## COMPUTATIONAL DETERMINATION OF THE LARGEST LATTICE POLYTOPE DIAMETER

# COMPUTATIONAL DETERMINATION OF THE LARGEST LATTICE POLYTOPE DIAMETER 

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# TITLE: <br> Computational determination of the largest lattice polytope diameter 

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## Abstract

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

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## List of Abbreviations and Symbols

| $d$ | $:$ dimension |
| :--- | :--- |
| $k$ | $:$ size of grid embedding |
| $P$ | $:$ a polytope |
| $F$ | $:$ a face of a polytope $P$ |
| $u, v$ | $:$ vertices of a polytope $P$ |
| $d(u, v)$ | $:$ the distance between vertices $u$ and $v$ on the edge-graph of $P$ |
| $d(u, F)$ | $:$ the distance between vertex $u$ and face $F$ on the edge-graph of $P$ |
| $\delta(P)$ | $:$ the diameter of polytope $P$; that is the diameter of its edge-graph |
| $\delta(d, k)$ | $:$ the largest diameter achieved by a lattice $(d, k)$-polytope |
| $F_{i}^{0}$ | $:$ the intersection of $P$ with the facet of the $[0, k]^{d}$ cube corresponding to $x_{i}=0$ |
| $F_{i}^{k}$ | $:$ the intersection of $P$ with the facet of the $[0, k]^{d}$ cube corresponding to $x_{i}=k$ |
| $\mathcal{F}_{d-1, k}^{*}$ | $:$ set of lattice $(d-1, k)$-polytopes achieving $\delta(d-1, k)$ |
| $\mathcal{I}_{d-1, k}^{*}$ | $:$ set of integer valued points inside the convex hull of any element in the set $\mathcal{F}_{d-1, k}^{*}$ |
| $e^{i}$ | $:$ the $i$-th vector in the standard basis of $\mathbb{R}^{d}$ |

## Chapter 1

## Introduction

### 1.1 Background

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

The convex hull of integer-valued points is called a lattice polytope and if all the vertices are drawn from $\{0,1, \ldots, k\}^{d}$, it is referred to as a lattice $(d, k)$-polytope. Let $\delta(d, k)$ be the largest edge-diameter over all lattice $(d, k)$-polytopes. Naddef [8] showed in 1989 that $\delta(d, 1)=d$. Kleinschmidt and Onn [7] generalized this result in 1992 showing that $\delta(d, k) \leq k d$. In 2016, Del Pia and Michini [4] strengthened the upper bound to $\delta(d, k) \leq k d-\lceil d / 2\rceil$ for $k \geq 2$, and showed that $\delta(d, 2)=$ $\lfloor 3 d / 2\rfloor$. Pursuing Del Pia and Michini's approach, Deza and Pournin [6] showed that $\delta(d, k) \leq k d-\lceil 2 d / 3\rceil-(k-3)$ for $k \geq 3$, and that $\delta(4,3)=8$. The determination of
$\delta(2, k)$ was investigated independently in the early nineties by Thiele [9], Balog and Bárány [2], and Acketa and Žunić [1]. Investigating the lower bound on $\delta(d, k)$, Deza, Manoussakis, and Onn [5] introduced the primitive lattice polytope $H_{1}(d, p)$ as the Minkowski sum of the following set of lattice vectors: $\left\{v \in \mathbb{Z}^{d}:\|v\|_{1} \leq p, \operatorname{gcd}(v)=\right.$ $1, v \succ 0\}$, where $\operatorname{gcd}(v)$ is the largest integer dividing all the coordinates of $v$, and $v \succ 0$ when the first non-zero coordinate of $v$ is positive. They showed that, for any $k \leq 2 d-1$, there exists a subset of the generators of $H_{1}(d, 2)$ whose Minkowski sum is, up to translation, a lattice $(d, k)$-polytope with diameter $\lfloor(k+1) d / 2\rfloor$. As a consequence, they obtained the lower bound $\delta(d, k) \geq\lfloor(k+1) d / 2\rfloor$ for $k \leq 2 d-1$, and proposed Conjecture 1.1 .

Conjecture 1.1. $\delta(d, k) \leq\lfloor(k+1) d / 2\rfloor$, and $\delta(d, k)$ is achieved, up to translation, by a Minkowski sum of lattice vectors.

Note that Conjecture 1.1 holds for all known values of $\delta(d, k)$ given in Table 1.2, and hypothesizes, in particular, that $\delta(d, 3)=2 d$.

| $k$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 2 | 2 | 3 | 4 | 4 | 5 | 6 | 6 | 7 | 8 | 8 |
| 3 | 3 | 4 | 6 | $\mathbf{7}$ | $\mathbf{9}$ |  |  |  |  |  |
| 4 | 4 | 6 | 8 |  |  |  |  |  |  |  |
| $\vdots$ | $\vdots$ | $\vdots$ |  |  |  |  |  |  |  |  |
| $d$ | $d$ | $\left\lfloor\frac{3 d}{2}\right\rfloor$ |  |  |  |  |  |  |  |  |

Table 1.2: The largest possible diameter $\delta(d, k)$ of a lattice $(d, k)$-polytope.

We develop a computational framework to investigate Conjecture 1.1 for challenging instances. While convex hull determination is a theoretically intractable question, instances of reasonable $d$ and $k$ can be computed by exploiting combinatorial and geometric properties. We propose Theorem 1.2.

Theorem 1.2. Conjecture 1.1 holds for $(d, k)=(3,4)$ and $(3,5)$; that is, $\delta(3,4)=7$ and $\delta(3,5)=9$, and both diameters are achieved, up to translation, by a Minkowski sum of lattice vectors.

### 1.2 Thesis Outline

In chapter 2, we use combinatorial and geometric properties to demonstrate a set of conditions given by [6] which any lattice $(d, k)$-polytope $P$ must meet in order to achieve $\delta(P)=\delta(d-1, k)+k$. In chapter 3, we use the conditions from chapter 2 to propose a computational framework which drastically reduces the search space for lattice $(d, k)$-polytopes achieving a large diameter. Applying this framework to $(d, k)=(3,4)$ and $(3,5)$, we determine in chapter 4 that $\delta(3,4)=7$ and $\delta(3,5)=9$, proving Theorem 1.2, and propose future work.

## Chapter 2

## Theoretical Background

In this chapter, we provide a theoretical background on the tools used to prove the upper bound on $\delta(d, k)$ and use it to demonstrate a set of conditions given by [6] which a lattice $(d, k)$-polytope must meet in order to reach $\delta(P)=\delta(d-1, k)+k$.

Our proof borrows techniques used by [4] in their proof for the upper bound of $\delta(d, k) \leq k d-\lceil d / 2\rceil$ for $k \geq 2$. Their proof, as well as our own, relies on the ability to bound the distance from a vertex to a face of a lattice polytope by using integrality and convexity. We begin by restating a key lemma and its proof from [4] to give an intuition for how this is done.

Lemma 2.1. Let $P$ be a lattice polytope, and let $u$ be a vertex of $P$. Let $c$ be an integral vector, $\gamma=\min \{c x: x \in P\}$, and $F=\{x \in P: c x=\gamma\}$. Then $d(u, F) \leq c u-\gamma$.

Proof. We show that there exists a vertex $v$ of $F$ such that $d(u, v) \leq c u-\gamma$. We prove this statement by induction on the integer value $c u-\gamma \geq 0$. The statement is trivial for $c u-\gamma=0$, as we can set $v=u$. Assume $c u-\gamma \geq 1$. Since $F$ is nonempty, there exists a neighbor $u^{\prime}$ of $u$ with $c u^{\prime}<c u$. The integrality of $c, u^{\prime}$ and $u$, implies $c u^{\prime} \leq c u-1$. As
$c u^{\prime}-\gamma \leq c u-\gamma-1$, by the induction hypothesis there exists a vertex $v$ of $F$ such that $d\left(u^{\prime}, v\right) \leq c u^{\prime}-\gamma$. Therefore $d(u, v) \leq d\left(u, u^{\prime}\right)+d\left(u^{\prime}, v\right) \leq 1+c u^{\prime}-\gamma \leq c u-\gamma$. 4]

The intuition for Lemma 2.1 comes from linear programming. If we look at this as an linear optimization problem, $c$ is the vector direction in which we are minimizing, $P$ is the feasible region for the problem, $\gamma$ is the minimum value achieved, $u$ is the starting point, and points $x \in F$ are optimal. The distance $d(u, F)$ is the minimum number of simplex pivots required to reach an optimal solution from $u . F$ must be nonempty, as our feasible region is bounded and convex, but it could be a single point, a face, a facet, or the entire polytope depending on $c$. Note then the strength of the argument: we can bound the distance from any vertex $u \in P$ to any face $F$ of $P$ just by choosing the appropriate optimization direction $c$.

We can use Lemma 2.1 to bound the distance between two vertices by bounding the length of the path between them through a face. If $u$ and $v$ are vertices of a polytope $P$ and $F$ is a face of $P$, then $d(u, v) \leq d(u, F)+d(v, F)+\delta(F)$. Applying this with Lemma 2.1 gives us:

Lemma 2.2. Let $P$ be a lattice polytope, and let $u$, $v$ be vertices of $P$. Let $c$ be an integral vector, $\gamma=\min \{c x: x \in P\}$, and $F=\{x \in P: c x=\gamma\}$. Then $d(u, v) \leq \delta(F)+c u+c v-2 \gamma$. [4]

We demonstrate the strength of Lemma 2.2 in the following example:

Example 2.3. Let $P$ be a lattice (3,4)-polytope, $u=(0,1,0)$ and $v=(4,1,4)$. If we choose $c=(0,-1,0)$, we can say that in the worst case $\gamma=-4$ and $F=\{x \in$ $\left.P: x_{2}=4\right\}$. Applying Lemma 2.2, we get $d(u, v) \leq \delta(F)+c u+c v-2 \gamma \leq \delta(2,4)-$ $1-1+8=10$. However, if we choose $c=(0,1,0)$, then we can say in the worst case $\gamma=0$ and $F=\left\{x \in P: x_{2}=0\right\}$. Applying Lemma 2.2 in this case gives us $d(u, v) \leq \delta(F)+c u+c v-2 \gamma \leq \delta(2,4)+1+1-0=6$.

Because we can choose $c$, we can bound the distance from $u$ to $v$ through any face of $P$. In this example, from the second case, we can already say without knowing what the rest of $P$ looks like that no path from $u=(0,1,0)$ to $v=(4,1,4)$ could ever reach the upper bound diameter of $\delta(3,4)=8$. Note that this does not rely on $P$ having a face $F=\left\{x \in P: x_{2}=0\right\}$. Instead, if $F=\emptyset$, then $u$ and $v$ must be even closer, as $\gamma$ would be larger. This example should illustrate the idea that although $u$ and $v$ were far from one facet, it created a short path through the opposing facet. Intuitively, then, if $u$ and $v$ are the points achieving $d(u, v)=\delta(d-1, k)+k$, we would expect $u$ and $v$ to have a combined distance equally far from all facets so as to not create such a shortcut between them. This idea leads to 2 additional conditions which a lattice $(d, k)$-polytope $P$ achieving $\delta(P)=\delta(d-1, k)+k$ must meet:

Lemma 2.4. Let $P$ be a lattice ( $d, k$ )-polytope. If $P$ does not intersect every facet of the $[0, k]^{d}$ hypercube, then $\delta(P) \leq \delta(d-1, k)+k-1$. [4]

Lemma 2.5. Let $P$ be a lattice ( $d, k$ )-polytope, and let $u$ and $v$ be vertices of $P$ achieving $d(u, v)=\delta(d, k)$. If $u+v \neq(k, k, \ldots, k), \delta(P) \leq \delta(d-1, k)+k-1$. [4]

We now apply these lemmas to prove Theorem 2.6 .

Theorem 2.6. For $d \geq 3$, let $d(u, v)$ denote the distance between two vertices $u$ and $v$ in the edge-graph of a lattice $(d, k)$-polytope $P$ such that $d(u, v)=\delta(d, k)$. For $i=1, \ldots, d$, let $F_{i}^{0}$, respectively $F_{i}^{k}$, denote the intersection of $P$ with the facet of the cube $[0, k]^{d}$ corresponding to $x_{i}=0$, respectively $x_{i}=k$. Then, $d(u, v) \leq \delta(d-1, k)+k$, and the following conditions are necessary for the inequality to hold with equality:
(1) $u+v=(k, k, \ldots, k)$,
(2) any edge of $P$ with $u$ or $v$ as vertex is $\{-1,0,1\}$-valued,
(3) for $i=1, \ldots, d$, $F_{i}^{0}$, respectively $F_{i}^{k}$, is a $(d-1)$-dimensional face of $P$ with diameter $\delta\left(F_{i}^{0}\right)=\delta(d-1, k)$, respectively $\delta\left(F_{i}^{k}\right)=\delta(d-1, k)$.

Proof. We define here $e^{i}$ to be the $i$-th vector in the standard basis of $\mathbb{R}^{d}$.
Condition (1) : Trivially true by Lemma 2.5 .
Condition (2) : Assume $u$ and $v$ are the points achieving $d(u, v)=\delta(d-1, k)+k$ and that there is an edge from $u$ of length $>1$ in direction $i$. Because Condition (1) must hold, by integrality there is a point $u^{\prime}$ such that $d\left(u, u^{\prime}\right)=1$ and either $u_{i}^{\prime}+v_{i} \leq k-2$ or $u_{i}^{\prime}+v_{i} \geq k+2$. In the first case, applying Lemma 2.2 we can bound the distance from $u^{\prime}$ to $v$ through $F_{i}^{0}$ with $c=e^{i}$. This gives a bound of $d\left(u^{\prime}, v\right) \leq \delta(d-1, k)+k-2$. In the second case, applying Lemma 2.2 we can bound the distance from $F_{i}^{k}$ with $c=-e^{i}$, which also gives a bound of $d\left(u^{\prime}, v\right) \leq \delta(d-1, k)+k-2$. Then we can say that $d(u, v) \leq d\left(u, u^{\prime}\right)+d\left(u^{\prime}, v\right) \leq \delta(d-1, k)+k-1$. Then $d(u, v)<\delta(d-1, k)+k$. The same reasoning holds for $v$.

Condition (3) : Assume $P$ has a diameter $\delta(P)=\delta(d-1, k)+k$ and has a face $F_{i}^{0}$ which is not a $(d-1)$-dimensional face with diameter $\delta\left(F_{i}^{0}\right)=\delta(d-1, k)$. By Lemma 2.4. $F_{i}^{0}$ must exist, else $\delta(P) \leq(d-1, k)+k-1$. Let $u$ and $v$ be the points of $P$ achieving $d(u, v)=\delta(P)$. Since Condition (1) must hold, $u+v=(k, k, \ldots, k)$. We can bound the distance from $u$ to $v$ by their path through $F_{i}^{0}$. Applying Lemma 2.2 with $c=e^{i}$, we get the bound $d(u, v) \leq \delta\left(F_{i}^{0}\right)+k$. But if $\delta\left(F_{i}^{0}\right)<\delta(d-1, k)$, this gives us $d(u, v) \leq \delta(d-1, k)+k-1$. Therefore $\delta(P)<\delta(d-1, k)+k$. The same proof holds for $F_{i}^{k}$ with $c=-e^{i}$.

## Chapter 3

## Computational Framework

In this chapter, we propose a computational framework to significantly decrease the search space to compute $\delta(d, k)$ for reasonable values of $d$ and $k$. We give a high level outline of the algorithm and then look at each step in detail, using $(d, k)=(3,4)$ and $(3,5)$ to illustrate each step.

Since $\delta(2, k)$ and $\delta(d, 2)$ are known, we consider in the remainder of the paper that $d \geq 3$ and $k \geq 3$. While the number of lattice $(d, k)$-lattice polytopes is finite, a brute force search is typically intractable, even for small instances. Consider the smallest unknown case, $\delta(3,4)$. As a combinatorial optimization problem, there are $5^{3}$ points to choose from, where each point is either included or not in the optimal solution. This means that complete enumeration would require $2^{125}$ convex hull computations and as many all-pairs shortest path computations to determine the largest diameter achieved. Both of these are known to be very expensive operations, making this computation far too inefficient to be practical. However, consider the known bounds on $\delta(3,4)$ and $\delta(3,5)$ :

$$
7 \leq \delta(3,4) \leq 8
$$

$$
9 \leq \delta(3,5) \leq 10
$$

In each case, there is a known Minkowski sum of lattice vectors achieving the lower bound, and a theoretical upper bound of $\delta(d, k)=\delta(d-1, k)+k$ which has not been ruled out. Thus, in either case, determining the maximum diameter only requires checking those lattice polytopes which could theoretically achieve a diameter of $\delta(P)=$ $\delta(d-1, k)+k$. If no polytope is found reaching this bound for either, then Theorem 1.2 has been shown to be true. With this in mind, recall the conditions in Theorem 2.6 which a lattice $(d, k)$-polytope must meet in order to achieve a diameter of $\delta(P)=$ $\delta(d-1, k)+k:$
(1) $u+v=(k, k, \ldots, k)$,
(2) any edge of $P$ with $u$ or $v$ as vertex is $\{-1,0,1\}$-valued,
(3) for $i=1, \ldots, d, F_{i}^{0}$, respectively $F_{i}^{k}$, is a $(d-1)$-dimensional face of $P$ with diameter $\delta\left(F_{i}^{0}\right)=\delta(d-1, k)$, respectively $\delta\left(F_{i}^{k}\right)=\delta(d-1, k)$.

Thus, to show that $\delta(d, k)<\delta(d-1, k)+k$, it is enough to show that there is no lattice $(d, k)$-polytope admitting a pair of vertices $(u, v)$ such that $d(u, v)=\delta(d, k)$ and the conditions (1), (2), and (3) are satisfied. The computational framework to determine, given $(d, k)$, whether $\delta(d, k)=\delta(d-1, k)+k$ is outlined in Algorithm 3.1,

```
Algorithm 3.1 Algorithm to determine whether \(\delta(d, k)<\delta(d-1, k)+k\)
Step 1: Initialization
Determine the set \(\mathcal{F}_{d-1, k}^{*}\) of all the lattice \((d-1, k)\)-polytopes \(P\) such that
\(\delta(P)=\delta(d-1, k)\).
```

Step 2: Symmetries
Determine, up to the symmetries of the cube $[0, k]^{d}$, the possible entries for a pair of vertices $(u, v)$ such that $u+v=\{k, k, \ldots, k\}$.

Step 3: Shelling
For each of the possible pairs $(u, v)$ determined during Step 2, consider all possible ways for $2 d$ elements of the set $\mathcal{F}_{d-1, k}^{*}$ determined during Step 1 to form the $2 d$ facets of $P$ lying on a facet of the cube $[0, k]^{d}$.

Step 4: Inner points
For each choice of $2 d$ elements of $\mathcal{F}_{d-1, k}^{*}$ forming a shelling obtained during Step 3 , consider each of the $\{1,2, \ldots, k-1\}$-valued points not in the convex hull of the vertices forming the shelling. Determine every possible lattice polytope that can be generated with the inclusion or exclusion of each of these as vertices.

For the remainder of the chapter, we will look at each of the 4 steps of Algorithm 3.1 in detail using $(d, k)=(3,4)$ and $(3,5)$ as an example.

### 3.1 Step 1: Initialization

Determine the set $\mathcal{F}_{d-1, k}^{*}$ of all the lattice $(d-1, k)$-polytopes $P$ such that $\delta(P)=$ $\delta(d-1, k)$.

For the cases we are considering, this means computing every lattice $(2,4)$-polytope with a diameter of 4 and every lattice (2,5)-polytope with a diameter of 5. 2dimensional convex hull computations are relatively inexpensive, so we form this as a branch and bound combinatorial optimization problem. We formulate a binary decision tree where each branch represents the decision of either adding or not adding the point at that depth.

Though there are $2^{25}$ different combinations of points in $[0,4]^{2}$ and $2^{36}$ in $[0,5]^{2}$, there are orders of magnitude fewer unique polytopes, with the convex hull of many different combinations of points achieving the same polytope. We speed up the computation by only seeking the combination where each point added represents a vertex in the polytope. To do this, we compute the convex hull every time a point is added by the decision tree. If any of the points is strictly inside the convex hull, then one of the points added will not be a vertex of the polytope, so we can prune the branch. We then only need to compute the diameter of each of the leaves of the tree that are reached.

At this stage, we may also compute the set $\mathcal{I}_{d-1, k}^{*}$, the integer valued points in the intersection of the convex hulls of elements in the set $\mathcal{F}_{d-1, k}^{*}$. In this way, we can determine any points which must be inside the convex hull of any facet of $\mathcal{F}_{d-1, k}^{*}$. If the set $\mathcal{I}_{d-1, k}^{*}$ is nonempty, then we may remove points from consideration as vertices at this stage, as the midpoint of 2 points inside the convex hull cannot be a vertex of a convex polytope.

### 3.2 Step 2: Symmetries

Determine, up to the symmetries of the cube $[0, k]^{d}$, the possible entries for a pair of vertices $(u, v)$ such that $u+v=\{k, k, \ldots, k\}$.

Considering the points $(0,0,1),(0,1,0)$, and $(1,0,0)$, it is easy to see that these points could all be treated as equivalent within some rotation of the $[0, k]^{3}$ cube. With this in mind, we only want to select $(u, v)$ pairs such that $u+v=\{k, k, \ldots, k\}$ which are all mutually distinct within symmetries of the cube. This condition on $(u, v)$ does not just give a pair of vertices which must be included in a polytope achieving $\delta(P)=\delta(d-1, k)+k$, but also that it is the distance from $u$ to $v$ that achieves $\delta(P)$ if $\delta(P)=\delta(d-1, k)+k$. Thus when generating these polytopes, we need not compute all pairs shortest paths for each polytope, but rather the single source shortest path from $u$ to $v$. We give here tables of possible vertex pairs which cover all distinct $(u, v)$ possibilities within the symmetries of the cube for $(d, k)=(3,4)$ and $(3,5)$.

| $u$ | $v$ |
| :---: | :---: |
| $(0,0,0)$ | $(4,4,4)$ |
| $(0,0,1)$ | $(4,4,3)$ |
| $(0,0,2)$ | $(4,4,2)$ |
| $(0,1,1)$ | $(4,3,3)$ |
| $(0,1,2)$ | $(4,3,2)$ |
| $(0,2,2)$ | $(4,2,2)$ |
| $(1,1,1)$ | $(3,3,3)$ |
| $(1,1,2)$ | $(3,3,2)$ |
| $(1,2,2)$ | $(3,2,2)$ |

Table 3.1: Vertex pairs for $(d, k)=(3,4)$

| $u$ | $v$ |
| :---: | :---: |
| $(0,0,0)$ | $(5,5,5)$ |
| $(0,0,1)$ | $(5,5,4)$ |
| $(0,0,2)$ | $(5,5,3)$ |
| $(0,1,1)$ | $(5,4,4)$ |
| $(0,1,2)$ | $(5,4,3)$ |
| $(0,2,2)$ | $(5,3,3)$ |
| $(1,1,1)$ | $(4,4,4)$ |
| $(1,1,2)$ | $(4,4,3)$ |
| $(1,2,2)$ | $(4,3,3)$ |
| $(2,2,2)$ | $(3,3,3)$ |

Table 3.2: Vertex pairs for $(d, k)=(3,5)$

### 3.3 Step 3: Shelling

For each of the possible pairs $(u, v)$ determined during Step 2, consider all possible ways for $2 d$ elements of the set $\mathcal{F}_{d-1, k}^{*}$ determined during Step 1 to form the $2 d$ facets of $P$ lying on a facet of the cube $[0, k]^{d}$.

While this would appear to generate $\left|\mathcal{F}_{d-1, k}^{*}\right|^{2 d}$ different possible shellings, there are several rules applied in this step which combat the exponential nature of this step of the algorithm:

## Rule 1: Mutually exclusive facets

Let $F_{i}$ and $F_{j}$ be facets of the $[0, k]^{d}$ hypercube, and let the edge $E=F_{i} \cap F_{j}$. When constructing a shelling to form a lattice polytope, if an element of $\mathcal{F}_{d-1, k}^{*}$ has already been selected for $F_{i}$, then an element of $\mathcal{F}_{d-1, k}^{*}$ may only be selected for $F_{j}$ if $\forall x \in E$ : x is a vertex of $F_{i} \Longleftrightarrow \mathrm{x}$ is a vertex of $F_{j}$.

## Rule 2: Shortcut through facets

This rule only applies when dealing with $(u, v)$ pairs which fall on the shelling of the polytope. It contains 2 parts:
i) If a facet is chosen from $\mathcal{F}_{d-1, k}^{*}$ which would give an edge of length $>1$ from $u$ or $v$, it can immediately be excluded by Condition (2) of Theorem 2.6.
ii) Let $u$ and $v$ be vertices of a lattice $(d, k)$-polytope $P$ such that $d(u, v)=\delta(P)$. Let $u^{\prime}$ and $v^{\prime}$ be two vertices in the same facet $F$ of $P$ such that $u^{\prime}$ also shares a facet with $u$ and $v^{\prime}$ also shares a facet with $v$. From Lemma 2.2 and Lemma 2.5 we know that $d\left(u, u^{\prime}\right)+d\left(v, v^{\prime}\right) \leq k$, and $d\left(u^{\prime}, v^{\prime}\right) \leq \delta(F)=\delta(d-1, k)$. If a path connects $u^{\prime}$ to $v^{\prime}$ with $d\left(u^{\prime}, v^{\prime}\right) \leq \delta(F)-1$, then $d(u, v) \leq \delta(d-1, k)+k-1$. If this is the case, then there exists a path from $u$ to $v$ in $P$ of length at most $\delta(d-1, k)+k-1$, so
$\delta(P)<\delta(d-1, k)+k$. Using this property, when a facet is added, shortest paths are computed from all vertices sharing a facet with $u$ to all vertices sharing a facet with $v$. If a path is discovered of distance $<\delta(d-1, k)$, then there is a short path from $u$ to $v$ through the polytope, so the facet should not be considered here and is removed.

Rule 3: Wide shelling excluding $u$ or $v$
This rule only applies when dealing with $(u, v)$ pairs which fall inside the shelling of the polytope. For such a pair, given the large size of the facets in $\mathcal{F}_{d-1, k}^{*}$, it is easy to see that trying to form a shelling of these facets is likely to create a shape in which $u$ and $v$ are strictly inside of the convex hull and not able to be vertices. To make efficient use of this, facets are added in the ordering $F_{1}^{0}, F_{1}^{k}, \ldots, F_{d}^{0}, F_{d}^{k}$. Every time 2 opposing facets are added to the shelling, the convex hull of the partial shelling is computed to see if $u$ or $v$ are inside the convex hull of the shape, and if so, the most recently added facet is removed.

### 3.4 Step 4: InNer points

For each choice of $2 d$ elements of $\mathcal{F}_{d-1, k}^{*}$ forming a shelling obtained during Step 3, consider each of the $\{1,2, \ldots, k-1\}$-valued points not in the convex hull of the vertices forming the shelling. Determine every possible lattice polytope that can be generated with the inclusion or exclusion of each of these as vertices.

Each $\{1,2, \ldots, k-1\}$-valued point must first be checked to see if it lies inside the convex hull of the shelling. If $\mathcal{I}_{d-1, k}^{*}$ is nonempty, some of these points will already have been determined to be inside the convex hull. To determine the rest of the $\{1,2, \ldots, k-1\}$ valued points, they are considered one by one, and a convex hull computation is required to determine if they are inside or outside the convex hull of the shelling. For reasonably small $k$, very few of the points will be outside the convex hull of the shelling, due to the size of the elements of $\mathcal{F}_{d-1, k}^{*}$. Each $\{1,2, \ldots, k-1\}$ valued point not in the convex hull is considered as a potential vertex of $P$ in a binary tree.

A convex hull and diameter computation are performed for each node of the obtained binary tree. If there is a node yielding a diameter of $\delta(d-1, k)+k$ we can conclude that $\delta(d, k)=\delta(d-1, k)+k$. Otherwise, we can conclude that $\delta(d, k)<\delta(d-1, k)+k$.

## Chapter 4

## Computational Results

In this chapter, we discuss the results of applying our computational framework to solve for $(d, k)=(3,4)$ and $(3,5)$, and potential strategies to extend the algorithm to solve for higher values of $d$ and $k$.
$4.1 \quad \delta(3,4)$

Step 1: We find 335 lattice (2,4)-polytopes with the maximum edge-diameter of 4. This number seems large, but when we consider that $\delta(2,4)=\delta(2,3)$, it makes sense that so many more polytopes can be formed in the larger box by extending edges and performing shifts in the grid to achieve the same diameter. We find that $\mathcal{I}_{2,4}^{*}=\{(1,2),(2,1),(3,2),(2,3),(2,2)\}$. From this we know that any $(*, 2,2)$-valued point or any $(*, 1,2)$-valued point, and their equivalent up to symmetry of the cube, is inside the convex hull of any shelling formed from elements in $\mathcal{F}_{2,4}^{*}$.

Step 2: We find the $9(u, v)$ pairs which are not equivalent by any symmetry given
in Table 3.1. We find 6 of these pairs lie on the exterior of the $[0,4]^{3}$ cube, and 3 lie strictly inside. Of these, we can immediately eliminate $u=\{(0,2,2),(1,1,2),(1,2,2)\}$ from consideration based on $\mathcal{I}_{2,4}^{*}$.

Step 3: A total of 7 full shellings are found, all from $(u, v)$ pairs which were on the outside of the $[0,4]^{3}$ cube. All other cases for these $(u, v)$ pairs were rapidly eliminated by finding short paths from facets containing $u$ to facets containing $v$. For the $u=(1,1,1), v=(3,3,3)$, we found that nearly all cases were able to be eliminated as soon as 2 opposing facets were in place. We are able to speed this part of the computation up slightly by noting that any facet containing the point $(0,0,0)$ or $(4,4,4)$ cannot be added based on convexity with $u$ and $v$. While these convex hull computations are cheaper than a full shelling, the requirement of nearly $\left|\mathcal{F}_{2,4}^{*}\right|^{2}$ made this part of the computation by far the most expensive.

Step 4: Of each of the shellings that were produced by Step 3, we found that none of the $\{1,2,3\}$-valued points were outside the convex hull of the shelling. Each of the 7 shellings consisted of some orientation of the same polytope, which is composed of the unique facet achieving $\delta(2,3)$ on all 6 sides (see Figure 4.1). Computing the convex hull, we find this shape has a diameter of 7 . We can then conclude that $\delta(3,4)<8$. Since the Minkowski sum of $(1,0,0),(0,1,0),(0,0,1),(0,1,1),(1,0,1),(1,1,0)$, and $(1,1,1)$ forms a lattice (3,4)-polytope with diameter 7 (see Figure 4.2), as does the polytope generated by the shellings we found, we conclude that $\delta(3,4)=7$. A summary of the computation for $(d, k)=(3,4)$ is given in Table 4.1.
total facets achieving $\delta(2,4): 335$

| $u$ | candidate facets for $u$ | full shellings found | convex hull computations |
| :---: | :---: | :---: | :---: |
| $(0,0,0)$ | 0 | 0 | 0 |
| $(0,0,1)$ | 9 | 1 | 9 |
| $(0,1,1)$ | 85 | 2 | 18 |
| $(0,0,2)$ | 8 | 2 | 18 |
| $(0,1,2)$ | 10 | 2 | 18 |
| $(1,1,1)$ | 297 | 0 | 94462 |

maximum diameter found : 7
total convex hull computations in dimension 3: 94525
Table 4.1: Computational results for $(d, k)=(3,4)$

## $4.2 \quad \delta(3,5)$

Step 1: We find 92 lattice $(2,5)$-polytopes belonging to the set $\mathcal{F}_{2,5}^{*}$. Compared to $(d, k)=(3,4)$, this means there are actually fewer possible shellings that need to be considered, despite the larger original search space. In the case of $(d, k)=(3,4)$, so many optimal facets were found because $\delta(2,4)=\delta(2,3)$, but we find less here because $\delta(2,5)>\delta(2,4)$. We find that $\mathcal{I}_{2,5}^{*}=\{(2,2),(2,3),(3,2),(3,3)\}$. We also find that none of the elements in $\mathcal{I}_{2,5}^{*}$ is a vertex for any element in $\mathcal{F}_{2,5}^{*}$. From this, we know that, up to symmetry of the cube, any ( $*, 2,2$ )-valued point is strictly inside the convex hull of any shelling formed from elements in $\mathcal{F}_{2,5}^{*}$.

Step 2: We find the $10(u, v)$ pairs which are not equivalent by any symmetry given in Table 3.2. We find 6 of these pairs lie on the exterior of the $[0,5]^{3}$ cube, and 4 lie strictly inside. Of these, we can immediately eliminate $u=\{(0,2,2),(1,2,2),(2,2,2)\}$ from consideration based on $\mathcal{I}_{2,5}^{*}$

Step 3: We find no full shellings which are not excluded by any of the pruning rules. In the cases of $(u, v)$ pairs where $u$ and $v$ lie on the outside of the $[0,5]^{3}$ cube, a short
total facets achieving $\delta(2,5): 92$

| $u$ | candidate facets for $u$ | full shellings found | convex hull computations |
| :---: | :---: | :---: | :---: |
| $(0,0,0)$ | 0 | 0 | 0 |
| $(0,0,1)$ | 1 | 0 | 0 |
| $(0,1,1)$ | 47 | 0 | 0 |
| $(0,0,2)$ | 1 | 0 | 0 |
| $(0,1,2)$ | 3 | 0 | 0 |
| $(1,1,1)$ | 91 | 0 | 8355 |
| $(1,1,2)$ | 92 |  | 8465 |

maximum diameter found : 0
total convex hull computations in dimension 3: 16820
Table 4.2: Computational results for $(d, k)=(3,5)$
path is able to be found through some facet before any shelling can be constructed, as all facets in $\mathcal{F}_{2,5}^{*}$ have vertices on at least 3 of the edges of a $[0,5]^{2}$ box. In the cases where $u$ and $v$ lie inside the cube, the large facets in $\mathcal{F}_{2,5}^{*}$ consistently create partial shellings for which $u$ or $v$ is strictly inside the convex hull.

Step 4: Because there are no shellings which make it through Step 3 of the algorithm, this step is never reached. From this we can conclude that no lattice $(3,5)$-polytope has a diameter of 10 , and since the Minkowski sum of $(1,0,0),(0,1,0),(0,0,1)$, $(0,1,1),(1,0,1),(1,1,0),(0,1,-1),(1,0,-1)$, and $(1,-1,0)$ forms, up to translation, a lattice $(3,5)$-polytope with diameter 9 (see Figure4.3), we conclude that $\delta(3,5)=9$. It is worth noting that this Minkowski sum is a truncated cuboctahedron, which is a well studied polyhedron named by Kepler. A summary of the computation for $(d, k)=(3,5)$ is given in Table 4.2.


Figure 4.1: Convex hull of shelling found achieving $\delta(3,4)=7$

### 4.3 Future Work

Computations for additional values of $\delta(d, k)$ are currently underway. In particular, the same algorithm may determine whether $\delta(d, k)=\delta(d-1, k)+k$ or $\delta(d-1, k)+k-1$ for $(d, k)=(5,3)$ and $(4,4)$ provided the set of all lattice $(d-1, k)$-polytopes achieving $\delta(d-1, k)$ is determined for $(d, k)=(5,3)$ and $(4,4)$. Similarly, the algorithm could be adapted to determine whether $\delta(d, k)<\delta(d-1, k)+k-1$ provided the set of all lattice $(d-1, k)$-polytopes achieving $\delta(d-1, k)$ or $\delta(d-1, k)-1$ is determined. For example, the adapted algorithm may determine whether $\delta(3,6)=10$.


Figure 4.2: Minkowski sum achieving $\delta(3,4)=7$


Figure 4.3: Minkowski sum, up to translation, achieving $\delta(3,5)=9$

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