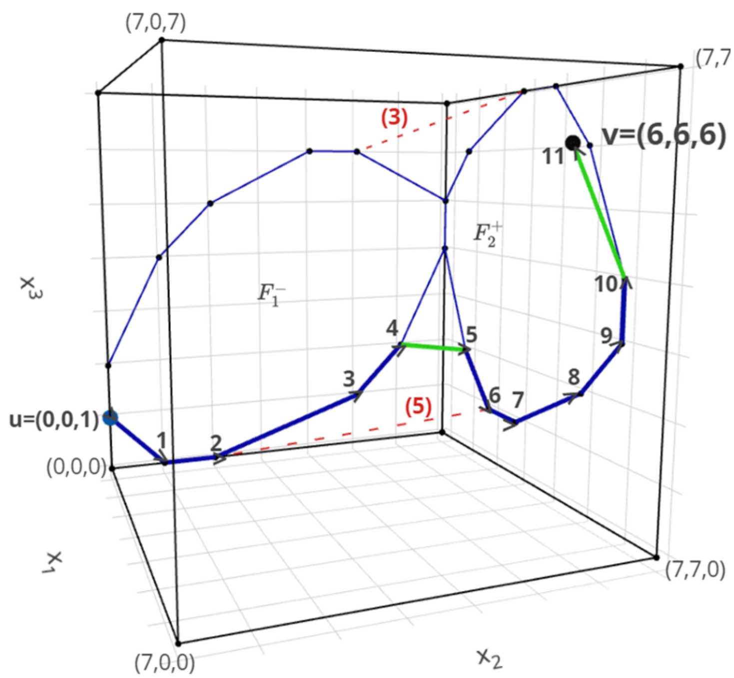

Figure 3.14: Shelling pruned due as $d(u,v) = 11$ for $(u,v) = ((0,0,1),(6,6,6))$. The point $w = (1,6,0)$ is assumed not to be a vertex. The virtual weighted edge $[(0,2,0),(2,7,1)]$ of length 5 is added to Γ.

Shelling step for $d = 4$

In this subsection we generalize the results presented in Section 3.1.5 for $d > 3$.

Lemma 3.1.6. *Let* P *a lattice* $(4,k)$*-polytope and* F_1^-*, satisfying the following conditions:*

(i) $F_1^- \cap F_2^- \cap F_3^- \cap F_4^- = \emptyset$.

(ii) *Let the vertices* $v^+ = (1,0,0,v_4^+)$, $v^- = (1,0,0,v_4^-)$, $w^+ = (1,0,0,w_4^+)$, $v^- = (1,0,0,w_4^-)$, $z^+ = (1,0,i,z_4^+)$, $z^- = (1,0,0,z_4^-)$ *where* $v_4^+ \geq v_4^-$, $w_4^+ \geq w_4^-$, $z_4^+ \geq z_4^-$ *respectively.*

(iii) *Point* $x = (0,0,x_3,x_4)$ *such as* $x_3 < i$*, is not a vertex of* P.

Then, plane $ix_1 + ix_2 + x_3 = i$ *defines a face of the hypercube* $[0,k]^4$ *and its edges can be added to* Γ.

Proof. Consider the problem $\min\{ix_1 + ix_2 + x_3 : x \in P\}$. Given that $\min\{ix_1 + ix_2 + x_3 : x \in P\} = i$, $\operatorname{argmin}\{ix_1 + x_2 + x_3 : x \in P\}$ forms a face f of P. To identify the vertices of f, we observe the $\{0,1,2,...,k\}$-valued vertices of P satisfying $ix_1 + ix_2 + x_3 = i$ are $(1,0,0,x_4)$, $(0,1,0,v_4)$, $(0,0,i,w_4)$. Since no more than two vertices can be aligned, we obtain that f has at most 6 vertices and edges can be added to Γ. $\square$

Note that we can assume without loss of generality that $P \cap F_i^{+/-} \neq \emptyset$ for $i = 1,\ldots,d$.

Lemma 3.1.7. *Assume that, up to the symmetries of the hypercube* $[0,k]^d$*,*

(i) $v = (0,1,0\ldots,0,v_d)$ *is a vertex of* P *for some* $v_d \in \{0,1,\ldots,k\}$

(ii) $w = (w_1,0,0\ldots,0,w_d)$ *is a vertex of* P *for some* $(w_1,w_d) \in \{0,1,\ldots,k\}^2$

(iii) $x = (0,\ldots,0,x_d)$ *is not a vertex of* P *for any* $x_d \in \{0,1,\ldots,k\}$

Then we can define the following two vertices of P

- *i* $v^- = argmin\{c^T x : x \in P, x_i = 0 \text{ for } i \notin \{2,d\}\}$
  where $c = (0, k+1, 0 \dots, 0, 1)$,
- *ii* $w^- = argmin\{c^T x : x \in P, x_i = 0 \text{ for } i \notin \{1,d\}\}$
  where $c = (k+1, 0 \dots, 0, 1)$,

and (v^-, w^-) *form an edge of* P*; that is* $d(v^-, w^-) = 1$.

Proof. Let $f^1 = \text{argmin}\{c^T x : x \in P, x_i = 0 \textit{ for } i \notin \{2,d\}\}$ where $c = (0, k+1, 0 \dots, 0, 1)$. Note that $f^1 \neq \emptyset$ due to item (i), item (iii) and the integrality of the coordinates of the vertices of P. f^1 consist of a unique vertex $v^- = (0, 1, 0 \dots, 0, v_d^-)$ such that $(0, 1, 0 \dots, 0, x_d)$ is not a vertex of P for $x_d < v_d^-$. Similarly, let $f^2 = \text{argmin}\{c^T x : x \in P, x_i = 0 \textit{ for } i \notin \{1,d\}\}$ where $c = (k+1, 0 \dots, 0, 1)$. Note that $f^2 \neq \emptyset$ by item (ii) and, by item (iii) and the integrality of the coordinates of the vertices of P, f^2 consist of a unique vertex $w^- = (w_1^-, 0 \dots, 0, w_d^-)$ such that $(w_1^-, 0 \dots, 0, x_d)$ is not a vertex of P for $x_d < w_d^-$. Consider $\gamma = \min\{c^T x : x \in P\}$ where $c = (1, w_1^-, k+1, \dots, k+1, 0)$. Note that $0 < \gamma \leq w_1^-$ by items (i) and (iii). In addition, by the integrality of the coordinates of the vertices of P, $\gamma = w_1^-$ and f is a face of P of dimension at most 2 that contains, besides the vertices v^- and w^-, at most 2 more vertices $v^+ = (0, 1, 0, \dots, 0, v_d^+)$ and $w^+ = (w_1^+, 0, 0, \dots, 0, w_d^+)$ such that $v_d^+ > v_d^-$ and $w_d^+ > w_d^-$. Consequently the vertices (v^-, w^-) form an edge. □

Lemma 3.1.8. *Assume that, up to the symmetry of the hypercube* $[0,k]^d$,

- (i) $v^- = (0, 1, 0 \dots, 0, v_d^-)$ *is a vertex of* P *for some* $v_d \in \{0, 1, \dots, k\}$, *and* $(0, 1, 0 \dots, 0, x_d)$ *is not a vertex of* P *for any* $x_d < v_d^-$
- (ii) $w = (w_1, 0, 0 \dots, 0)$ *is a vertex of* P *for some* $w_1 \in \{0, 1, \dots, k\}$
- (iii) $x = (0, \dots, 0, x_d)$ *is not a vertex of* P *for any* $x_d \in \{0, 1, \dots, k\}$

Then $d(v^-, w) \leq w_1$.

Proof. Note that the vertex v^- corresponds to the vertex v^- used in the proof of Proposition 3.1.7. Similarly, items (ii) and (iii) yield a vertex $w^- = (w_1^-, 0\ldots, 0, w_d^-)$ such that $(w_1^-, 0\ldots, 0, x_d)$ is not a vertex of P for $x_d < w_d^-$. By Proposition 3.1.7, $d(v^-, w^-) = 1$. Note w^- and w both belong to the face f of P of dimension at most 2 defined by $f = \text{argmin}\{c^T x : x \in P\}$ where $c = (0, 1, \ldots, 1, 0)$. Note that $w_1 = w_1^-$ if only if $w = w^-$ and then $d(w^-, w) \leq w_1 - w_1^- = 0$. If $w_1 \neq w_1^-$ then $d(v^-, w) \leq d(v, w^-) + d(w^-, w)$ and $d(v^-, w) \leq w_1$. Finally, $d(v^-, w) = 1$ if $w_1 = w_1^-$ and this occurs only if $w^- = w$.

□

3.1.6 Enhanced inner step

In this subsection we propose an efficient examination of the inner points in the search space for performing convex hull computations only when it is strictly necessary. Given a shelling and its graph Γ, denote by G the vertex set of Γ. The following enhancements are part of inner step in the new framework:

- We know by convexity that at most two points can be aligned in P. Thus some inner points of the hypercube can be removed from consideration. Let v^1 and v^2 be 2 vertices in G such as they differ only in one coordinate. Under this condition all inner points of $[0,k]^d$ belonging to the line defined by v^1 and v^2 can be removed.

- The next idea consists of building paths on Γ considering some inner points of $[0,k]^d$. Let p an inner point of $[0,k]^d$ and without loss of generality assume that $p_i = 1$. We note that there is an edge between p and one of the vertex of F_i^-. In this case, a branching process can be performed connecting p with F_i^-, one vertex at a time. Certificates can be verified to determine whether target diameter can be achieved or not. Thus, it is possible to remove additional inner points without invoking a convex hull subroutine.

- For the inner points of hypercube p that satisfy the previous two verifications, we check the condition whether the number of vertices in convex hull of $G \cup \{p\}$ is equal to $|G|+1$. Denote by V the set of points for which $|G \cup \{p\}| = |G|+1$. In order to avoid verifying the $2^{|V|}$ subsets of V, the algorithm will not consider redundant examinations. As illustration let p and q the two points in V, if $|G \cup \{p,q\}| < |G|+2$ for $\{p,q\}$, then any subset of V containing $\{p,q\}$ will not be examined. Hence, this allows to decrease the number of convex hull function callings and speed up the computations during the inner step.

3.2 Results

In this section, we detail the result that was obtained using the new framework. The main result is Theorem 3.2.1 which provided the value for $\delta(3,7)$.

Theorem 3.2.1. $\delta(3,7)$ *is equal to* 11.

Theorem 3.2.1 is obtained by computationally verifying that the output of the shelling step is empty for $(d,k,g) = (3,7,0)$ and $(d,k,g) = (3,7,1)$. Therefore, $\delta(3,7) < 12$ and since we can verify the Minkowski sum of the vectors $\{(0,0,1),$ $(0,1,0),(1,0,0),(0,1,1),(0,1,1),(1,0,1),(1,0,1),(1,1,0),(1,1,0),(1,1,1),$ $(1,1,1)\}$ forms, up to translation, a lattice $(3,7)$-polytope with diameter 11 therefore $\delta(3,7) = 11$. Running the algorithm for $(3,7,1)$ requires the determination of all lattice $(2,7)$-polytopes of diameter 5 or 6.

The algorithm is implemented in *C#* and *SQL Server* database. Calculations were carried out on a Dell G3 with a 2.2GHz i7 processor and 32GB of RAM.

3.2.1 Determination of $\delta(3,7)$

The number of lattice $(2,7)$-polygons with diameter 5 or 6 to be checked during each attempt to embed onto the cube's facets is large. This is an intractable task for the algorithm developed by Deza et al. [8] due to the following reasons:

- Given a pair (u,v) where both points belong to the cube facets, the search space tree significantly grew up from the second embedding.
- The input of inner step contained shellings that can not be the skeleton of lattice $(3,7)$-polytopes with diameter 12. Therefore, unnecessary convex hull computations were performed during this step, making the problem computationally intractable.
- Given a pair (u,v) with at least one vertex as inner point of the cube, the

verification of Certificate 2 was performed at every attempt of embedding. The verification of Certificate 2 requires a convex hull computation, that is performing the most time consuming operation a large amount of time.

As presented in Table 3.2, there are 804 646 lattice $(2,7)$-polygons with diameter 5 or diameter 6. During the shelling step, it is important to determine whether there is a path connecting u and v in Γ graph with at most 3 intersections with the cube $[0,7]^3$. Otherwise the problem becomes computationally intractable. The first step is to generate the sets $\mathscr{V}_{2,7,0}$, $\mathscr{V}_{2,7,1}$, and all potential pairs (u,v) for $(d,k,g) = (3,7,1)$.

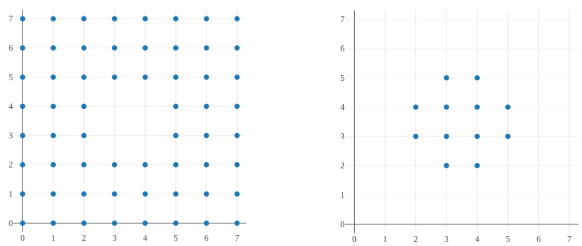

Figure 3.15: The sets $\mathscr{V}_{2,7,0}$ and $\mathscr{P}_{2,7,0}$

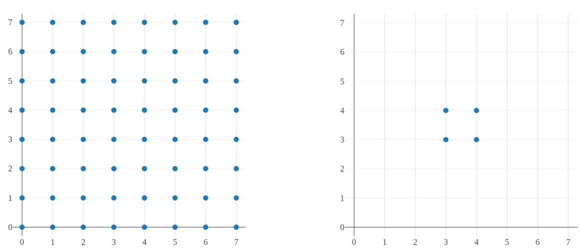

Figure 3.16: The sets $\mathscr{V}_{2,7,1}$ and $\mathscr{P}_{2,7,1}$

Table 3.6 lists the 91 considered pairs (u,v) of vertices of a lattice $(3,7)$-polytope P such that $d(u,v)$ could be potentially equal to 12 and P is assumed to have a non-empty intersection with each facet of the cube $[0,7]^3$.

Because the shelling step output is empty, the inner step is never reached. Thus we state that no lattice $(3,7)$-polytope has a diameter of 12. As we mentioned in the previous section a Minkowski sum of 11 vectors forms, up to translation, a lattice

u	v
$(0,0,0)$	$(6,6,6)$, $(6,6,7)$, $(6,7,7)$, $(7,7,7)$
$(0,0,1)$	$(6,6,5)$, $(6,6,6)$, $(6,6,7)$, $(6,7,5)$, $(6,7,6)$, $(6,7,7)$, $(7,7,5)$, $(7,7,6)$
$(0,0,2)$	$(6,6,4)$, $(6,6,5)$, $(6,6,6)$, $(6,7,4)$, $(6,7,5)$, $(6,7,6)$, $(7,7,4)$, $(7,7,5)$
$(0,0,3)$	$(6,6,3)$, $(6,6,4)$, $(6,6,5)$, $(6,7,3)$, $(6,7,4)$, $(6,7,5)$, $(7,7,3)$, $(7,7,4)$
$(0,1,1)$	$(6,5,5)$, $(6,5,6)$, $(6,5,7)$, $(6,6,6)$, $(6,6,7)$, $(7,5,5)$, $(7,5,6)$, $(7,6,6)$
$(0,1,2)$	$(6,5,5)$, $(6,5,6)$, $(6,6,4)$, $(6,6,5)$, $(6,6,6)$, $(6,7,4)$, $(6,7,5)$, $(7,5,4)$ $(7,5,5)$, $(7,5,6)$, $(7,6,4)$, $(7,6,5)$
$(0,1,3)$	$(6,5,5)$, $(6,6,3)$, $(6,6,4)$, $(6,6,5)$, $(6,7,3)$, $(6,7,4)$, $(7,5,3)$, $(7,5,4)$ $(7,5,5)$, $(7,6,3)$, $(7,6,4)$
$(0,2,2)$	$(6,4,6)$, $(6,5,5)$, $(6,5,6)$, $(6,6,6)$, $(7,4,4)$, $(7,4,5)$, $(7,5,5)$
$(0,2,3)$	$(6,5,5)$, $(6,6,3)$, $(6,6,4)$, $(6,6,5)$, $(7,4,3)$, $(7,4,4)$, $(7,4,5)$, $(7,5,3)$ $(7,5,4)$
$(0,3,3)$	$(7,3,3)$, $(7,3,4)$, $(7,4,4)$
$(1,1,1)$	$(5,5,6)$, $(5,6,6)$, $(6,6,6)$
$(1,1,2)$	$(5,5,6)$, $(5,6,5)$, $(5,6,6)$, $(6,6,4)$, $(6,6,5)$
$(1,1,3)$	$(5,6,5)$, $(6,6,3)$, $(6,6,4)$
$(1,2,2)$	$(5,5,6)$, $(6,5,5)$

Table 3.6: All pairs (u,v) for $(d,k,g) = (3,7,1)$

$(3,7)$-polytope with diameter 11 (see Figure 3.17), we conclude that $\delta(3,7) = 11$.

Considerations during Implementation

It should be emphasized that performing convex hull computations thousands of times has a significant impact on the algorithm performance. During the implementation, the convex hull subroutine was invoked only when it was strictly necessary.

When at least one of the vertices u, v is an inner point of the cube $[0,7]^3$, the execution time increases, due to the following two reasons.

- Assume that v is an inner point of the cube. The first reason is that the

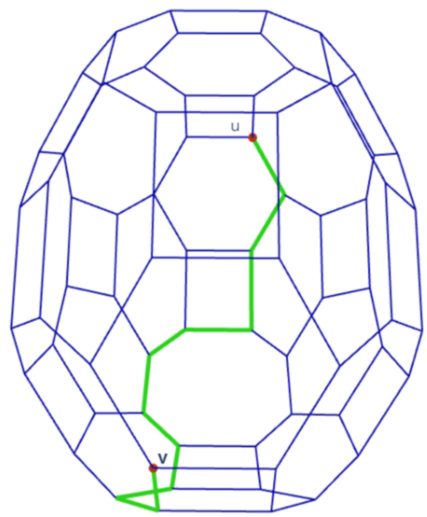

Figure 3.17: A lattice $(3,7)$-polytope of diameter 11 for $(u,v) = ((0,1,3),(7,6,4))$.

certificate 2 is evaluated every time the algorithm tries to embed a lattice $(2,7)$-polygon onto a facet of the cube. This is to determine if v is vertex of the convex cell of $\mathscr{C}^{\Gamma}_{d,k,g}$.

- Second reason, for each v_i equal to $k-1$, an attempt is made to connect via Γ with vertices of F_i^+, using the process described in the section 3.1.5.

Out of 91 pairs presented in Table 3.6, pair $(u,v) = ((1,1,2),(6,6,5))$ was the one that took by far the largest computational time to determine the shelling step output. During the preprocessing stage we determined that the points showed in Table 3.7 can not be vertices of a lattice (d,k)-polytope P for the pair $(u,v) = ((1,1,2),(6,6,5))$ as vertices. Table 3.7 presents these points organized according to the intersections with the cube $[0,7]^3$ for which they belong.

The first facet of the cube $[0,7]^3$ to intersect is F_1^-. We note from Table 3.7 that 7 points cannot be vertices, as a result there are 154 007 lattice $(2,7)$-polygons available to intersect. This gives us an idea about the search space size. If the second intersection with the cube $[0,7]^3$ to consider is F_2^+, similarly, we know beforehand which points can not be considered as vertices.

F	Points
F_1^-, F_2^-	$(0,0,0)$, $(0,0,1)$, $(0,0,2)$, $(0,0,3)$
F_1^-, F_3^-	$(0,1,0)$
F_1^-	$(0,1,1)$, $(0,1,2)$
F_2^-, F_3^-	$(1,0,0)$
F_2^-	$(1,0,1)$, $(1,0,2)$
F_1^+	$(7,6,5)$, $(7,6,6)$
F_1^+, F_3^+	$(7,6,7)$
F_1^+, F_2^+	$(7,7,4)$, $(7,7,5)$, $(7,7,6)$, $(7,7,7)$
F_2^+	$(6,7,5)$, $(6,7,6)$
F_2^+, F_3^+	$(6,7,7)$

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Table 3.7: Points for pair $(u,v) = ((1,1,2),(6,6,5))$ that can not be vertices for $(d,k,g) = (3,7,1)$.

3.3 Future Work

Further research can focus on how to exploit the problem $\min\{c \cdot x : x \in P\}$ and the integrality of coordinates of the search space to identify properties or patterns of lattice (d,k)-polytopes for higher dimensions and values of k equal to 4 or less. Such properties could allow to discover more results for introducing new certificates and identifying new faces of P and tightening the current upper bounds. The next two strategies, which are not exclusive, are proposed for further research:

- Considering values of $k \in 2,3,4$ and for $d \geq 4$, to try to identify new faces of P with the lowest possible number of embeddings.
- Given a fixed dimension d, to explore the search space in order to find more patterns for adding virtual weighted edges to Γ.

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