Size bounds and classification results for integral polyhedra with at most one interior integral point

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Zusammenfassung

Gegenstand der vorliegenden Dissertationsschrift sind ganzzahlige Polyeder, welche höchstens einen ganzzahligen Punkt in ihrem Inneren enthalten. Dabei nennen wir Polyeder ohne ganzzahlige Punkte im Innern gitterpunktfrei. Motiviert durch mögliche Anwendungen in der gemischt-ganzzahligen Optimierung liegt die Aufmerksamkeit in erster Linie auf ganzzahligen gitterpunktfreien Polyedern.

In der gemischt-ganzzahligen Optimierung geht es darum, ein lineares Optimierungsproblem unter zusätzlichen Ganzzahligkeitsbedingungen an einen Teil der Variablen zu lösen. Viele Probleme aus der Industrie lassen sich als solche gemischt-ganzzahlige lineare Probleme formulieren. Ein weit verbreiteter Ansatz ist, zunächst das lineare Optimierungsproblem ohne Berücksichtigung der Ganzzahligkeitsbedingungen zu lösen. Erfüllt die auf diese Weise gefundene Lösung die Ganzzahligkeitsbedingungen nicht, so sucht man eine lineare Ungleichung, die für die gefundene Lösung nicht erfüllt ist, aber gültig ist für alle zulässigen Punkte, welche die Ganzzahligkeitsbedingungen erfüllen. Eine solche Ungleichung nennt man einen Schnitt, da das Hinzufügen dieser Ungleichung zur Beschreibung des zugrunde liegenden linearen Problems die gefundene, nicht zulässige Lösung abschneidet. Nun wiederholt man obiges Vorgehen für das durch Hinzufügen der Ungleichung entstandene lineare Problem, bis man idealerweise eine Lösung erhält, welche die Ganzzahligkeitsbedingungen erfüllt.

Die Frage, wie man solche Schnitte systematisch generiert, ist seit den 1960er Jahren Gegenstand der Forschung. Seit der grundlegenden Arbeit von Balas (1971) ist bekannt, dass sich gitterpunktfreie Polyeder zum Generieren von Schnitten verwenden lassen. Eine besondere Rolle kommt dabei den inklusionsmaximalen gitterpunktfreien ganzzahligen Polyedern zu, also denjenigen, welche nicht echt in einem anderen gitterpunktfreien ganzzahligen Polyeder enthalten sind. Solche Polyeder nennen wir $\mathbb{Z}^d$-maximal. Zum einen generieren solche Polyeder unter allen ganzzahligen gitterpunktfreien Polyedern die stärksten Schnitte. Zum anderen ist die Klasse dieser Polyeder in gegebener Dimension bis auf Äquivalenz bzgl. gittererhaltender affiner Transformationen endlich. Außerdem lässt sich jedes unbeschränkte gitterpunktfreie ganzzahlige Polyeder auf ein gitterpunktfreies ganzzahliges Polytop (d.h. beschränktes Polyeder) niedrigerer Dimension zurückführen. Dies lässt darauf hoffen, dass diese Klasse von Polyedern sich zukünftig tatsächlich zur Entwicklung eines Schnittebenenverfahrens zur Lösung gemischt-ganzzahliger Optimierungsprobleme verwenden lässt.

Die Schwierigkeit besteht allerdings darin, dass über die Klasse der $\mathbb{Z}^d$-maximalen gitterpunktfreien ganzzahligen Polyeder wenig bekannt ist. So war bislang nur in den Dimensionen eins und zwei eine vollständige Klassifizierung dieser Klasse bekannt. Eine stärkere Eigenschaft als $\mathbb{Z}^d$-Maximalität ist die folgende: wir nennen ein gitterpunktfreies Polyeder $\mathbb{R}^d$-maximal, wenn es nicht echt in irgendeiner gitterpunktfreien konvexen Menge enthalten ist. Offenbar ist jedes $\mathbb{R}^d$-maximale gitterpunktfreie ganzzahlige Polyeder auch $\mathbb{Z}^d$-maximal. Die Frage, für welche Dimensionen d auch die Umkehrung gilt, ist besonders aus dem Grund interessant, weil die Eigenschaften von $\mathbb{R}^d$-Maximalität gut zu charakterisieren sind. Dass diese Äquivalenz für $d \geq 4$ nicht gilt, zeigten Nill und Ziegler (2011). Für $d = 3$ dagegen wurden alle $\mathbb{R}^3$-maximalen gitterpunktfreien ganzzahligen Polyeder von Averkov, Wagner und Weismantel (2011) klassifiziert. Hätte man also die Äquivalenz von $\mathbb{R}^3$-Maximalität und $\mathbb{Z}^3$-Maximalität, so erhielte man daraus direkt eine Klassifikation aller $\mathbb{Z}^3$-maximalen gitterpunktfreien ganzzahligen Polyeder in Dimension drei.

In dieser Dissertationsschrift wird gezeigt, dass die Äquivalenz von $\mathbb{Z}^3$-Maximalität

und $\mathbb{R}^3$-Maximalität tatsächlich gilt. Betrachtet man statt ganzzahligen Polyedern rationale Polyeder, so lässt sich folgende verallgemeinerte Frage stellen: für welche natürlichen Zahlen s, d gilt, dass jedes $\mathbb{Z}^d$-maximale Polyeder, welches in $\frac{1}{s}\mathbb{Z}^d$ erzeugt ist, auch $\mathbb{R}^d$-maximal ist? Diese Frage wird ebenfalls vollständig beantwortet.

In höheren Dimensionen scheint eine vollständige Klassifizierung $\mathbb{Z}^d$-maximaler gitterpunktfreier ganzzahliger Polyeder momentan noch in weiter Ferne zu sein. Um mehr über die Struktur dieser Klasse in höheren Dimensionen in Erfahrung zu bringen, konzentriert man sich auf Polytope in dieser Klasse und untersucht Parameter, welche die Größe dieser Polytope beschreiben. Ein solcher Parameter ist der Gitterdurchmesser eines $\mathbb{Z}^d$-maximalen gitterpunktfreien ganzzahligen Polytops der Dimension d. Kennt man diesen, folgt daraus auch direkt eine Schranke an die Zahl der ganzzahligen Punkte des Polytops. Eine obere Schranke an den Gitterdurchmesser kann man dadurch erhalten, dass man für einen ganzzahligen Simplex S der Dimension $d - 1$ mit genau einem inneren ganzzahligen Punkt x eine obere Schranke an den Asymmetriekoeffizienten von S bzgl. x nachweist. Hensley hat 1983 eine erste obere Schranke an den Asymmetriekoeffizienten von S bzgl. x bewiesen. Darüber hinaus stellte er eine Vermutung auf, wie groß dieser Asymmetriekoeffizient für gegebenes d tatsächlich höchstens sein kann und gab eine Familie von Simplizes an, für welche diese Schranke auch angenommen wird. Die von Hensley bewiesene obere Schranke an den Asymmetriekoeffizienten war allerdings von der von ihm vermuteten Schranke noch weit entfernt. In der Zwischenzeit konnte die Lücke zwischen bester bekannter Schranke und vermuteter Schranke bzw. größtem bekannten Beispiel zwar verringert, aber nicht geschlossen werden.

In dieser Arbeit wird Hensleys Vermutung bestätigt. Mit den Methoden, welche im Beweis dieser Aussage verwendet werden, lassen sich aber eine ganze Reihe weiterer Eigenschaften von Simplizes (und in einigen Fällen allgemeiner Polytope) mit genau einem inneren ganzzahligen Punkt nachweisen. Daher enthält diese Arbeit außerdem für solche Simplizes Schranken an das Volumen des Simplex und das Volumen seiner Seitenflächen sowie, unter der Annahme, dass der innere ganzzahlige Punkt der Ursprung ist, an das Mahlervolumen sowie das Volumen des Dualen. Wo immer möglich, wurden auch die Simplizes charakterisiert, für welche diese Schranken tatsächlich angenommen werden. Ferner wird gezeigt, dass die Schranke an den Asymmetriekoeffizienten auch für allgemeine ganzzahlige Polytope mit genau einem inneren ganzzahligen Punkt gilt. Abschließend wird dann aus der Schranke an den Asymmetriekoeffizienten eine Schranke an den Gitterdurchmesser $\mathbb{Z}^d$-maximaler gitterpunktfreier ganzzahliger Polytope (tatsächlich wird nur eine etwas schwächere Maximalitätsvoraussetzung verwendet) bewiesen und ebenfalls gezeigt, dass diese Schranke angenommen wird.

Summary

The subject of this thesis is the analysis of integral polyhedra with at most one interior integral point. Polyhedra with no interior integral points are called lattice-free. The interest in integral lattice-free polyhedra is motivated by applications in mixed-integer optimization.

A mixed-integer linear optimization problem is a linear optimization problem with additional integrality constraints on some of the variables. Many problems arising from industrial applications can be formulated as mixed-integer linear optimization problems. A well-known approach to solving such problems is the following. First, one solves the linear programme without considering the integrality constraints. If the solution found in this way does not fulfil the integrality constraints, one wants to find a linear inequality which is violated by this solution but satisfied by all feasible points of the linear programme fulfilling the integrality constraints. Since adding such an inequality to the formulation of the underlying linear programme cuts off the previous solution, we call such an inequality a cut. One can now repeat this process for the new linear programme, hoping to eventually find a solution which fulfils the integrality constraints. The development of algorithms generating cuts has been a research topic since the 1960s. In particular, it has been known that lattice-free polyhedra can be used for cut generation since the seminal work of Balas (1971). Among lattice-free polyhedra there is a particular focus on $\mathbb{Z}^d$-maximal lattice-free integral polyhedra, i.e. those polyhedra which are not properly contained in another lattice-free integral polyhedron. The reason for the focus on this class is that on the one hand these polyhedra generate the strongest cuts among all integral lattice-free polyhedra. On the other hand, for fixed dimension, this class is finite up to lattice-preserving affine transformations. Additionally, every unbounded lattice-free integral polyhedron can be constructed as the direct product of an affine space and an integral lattice-free polytope of lower dimension. These properties suggest that the class of $\mathbb{Z}^d$-maximal lattice-free integral polyhedra could be used in future cutting-plane methods for mixed-integer linear optimization problems.

The drawback is that there is very little known about this class. In fact, a full classification has so far been available only for dimensions one and two. We introduce the following stronger maximality property: a lattice-free polyhedron is said to be $\mathbb{R}^d$-maximal if it is not properly contained in a lattice-free convex set. It is obvious that this condition is indeed stronger and that every $\mathbb{R}^d$-maximal lattice-free integral polyhedron is also $\mathbb{Z}^d$-maximal. Since the properties of $\mathbb{R}^d$-maximal polyhedra can be characterized in a relatively simple way, one is interested to know for which dimensions d the reverse assertion is also true, i.e. for which dimension d every $\mathbb{Z}^d$-maximal lattice-free integral polyhedron is also $\mathbb{R}^d$-maximal. It was shown by Nill and Ziegler (2011) that this does not hold for $d \geq 4$. The case of $d = 3$, on the other hand, is of particular interest as there exists a full classification of $\mathbb{R}^3$-maximal lattice-free integral polyhedra due to Averkov, Wagner and Weismantel (2011). Thus, if one could show the equivalence of $\mathbb{R}^3$-maximality and $\mathbb{Z}^3$-maximality for integral polyhedra of dimension three, this would immediately yield a full classification of $\mathbb{Z}^3$-maximal integral polyhedra.

One of the main results of this thesis is that this equivalence does indeed hold. Furthermore, the following generalization for rational polyhedra is discussed: for which values of d and s is every $\mathbb{Z}^d$-maximal polytope which is generated within $\frac{1}{s}\mathbb{Z}^d$ also $\mathbb{R}^d$-maximal? A complete list of all such pairs d, s is also given in this thesis.

Since in higher dimensions a full classification of $\mathbb{Z}^d$-maximal lattice-free integral polyhedra seems to be beyond reach at the moment, it is necessary to understand more

about the structure of the elements of this class. Focusing on polytopes, one is therefore interested in analyzing parameters describing their size. One such parameter is the lattice diameter. An upper bound on the lattice diameter of a $\mathbb{Z}^d$-maximal lattice-free integral polytope can be derived by providing an upper bound for the coefficient of asymmetry of an integral simplex S of dimension $d-1$ about its only interior integral point x. In 1983, Hensley proved a first upper bound on the coefficient of asymmetry of S about x. Moreover, he conjectured what the sharp bound should be and named a family of simplices for which his conjectured bound is indeed attained. However, there was a significant gap between his upper bound and the bound he conjectured. In the meantime, improvements to Hensley's upper bound have been made, none of which fully closed the gap to the conjectured bound.

In this thesis, it is confirmed that Hensley's conjecture is indeed true. As a natural consequence of the methods used in the proof of this statement, several other properties of simplices (and in some cases, arbitrary polytopes) with precisely one interior integral point are also analyzed. More precisely, this thesis contains bounds on the volume and the volume of the faces of such a simplex as well as, assuming the origin to be the interior integral point, on the Mahler volume and the volume of the dual of the simplex. Where possible, the simplices for which the bounds are attained are characterized. Furthermore, it is shown that the bound on the coefficient of asymmetry remains valid for arbitrary integral polytopes with precisely one interior integral point. Finally, from the bound on the coefficient of asymmetry, the aforementioned bound on the lattice diameter of $\mathbb{Z}^d$-maximal lattice-free integral polytopes (in fact, a slightly weaker maximality assumption is used) is proved and the polytopes for which this bound is attained are characterized.

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It goes without saying that without the help and support of numerous people this thesis could not have been written.

In fact, all the results presented in this thesis were obtained during two different collaborations, one of which, with Gennadiy Averkov and Benjamin Nill, yielded the results published in [AKN15], while the results of the other, with Gennadiy Averkov and Stefan Weltge, have not yet been published. I am very thankful to all three of them for giving me the permission to use our results in this thesis.

To my supervisor Gennadiy Averkov I am deeply indebted on several accounts: for introducing me to the subjects of this thesis and pointing out the interesting research questions with which my studies were then concerned; for guiding me expertly throughout my research on these questions, sharing plenty of invaluable advice in the process; for the many, many hours spent discussing mathematical details of the topics I have been working on; and for numerous comments on how to structure and present mathematical facts in the best possible way.

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Contents

Chapter 1

Background and results

Introduction

The original aim of the research project leading to this thesis was to investigate properties of *lattice-free* integral polyhedra, i.e. integral polyhedra[1] which contain no integral points in their interiors. A polyhedron is called *integral* if it coincides with the convex hull of its integral points. In particular, applications in mixed-integer optimization outlined in recent publications had raised interest in lattice-free integral polyhedra satisfying certain maximality conditions. During the research on those polyhedra, a second class of polyhedra came into focus, which proved to be useful for the analysis of lattice-free polytopes: integral simplices with precisely one interior integral point. As a consequence, an in-depth analysis of these polytopes was also conducted.

Therefore, this thesis is concerned with two main subjects: results on lattice-free integral polyhedra and results on integral polytopes with one interior integral point. I wish to point out that the results on the former topic presented in this thesis were obtained during joint work with Gennadiy Averkov and Stefan Weltge, while the contributions regarding the second topic are the result of joint work with Gennadiy Averkov and Benjamin Nill. The results of the latter collaboration have been published in [AKN15]. More precisely, [AKN15] contains Chapter 3 as well as Section 1.4 and most of the content of Section 1.3 of this thesis. A manuscript containing the results of the collaboration with Gennadiy Averkov and Stefan Weltge ([AKW15]) has been submitted for publication and is available online as a preprint. This manuscript forms the basis of Chapter 2 and Section 1.2.

The introduction is structured as follows: in the following section, the motivation for analyzing lattice-free sets in general and integral lattice-free polytopes with maximality properties in particular will be outlined and an overview of existing results will be given. The new results on this topic are then presented. Next, a link between lattice-free integral polytopes and integral simplices with one interior integral point is described, motivating our interest in the latter class of polytopes. Previous research on this topic is highlighted and connections to other fields of research are outlined, before the new contributions made in [AKN15] are given. The chapter is completed by providing definitions and notation used in the remainder of this thesis.

[1] In the introduction, familiarity of the reader with standard terminology from polyhedra theory, optimization, convex geometry and the geometry of numbers is assumed.

1.1 Lattice-free polyhedra in mixed-integer optimization

The theory of linear optimization is concerned with the following general problem: to find the minimal value of a linear objective function $c^\top x$, where c is a given vector with n rational entries and x is the vector of variables $x_1, \dots, x_n$, such that x satisfies a set of given linear constraints. This set of constraints can be expressed by $Ax \leq b$, where A is a rational matrix A of size $m \times n$, with m being the number of constraints, and b is a rational vector with m entries. The system $Ax \leq b$ describes a polyhedron $P = \{x \in \mathbb{R}^n : Ax \leq b\}$ in dimension n. For the avoidance of degenerate cases we will assume that P is non-empty and bounded, i.e. P is a polytope.

Therefore, we can formulate the *linear optimization problem* (short: LP) as follows:

$$\text{minimize} \qquad c^\top x \qquad \text{s. t.} \qquad x \in P. \tag{1.1}$$

Since P is non-empty and bounded, the optimal value of the objective function is attained in a vertex of P. A well-known method to solve a linear optimization problem which makes use of this fact is the *simplex method* first introduced by Dantzig [Dan51]. While it is not within the scope of this thesis to elaborate further on how the simplex method works, it should be pointed out that the simplex method can be implemented in such a way that it is guaranteed to terminate, yielding the optimal solution of an LP. Furthermore, while there are examples of LPs where the running time of the simplex method is exponential in m, it turns out that in practice, for most LPs the running time is polynomial in m.

We now switch our focus to mixed-integer linear optimization problems. A *mixed-integer linear optimization problem* (short MILP) is a linear optimization problem with additional integrality constraints on some of the variables. In the following, we always assume the variables to be ordered in such a way that the integrally constrained variables are the first d variables, i.e. $x_1, \dots, x_d$, for some $d \in \{1, \dots, n\}$. Note that in the special case $d = n$, our optimization problem is in fact an *integer linear optimization problem* (ILP). An MILP which has the same linear constraints $Ax \leq b$ as (1.1) and additional integrality constrains on the first d variables can be written as

$$\text{minimize} \qquad c^\top x \qquad \text{s. t.} \qquad x \in P \cap (\mathbb{Z}^d \times \mathbb{R}^{n-d}). \tag{1.2}$$

Equivalently, one can formulate this as

$$\text{minimize} \qquad c^\top x \qquad \text{s. t.} \qquad x \in P_{MI}, \tag{1.3}$$

where

$$P_{MI} := \operatorname{conv}\left(P \cap (\mathbb{Z}^n \times \mathbb{R}^{d-n})\right).$$

We call P_{MI} the *mixed-integer hull* of P. Then P_{MI} is a rational polyhedron (see [Sch86, §16.7]) with the property that all of its vertices are feasible solutions of the MILP. Therefore, if one had a description of P_{MI} by means of linear inequalities, one could formulate the MILP as LP. In particular, this would enable us to solve the MILP using methods of linear optimization, e.g. the simplex method.

The problem is that an inequality description of P_{MI} can usually not be derived immediately from the inequality description of P. An approach to the solution of this problem are the so-called *cutting-plane* methods, the foundations for which were laid in the fundamental work of Gomory [Gom58, Gom63]. The gist of cutting-plane methods is the following: first, solve the linear optimization problem (1.1) to obtain an optimal solution x^*. If $x^* \in \mathbb{Z}^d \times \mathbb{R}^{n-d}$, this is also an optimal solution of (1.2). If not, we want to determine a rational vector $\alpha \in \mathbb{R}^n$ and a rational number β such that the inequality

$\alpha^\top x \leq \beta$ is violated for x^* but is valid for every $x \in P_{MI}$. Adding the inequality $\alpha^\top x \leq \beta$ to the inequality description $Ax \leq b$ of P therefore cuts off the optimal solution x^* of (1.1). We call an inequality which is valid for P_{MI} a *cut*. For the ILP case, i.e. $d = n$, cuts can be generated from an inequality $a^\top x \leq b$ with $a \in \mathbb{Z}^n$ which is valid for P and fulfilled with equality for x^* (i.e. $a^\top x^* = b$) by rounding down the right hand side b to the nearest integer. These cuts constitute the so-called *Gomory cuts*. The theoretical framework for Gomory cuts was established by Chvátal [Chv73] and Schrijver [Sch80]: let H be a halfspace given by $H = \{x \in \mathbb{R}^n : \gamma^\top x \leq \delta\}$, where $\gamma \in \mathbb{Q}^n$ and $\delta \in \mathbb{Q}$, and set $H_I := \{x \in \mathbb{R}^n : \gamma^\top x \leq \lfloor \delta \rfloor\}$. Then we call $C_{\mathrm{CG}} := \bigcap_{H \supseteq P} H_I$ the *Chvátal-Gomory closure* of P. The Chvátal-Gomory closure of a rational polyhedron is again a polyhedron (see [Sch86, §23.1]). Furthermore, let $C^0_{\mathrm{CG}}(P) := P$ and $C^i_{\mathrm{CG}}(P) := C_{\mathrm{CG}}(C^{i-1}_{\mathrm{CG}}(P))$ for $i \in \mathbb{N}$. Then there exists some $k \in \mathbb{N} \cup \{0\}$ such that $C^k_{\mathrm{CG}} = P_{MI}$ (see [Sch86, §23.2]). In other words, by taking the closure finitely many times, i.e. $C_{\mathrm{CG}}(P), C_{\mathrm{CG}}(C_{\mathrm{CG}}(P)), \ldots$ one obtains the integer hull of P, thus making Gomory cuts a very powerful tool in the ILP case.

In the general mixed-integer case, i.e. (1.2) with $d \leq n$, it is obvious that the Gomory cuts as introduced before are not necessarily valid for all points of P_{MI}. Several ways to generate cuts in the mixed-integer case have been introduced in the literature; see e.g. [BCC93], [Gom60], [NW90] and [CKS90]. For a detailed survey of the different types of cuts, see [MMWW02]. The downside is that there is no finitely converging cutting-plane algorithm based only on cuts of one of those types; see again [MMWW02]. In recent literature, however, cuts generated by lattice-free polyhedra have come into focus as a possible solution for the development of a finitely converging cutting plane algorithm for the MILP case. We say that a d-dimensional convex set in $\mathbb{R}^d$ is *lattice-free* if it does not contain any points of $\mathbb{Z}^d$ in its interior. In principle, it is known since the seminal work of Balas [Bal71] that lattice-free polyhedra can be used to generate cuts for the MILP (for a more direct link between lattice-free sets and disjunctive cuts of Balas, we refer to [Del12]). The basic idea behind this is as follows: let $L \subseteq \mathbb{R}^d$ be a lattice-free convex set. Then $\mathbb{Z}^d \subseteq \mathbb{R}^d \setminus \mathrm{int}(L)$ and hence, $P_{MI} \subseteq P \setminus (\mathrm{int}(L) \times \mathbb{R}^{n-d})$. Therefore, every half-space H satisfying $P \setminus (\mathrm{int}(L) \times \mathbb{R}^{n-d}) \subseteq H$ yields a cut in the sense that $P_{MI} \subseteq P \cap H$. We call a half-space H satisfying this, or more precisely an inequality describing it, a *lattice-free cut* generated by the lattice-free convex set L.

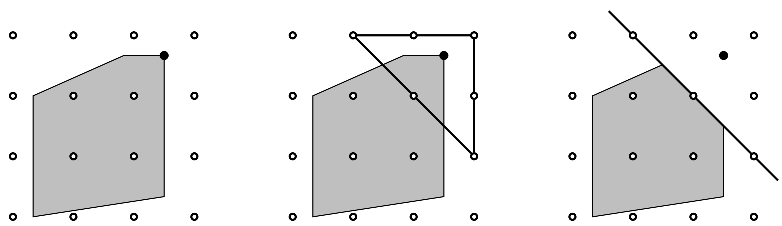

Figure 1.1: Using a lattice-free set to generate a cut in an ILP. The optimal solution of minimizing $-x_1 - x_2$ over the polygon P shaded in grey is non-integral (left). The lattice-free triangle (middle) contains this optimal solution in its interior and thus generates a cut which separates it from the feasible integral points (right).

We point out that the cuts introduced in [CKS90], which were mentioned above, are the so-called *split cuts*, which are a special case of lattice-free cuts. A *split* is the lattice-free convex set obtained by taking the convex hull of two parallel lattice hyperplanes. However, it was shown in [CKS90, Example 2] that there is no finitely converging cutting-plane algorithm using only split cuts. On the other hand, if one instead considers *all* lattice-free sets for generating cuts, one can even show the following correspondence between valid inequalities for P_{MI} and lattice-free convex sets: if $\alpha x \leq \beta$ is an inequality (with rational vector α and rational number β) which is valid for P_{MI}, then there exists a rational lattice-free polyhedron $L \subseteq \mathbb{R}^d$ such that $\alpha x \leq \beta$ is valid for the closed convex hull[2] of $P \setminus \operatorname{int}(L \times \mathbb{R}^{n-d})$; see [Jör08, Lemma 3.5] and [CCZ10]. As a consequence, one obtains that P_{MI} can be written as

$$P_{MI} = \bigcap_{L \in \mathcal{L}} \overline{\operatorname{conv}}\Big(P \setminus \operatorname{int}(L \times \mathbb{R}^{n-d})\Big), \tag{1.4}$$

where $\mathcal{L}$ denotes the set of all rational lattice-free convex sets in $\mathbb{R}^d$ and $\overline{\operatorname{conv}}$ is short for closed convex hull; see [DW12b, p. 10]. There is a major drawback to this type of results, of course: the family of general rational lattice-free convex sets is infinite. Hence, one cannot expect to make any practical use of this result. One important observation, by which one can reduce the class of polyhedra which need to be considered, is that if L, L' are lattice-free convex sets with $L' \subseteq L$, then $P \setminus (\operatorname{int}(L) \times \mathbb{R}^{n-d}) \subseteq P \setminus (\operatorname{int}(L') \times \mathbb{R}^{n-d})$. As a consequence, for generating cuts it suffices to consider only those lattice-free convex sets which are not properly included in another lattice-free set.

This leads to the following definition of maximality introduced by Lovász in [Lov89]: according to Lovász, a lattice-free convex subset of $\mathbb{R}^d$ is called *maximal* if this set cannot be extended to a strictly larger lattice free set by adding points of $\mathbb{R}^d$, i.e., is not properly contained in another lattice-free subset of $\mathbb{R}^d$. Maximal lattice-free convex sets have several favourable properties, which we will outline in the next theorem. Proofs of this result can be found in [Ave13] and [BCCZ10]. For this theorem we need the notion of *unimodular equivalence*: we call an affine transformation $\phi\colon \mathbb{R}^d \to \mathbb{R}^d$ with the property $\phi(\mathbb{Z}^d) = \mathbb{Z}^d$ a *unimodular* transformation and two sets $X, Y \subseteq \mathbb{R}^d$ are said to be unimodularly equivalent (short: $X \simeq Y$) if there exists a unimodular map $\phi\colon \mathbb{R}^d \to \mathbb{R}^d$ such that $\phi(X) = Y$.

Theorem 1.1 ([Lov89, §3]). *Let $d \in \mathbb{N}$ and let L be a d-dimensional maximal lattice-free convex set. Then, the following statements hold:*

(a) The set L is a polyhedron with at most 2^d facets.

(b) If L is unbounded, then there exists a $k \in \{1, \dots, d-1\}$ such that L is unimodularly equivalent to $L' \times \mathbb{R}^k$, where $L' \subseteq \mathbb{R}^{d-k}$ is a bounded maximal lattice-free set.

(c) Every facet of L contains a point of $\mathbb{Z}^d$ in its relative interior.

From a mixed-integer optimization viewpoint, the favourable properties of maximal lattice-free convex sets therefore are the following: first, in view of assertion (a), instead of arbitrary convex sets one can focus on cuts derived from lattice-free polyhedra. Furthermore, in view of assertion (b), it suffices to employ cuts derived from (lower-dimensional) bounded polyhedra, i.e. polytopes. Assertion (c) gives rise to the following definition: we call a facet F of a polyhedron L *blocked* if $\operatorname{relint}(F) \cap \mathbb{Z}^d \neq \emptyset$. It is easy to see that one can use this notion to give a rather simple characterization of the property of maximality: a d-dimensional lattice-free set L is maximal lattice-free if and only if it is a polyhedron with the property that each of its facets is blocked. However, for practical purposes, one would want to have some form of finiteness of the class of polytopes to consider. Since unimodular transformations maintain the properties of convex sets with regard to their integral points (e.g. lattice-freeness and structure of integral points in the boundary), it

[2]The closed convex hull of a set $X \subseteq \mathbb{R}^d$ is the closure of the convex hull of X, for a precise definition see [Roc97].

seems reasonable to aim for replacing the set $\mathcal{L}$ in (1.4) by some set which is finite up to unimodular equivalence. Since there are infinitely many maximal lattice-free convex sets in $\mathbb{R}^d$, even up to unimodular transformations, this class does not appear to be useful for the potential development of cutting-plane algorithms.

As a consequence, one is interested in other families of lattice-free polyhedra which generate strong cuts but might be of more practical use. One class that has been studied in the literature is a class of all lattice-free integral polyhedra that fulfil a weaker maximality condition which we introduce now. In what follows, we will call maximality in the sense of Lovász $\mathbb{R}^d$-*maximality*. Accordingly, for a subset X of $\mathbb{R}^d$, we will say that a lattice-free set L is X-*maximal* if for every $x \in X \setminus L$, the set $\operatorname{conv}(L \cup \{x\})$ is not lattice-free. Furthermore, for a subset Y of $\mathbb{R}^d$, we say that a polyhedron P is a Y-polyhedron if P is generated within the set Y, i.e. if $P = \operatorname{conv}(P \cap Y)$ holds. By $\mathcal{P}(Y)$ we denote the set of all Y-polyhedra. In particular, $\mathcal{P}(\mathbb{Z}^d)$ are the integral polyhedra in $\mathbb{R}^d$, while the elements of $\mathcal{P}(\frac{1}{2}\mathbb{Z}^d)$ are called *half-integral*. We will now consider the class of all $\mathbb{Z}^d$-maximal lattice-free polyhedra in $\mathcal{P}(\mathbb{Z}^d)$. By definition, such a polyhedron is not properly contained in another lattice-free polyhedron in $\mathcal{P}(\mathbb{Z}^d)$. Therefore, among the class of integral polytopes, the $\mathbb{Z}^d$-maximal ones generate the strongest cuts. The following theorem collects some important properties of this class.

Theorem 1.2 ([AWW11],[NZ11]). *Let $d \in \mathbb{N}$. Then, the following statements hold:*

(a) Let $P \in \mathcal{P}(\mathbb{Z}^d)$ be lattice-free. Then there exists a $\mathbb{Z}^d$-maximal lattice-free polyhedron $L \in \mathcal{P}(\mathbb{Z}^d)$ such that $P \subseteq L$.

(b) Every unbounded $\mathbb{Z}^d$-maximal lattice-free polyhedron $P \in \mathcal{P}(\mathbb{Z}^d)$ is unimodularly equivalent to a polyhedron of the form $P' \times \mathbb{R}^k$, where $1 \le k \le d-1$ and P' is a $\mathbb{Z}^{d-k}$-maximal lattice-free polytope in $\mathcal{P}(\mathbb{Z}^{d-k})$.

(c) Up to unimodular equivalence, there exist only finitely many $\mathbb{Z}^d$-maximal lattice-free polyhedra in $\mathcal{P}(\mathbb{Z}^d)$.

Let us now consider only cuts derived from the family of $\mathbb{Z}^d$-maximal lattice-free integral polyhedra and denote by $C_{\mathrm{IL}}(P)$ the *integral lattice-free closure* of P, which is defined as the set of points in P satisfying every cut derived from a $\mathbb{Z}^d$-maximal lattice-free integral polyhedron. It was shown in [DW12a, Theorem 3] that $C_{\mathrm{IL}}(P)$ is again a polyhedron. Analogously to the ILP case, we set $C^0_{\mathrm{IL}}(P) = P$ and $C^j_{\mathrm{IL}}(P) = C_{\mathrm{IL}}(C^{j-1}_{\mathrm{IL}}(P))$ for $j \ge 1$. In [DW12a, Theorem 4] it was shown that there exists some $k \in \mathbb{N} \cup \{0\}$ such that $C^k_{\mathrm{IL}}(P) = P_{MI}$. On the other hand, it was shown in [Del12] that in order to guarantee convergence, one cannot omit any of the $\mathbb{Z}^d$-maximal lattice-free integral polyhedra in $\mathbb{R}^d$ in the definition of the lattice-free integral closure.

Motivated by the possibility of devising a mixed-integer cutting-plane algorithm with the help of $\mathbb{Z}^d$-maximal lattice-free integral polyhedra, one is interested in characterizing the family of those polyhedra. Previously to our results presented here, a full classification of $\mathbb{Z}^d$-maximal lattice-free integral polyhedra was known only for dimensions one and two. Among other contributions, this thesis contains a full classification of $\mathbb{Z}^3$-maximal lattice-free integral polyhedra in dimension three, which will be given in the next section.

It should be pointed out that even though lattice-free integral polyhedra promise to be helpful objects for devising cutting-plane methods in mixed integer optimization, this thesis is concerned solely with the theoretical analysis of these (and related) polyhedra. No computational aspects are discussed. In fact, to the best of my knowledge, a way to use the convergence result cited above has not yet been found. To do so, one would have to decide three questions for a given optimal solution x^* of our LP (1.1) which is not feasible for (1.2): which lattice-free integral polyhedron L to use for generating a cut, which position to choose for this polyhedron (i.e. which unimodular transformation φ to apply to a polyhedron chosen from the finite list of lattice-free integral polyhedra) and finally, how to efficiently determine an inequality describing a cut obtained from given $\varphi(L)$. None of these questions is discussed in this thesis. Instead, we focus purely on trying to characterize the geometrical properties of lattice-free integral polyhedra.

This section is closed by remarking that interest in lattice-free (integral) polyhedra is not restricted to the motivation outlined above. Even in cutting-plane theory, there is another link to lattice-free integral polyhedra, as they appear as extremal examples for the *reverse Chvátal-Gomory rank*, or reverse CG rank for short. Let $Q \subseteq \mathbb{R}^d$ be an integral polyhedron and for a polyhedron $Q' \subseteq \mathbb{R}^d$ such that $Q = \operatorname{conv}(Q' \cap \mathbb{Z}^d)$, denote by $r(Q')$ the minimal number k such that $C^k_{\mathrm{CG}}(Q') = Q$ (see above). Then the reverse Chvátal-Gomory rank of Q is

$$r^*(Q) = \sup\left\{ r(Q') \,:\, Q \text{ is a polyhedron in } \mathbb{R}^d \text{ s.t. } Q = \operatorname{conv}(Q' \cap \mathbb{Z}^d)\right\}.$$

It was shown in [CDD+13, Theorem 1] that $r^*(Q) = +\infty$ if and only if Q belongs to a special class of lattice-free polyhedra. For more information on this topic, see [CDD+13] and [ACD+13]. Applications of lattice-free polyhedra can also be found in algebraic geometry; see, for instance, [Seb99], [BN07], [MS84] and [BBBK11].

1.2 New results on $\mathbb{Z}^d$-maximal polyhedra

$\mathbb{Z}^3$-maximal integral polyhedra in dimension three

It is obvious that every $\mathbb{R}^d$-maximal lattice-free set is also $\mathbb{Z}^d$-maximal. The converse is not true in general: see Figure 1.2 for an illustration of the notions of $\mathbb{R}^d$-maximality and $\mathbb{Z}^d$-maximality.

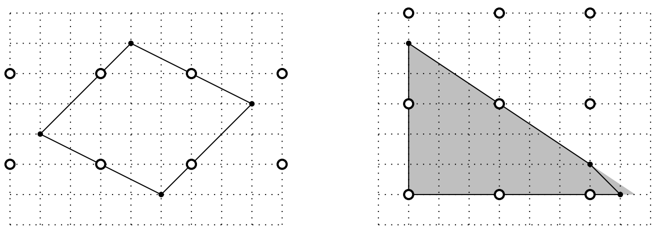

Figure 1.2: Two $\frac{1}{3}\mathbb{Z}^2$-polygons: the one on the left is $\mathbb{R}^2$-maximal and $\mathbb{Z}^2$-maximal; the one on the right is $\mathbb{Z}^2$-maximal but not $\mathbb{R}^2$-maximal since it is properly contained in the lattice-free polygon shaded in grey.

The geometry of $\mathbb{Z}^d$-maximal lattice-free polyhedra is less well understood than that of $\mathbb{R}^d$-maximal lattice-free ones. In particular, there is no characterization of $\mathbb{Z}^d$-maximality known which is comparable to the characterization of $\mathbb{R}^d$-maximality via blocked facets. This leads to the following challenge in the study of $\mathbb{Z}^d$-maximal lattice-free sets: while it is possible to decide whether a given d-dimensional polyhedron is $\mathbb{R}^d$-maximal if the dimension d is not too large (by solving several linear integer optimization problems of relatively small size to check for integral points in the relative interior of the facets), it is much more difficult to decide whether a given polyhedron is $\mathbb{Z}^d$-maximal. As a consequence, carrying out a classification of $\mathbb{Z}^d$-maximal lattice-free polyhedra turns out to be a very challenging task. As mentioned above, a complete classification of $\mathbb{Z}^d$-maximal polyhedra in $\mathcal{P}(\mathbb{Z}^d)$ previously existed only for $d = 1, 2$ (and is straightforward to obtain in these cases). As it turns out, the $\mathbb{Z}^d$-maximal polytopes in dimensions one and two are exactly the $\mathbb{R}^d$-maximal ones. This raises the following question: for which dimensions d is every $\mathbb{Z}^d$-maximal integral polyhedron also $\mathbb{R}^d$-maximal? In other words, for which dimensions would a classification of $\mathbb{R}^d$-maximal integral polyhedra also provide a classification of $\mathbb{Z}^d$-maximal integral polyhedra? It was shown in [NZ11, Theorem 3.2] that there exist $\mathbb{Z}^d$-maximal integral polyhedra which are not $\mathbb{R}^d$-maximal for every $d \geq 4$. For $d = 3$, however, the equivalence of $\mathbb{Z}^3$-maximality and $\mathbb{R}^3$-maximality was an open question; see [NZ11, Question 1.5] and also [Wag11, Section 7.4]. The following theorem provides an answer to this question.

Theorem 1.3 (Equivalence of maximality notions for lattice-free polyhedra in $\mathcal{P}(\mathbb{Z}^3)$). *Let $P \in \mathcal{P}(\mathbb{Z}^3)$ be a lattice-free polyhedron. Then, P is $\mathbb{Z}^3$-maximal if and only if P is $\mathbb{R}^3$-maximal.*

This theorem is of particular interest since for $\mathbb{R}^3$-maximal polyhedra in $\mathcal{P}(\mathbb{Z}^3)$ a complete classification was achieved in [AWW11]; see also [Tre08], [Tre10]. In view of this classification, Theorem 1.3 also provides a complete classification of $\mathbb{Z}^3$-maximal lattice-free polyhedra $P \in \mathcal{P}(\mathbb{Z}^3)$, where part (a) of the following corollary is a consequence of Theorem 1.2 (b) and the well-known classification of $\mathbb{Z}^d$-maximal elements of $\mathcal{P}(\mathbb{Z}^d)$ for $d \in \{1, 2\}$.

Corollary 1.4 (Classification of $\mathbb{Z}^3$-maximal lattice-free polyhedra in $\mathcal{P}(\mathbb{Z}^3)$). *Let $P \in \mathcal{P}(\mathbb{Z}^3)$ be $\mathbb{Z}^3$-maximal lattice-free. Then, the following statements hold:*

(a) If P is unbounded, then P is unimodularly equivalent to $[0, 1]\times\mathbb{R}^2$ *or to* $\operatorname{conv}(o, 2e_1, 2e_2)\times\mathbb{R}$.

(b) If P is bounded, then P is unimodularly equivalent to one of the following twelve polytopes:

- *the simplex* $\operatorname{conv}(-2e_1, 4e_1, e_1 + 3e_2, 2e_3)$,
- *the simplex* $\operatorname{conv}(o, 4e_1, 4e_2, 2e_3)$,
- *the simplex* $\operatorname{conv}(-e_1 + e_2, e_1 + 3e_2, 2e_3, 2e_1 - 2e_2 + 2e_3)$,
- *the simplex* $\operatorname{conv}(-e_1, 3e_1, e_1 + 4e_2, 2e_3)$,
- *the pyramid* $\operatorname{conv}(\pm 2e_1, \pm 2e_2, 2e_3)$,
- *the prism* $\operatorname{conv}(e_1, 3e_1, 2e_1 + 2e_2, 2e_3, 2e_1 + 2e_3, e_1 + 2e_2 + 2e_3)$,
- *the parallelepiped* $\operatorname{conv}(o, -e_1 + e_2, 2e_2, e_1 + e_2, 2e_3, e_1 + e_2 + 2e_3, 2e_1 + 2e_3, e_1 - e_2 + 2e_3)$,
- *the simplex* $\operatorname{conv}(o, 3e_1, 3e_2, 3e_3)$,
- *the simplex* $\operatorname{conv}(o, e_3, 5e_2 + 2e_3, 5e_1 + 3e_3)$,
- *the simplex* $\operatorname{conv}(o, e_1 + 3e_2, 3e_1, 2e_1 + 3e_3)$,
- *the pyramid* $\operatorname{conv}(-e_1, -e_2, 2e_1, 2e_2, e_1 + e_2 + 3e_3)$,
- *the prism* $\operatorname{conv}(-e_1, 2e_1, e_2, e_1 - e_2, e_1 + 2e_2 + 3e_3, 3e_1 + e_2 + 3e_3)$.

The twelve polytopes of Corollary 1.4(b) are depicted in Figures 1.3 and 1.4.

$\mathbb{Z}^d$-maximal lattice-free polyhedra in $\mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$

During the proof of Theorem 1.3, another, more general question arose. It turns out that in order to classify $\mathbb{Z}^3$-maximal lattice-free polytopes in $\mathcal{P}(\mathbb{Z}^3)$, we need a classification of $\mathbb{Z}^2$-maximal lattice-free polytopes in $\mathcal{P}(\frac{1}{2}\mathbb{Z}^2)$. More precisely, polytopes of this kind appear as hyperplane cross-sections of $\mathbb{Z}^3$-maximal lattice-free polytopes having lattice width two with certain hyperplanes (see also Figure 1.3: the intersections in question

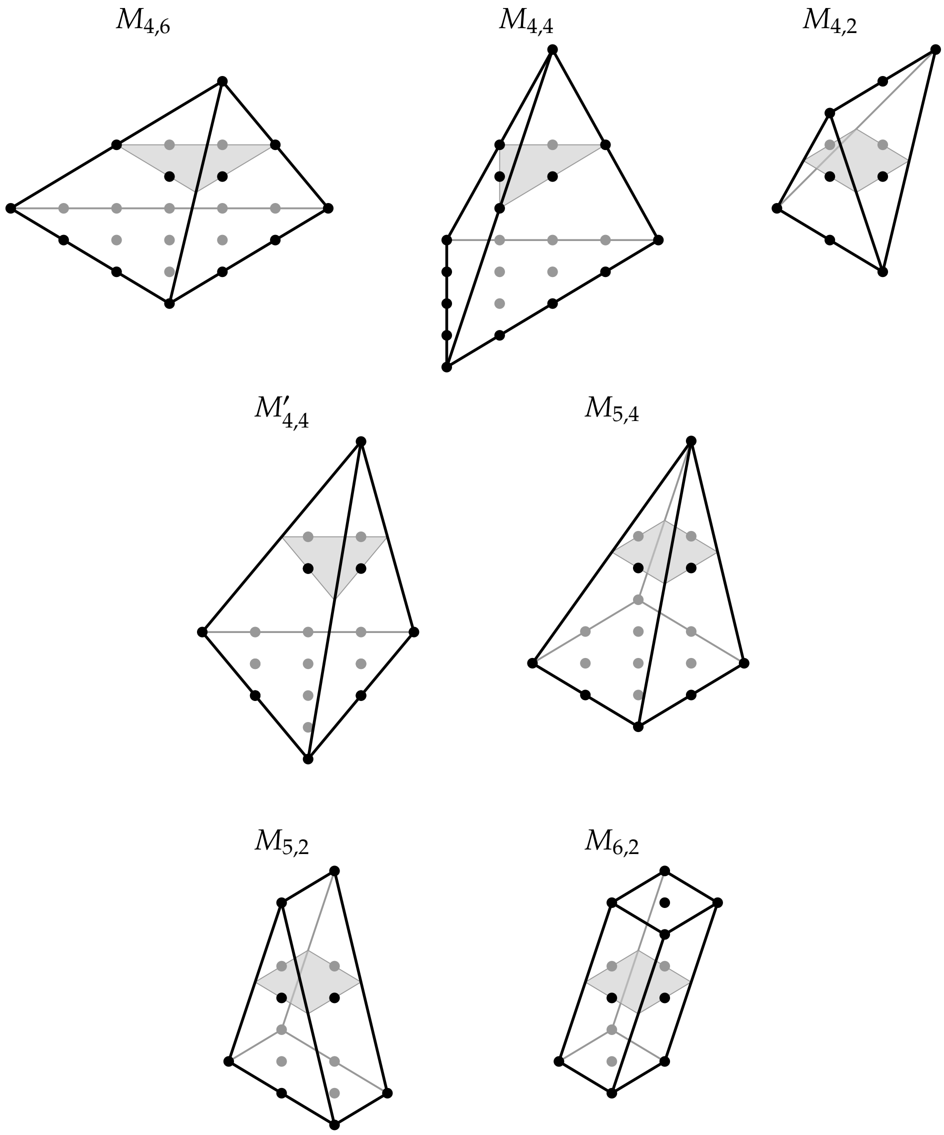

Figure 1.3: The $\mathbb{Z}^3$-maximal $\mathbb{Z}^3$-polytopes with lattice width two. For further reference, the polytopes have been labeled by a pair of indices (i, j), where i is the number of facets and j the lattice diameter.

are shaded in grey). Likewise, one can observe that $\mathbb{Z}^2$-maximal lattice-free polytopes in $\mathcal{P}(\frac{1}{3}\mathbb{Z}^2)$ appear as hyperplane cross-sections of $\mathbb{Z}^3$-maximal lattice-free polytopes with lattice width three (see also Figure 1.4: these cross-sections are again shaded in grey). We therefore extended our analysis as follows: for a fixed pair $(d, s) \in \mathbb{N}^2$, we want to know whether every $\mathbb{Z}^d$-maximal lattice-free polyhedron in $\mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$ is also $\mathbb{R}^d$-maximal. To my best knowledge, these polyhedra have not been studied in the literature, but a similar class of polyhedra has: the set of all $\frac{1}{s}\mathbb{Z}^d$-maximal lattice-free polyhedra in $\mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$ for a fixed pair d, s. This family could be interpreted as a 'discretized' version of Lovász's notion of maximality, as here $\mathbb{R}^d$ is replaced by $\frac{1}{s}\mathbb{Z}^d$. In a sense, the class of convex lattice-free sets is therefore 'sampled' by rational polyhedra and s denotes the 'precision' of those

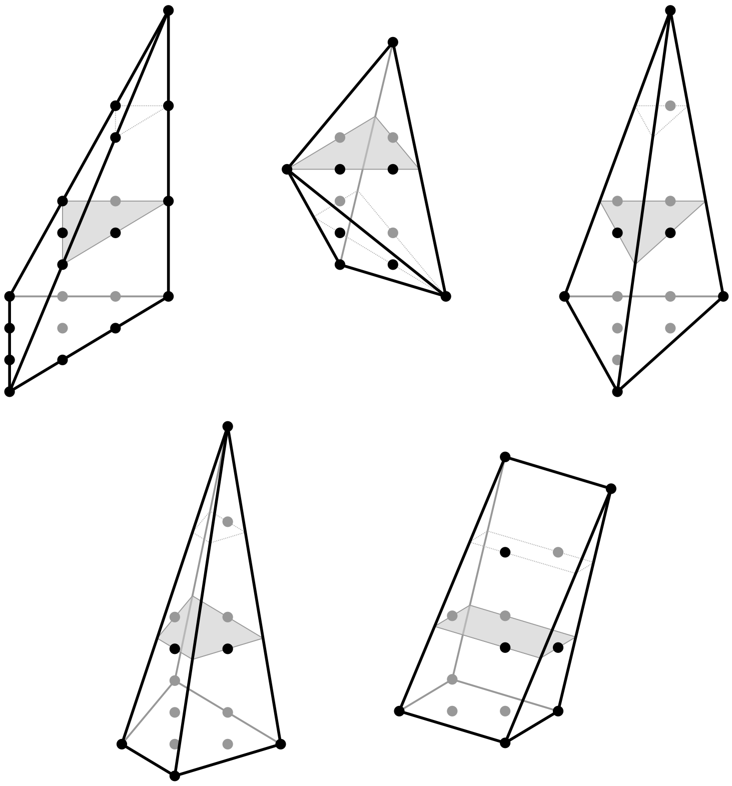

Figure 1.4: The $\mathbb{Z}^3$-maximal $\mathbb{Z}^3$-polytopes with lattice width three.

samples. This generalization of $\mathbb{R}^d$-maximality has been the subject of [AWW11] and [NZ11]. In fact, Theorem 1.2 as stated here is only a special case of the results presented there: Theorem 1.2 (b) was proven more generally for $\frac{1}{s}\mathbb{Z}^d$-maximal lattice-free polyhedra in $\mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$ in [AWW11, Proposition 3.1], while Theorem 1.2 (c) was proven for the same class in [AWW11, Theorem 2.1] and, independently, in [NZ11, Corollary 2.2]. The results and proofs from these publications can be modified to fit our setting, which yields the following theorem.

Theorem 1.5 (Properties of $\mathbb{Z}^d$-maximal polyhedra in $\mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$). *Let $s, d \in \mathbb{N}$. Then, the following statements hold:*

(a) Let $P \in \mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$ be lattice-free. Then there exists a $\mathbb{Z}^d$-maximal lattice-free polyhedron $L \in \mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$ such that $P \subseteq L$.

(b) Every unbounded $\mathbb{Z}^d$-maximal lattice-free polyhedron $P \in \mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$ is unimodularly equivalent to a polyhedron of the form $P' \times \mathbb{R}^k$, where $1 \le k \le d-1$ and P' is a $\mathbb{Z}^{d-k}$-maximal lattice-free polytope in $\mathcal{P}(\frac{1}{s}\mathbb{Z}^{d-k})$.

(c) Up to unimodular equivalence, there exist only finitely many $\mathbb{Z}^d$-maximal lattice-free polyhedra in $\mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$.

Theorem 1.5 can be proved using arguments and results from [AWW11] and [NZ11]. Since it has not been around in the literature in this form, we give a proof of Theorem 1.5 at the end of Chapter 2.

Motivated by our proof methods for Theorem 1.3, we extend Theorem 1.3 to the following theorem.

Theorem 1.6 (Equivalence of maximality notions for rational lattice-free polyhedra). *Let $d, s \in \mathbb{N}$. If $d = 3$, $s = 1$ or $d = 2$, $s \in \{1, 2\}$ or $d = 1$, then the following holds:*

$$\text{For every lattice-free } P \in \mathcal{P}\left(\tfrac{1}{s}\mathbb{Z}^d\right) \text{ one has:} \\ P \text{ is } \mathbb{Z}^d\text{-maximal if and only if } P \text{ is } \mathbb{R}^d\text{-maximal.} \tag{1.5}$$

Furthermore, for all other choices of (d, s), property (1.5) *does not hold, i.e. there exist lattice-free polyhedra in $\mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$ that are $\mathbb{Z}^d$-maximal but not $\mathbb{R}^d$-maximal.*

We remark that our contribution essentially consists of the cases $d = 3$, $s = 1$ (our Theorem 1.3) and $d = 2$, $s = 2$. The $\mathbb{Z}^2$-maximal polytopes in $\mathcal{P}(\frac{1}{2}\mathbb{Z}^2)$ are depicted in Figure 1.5. The other cases up to dimension three are straightforward (and were mostly known before), while we have already pointed out that Nill & Ziegler gave counterexamples for the case $d \geq 4$ and $s = 1$ in [NZ11]. Obviously, this also provides counterexamples for every $s \geq 2$ since every integral polyhedron is also in $\mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$ for every $s \geq 2$.

We also point out that for the cases $d = 3$, $s = 1$ and $d = 2$, $s = 2$, Theorem 1.6 also answers an open question from [Wag11, Section 7.4]. There, the question was raised for which pairs s, d every $\frac{1}{s}\mathbb{Z}^d$-maximal lattice-free integral polytope is also $\mathbb{R}^d$-maximal, and these two cases as well as the case $d = 3$, $s = 2$ were identified as the only open ones. We point out that since $\mathbb{Z}^d$-maximality is a weaker condition than $\frac{1}{s}\mathbb{Z}^d$-maximality for fixed $s \geq 2$, our results prove that equivalence of $\frac{1}{s}\mathbb{Z}^d$-maximality and $\mathbb{R}^d$-maximality holds for $d = 3$, $s = 1$ as well as $d = 2$, $s = 2$. Furthermore, we remark that the polytope we present in the proof of Theorem 1.6 as an example of a $\mathbb{Z}^3$-maximal lattice-free polytope in $\mathcal{P}(\frac{1}{2}\mathbb{Z}^3)$ which is not $\mathbb{R}^3$-maximal is also an example why $\frac{1}{2}\mathbb{Z}^3$-maximality and $\mathbb{R}^3$-maximality are not equivalent for elements of $\mathcal{P}(\frac{1}{2}\mathbb{Z}^3)$. Therefore, our results provide the answers to all three open cases mentioned in [Wag11].

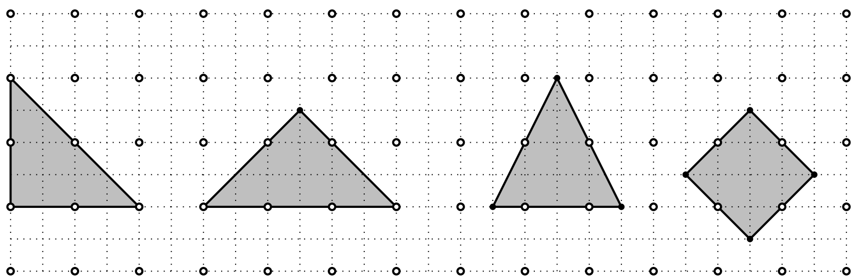

Figure 1.5: All $\mathbb{Z}^2$-maximal $\frac{1}{2}\mathbb{Z}^2$-polytopes.

The proofs of the results of this section are given in Chapter 2.

1.3 Integral simplices with one interior integral point and their link to lattice-free polytopes

For the characterization of $\mathbb{Z}^d$-maximal lattice-free polyhedra in $\mathcal{P}(\mathbb{Z}^d)$ in higher dimensions, but also en route to the eventual proof of Theorem 1.3, we looked at various parameters of lattice-free polytopes in order to bound their size. As parameters for the size, we considered the volume, the number of integral points and the lattice width, but we were also particularly interested in the *lattice diameter*: for a polyhedron $P \subseteq \mathbb{R}^d$, the lattice diameter $\mathrm{ld}(P)$ is defined as the maximum of $|P \cap \mathbb{Z}^d \cap g| - 1$ over all rational lines g. In other words, the largest number of collinear integral points contained in P is $\mathrm{ld}(P) + 1$. This parameter is helpful for the analysis of lattice-free integral polytopes in $\mathcal{P}(\mathbb{Z}^d)$ on several accounts. First, $\mathrm{ld}(P)$ contains information about the edges of P: each edge can contain at most $\mathrm{ld}(P) + 1$ points of $\mathbb{Z}^d$. Second, it yields an upper bound on the so-called *lattice point enumerator*, which is defined as $G(P) := |P \cap \mathbb{Z}^d|$. This can be bounded in terms of the lattice diameter, as

$$\mathrm{ld}(P) + 1 \leq G(P) \leq (\mathrm{ld}(P) + 1)^d. \tag{1.6}$$

The lower bound follows from the definitions of $\mathrm{ld}(P)$ and $G(P)$, while the upper bound can be proved using the so-called parity argument; see [Rab89b, Theorem 1]. Furthermore, the lattice diameter provides not only information about the properties of P, but also about those of its faces: obviously, every face of P has lattice diameter at most $\mathrm{ld}(P)$.

We point out that the lattice diameter of a lattice-free integral polyhedron can be arbitrarily large. In particular, it can even be infinite if the polyhedron is unbounded: $[0,1] \times \mathbb{R}$ contains the line $\{0\} \times \mathbb{R}$, which contains infinitely many points of $\mathbb{Z}^2$. For every $k \in \mathbb{N}$, the bounded set $\mathrm{conv}(o, e_1, ke_2)$ is lattice-free and has lattice diameter k. Therefore, we can obtain an upper bound on the lattice diameter of integral lattice-free polyhedra only under some additional assumption. We will call a lattice-free polyhedron $P \subseteq \mathbb{R}^d$ *ℓ-maximal* (for 'lineality space maximal') lattice-free if for every $u \in \mathbb{Z}^d \setminus \{o\}$, the polyhedron $P + \mathrm{lin}(u)$ is not lattice-free. Obviously, every ℓ-maximal lattice-free integral polyhedron is in fact a polytope: by Theorem 1.2(a), every unbounded lattice-free integral polyhedron P is contained in an unbounded $\mathbb{Z}^d$-maximal lattice-free integral polyhedron L. In turn, by Theorem 1.2(b), L is a polyhedron containing $\mathrm{lin}(u)$ for some $u \in \mathbb{Z}^d \setminus \{o\}$. Thus, $P + \mathrm{lin}(u)$ is lattice-free and thus P is not ℓ-maximal. ℓ-maximality is equivalent to the condition of 'not allowing a lattice projection onto a $(d-1)$-dimensional lattice-free polytope' used in [NZ11]. Moreover, every bounded $\mathbb{Z}^d$-maximal lattice-free set is also ℓ-maximal, whereas the reverse statement is not true for $d \geq 3$: for instance, the d-dimensional integral simplex $\mathrm{conv}(o, de_1, \dots, de_{d-1}, (d-1)e_d)$ is ℓ-maximal but not $\mathbb{Z}^d$-maximal for every $d \geq 3$.

A way to bound the lattice diameter of a $\mathbb{Z}^d$-maximal lattice-free polytope P in $\mathcal{P}(\mathbb{Z}^d)$ from above was given in [AWW11]. We repeated the argumentation to show the statement for ℓ-maximal polytopes in [AKN15, Theorem 2.9], which is also part of this thesis as Theorem 1.15; see the proof of this theorem for a detailed explanation. In short, the idea is as follows: assuming that the line g for which the lattice diameter is attained is orthogonal to $\mathbb{R}^{d-1} \times \{0\}$ (which can be achieved by applying a suitable unimodular transformation), we project P onto $\mathbb{R}^{d-1}$. Then by a result from [AWW11], one can find an integral simplex S of dimension at most $d-1$ contained in the projection which has precisely one point of $\mathbb{Z}^{d-1}$, say p, in its (relative) interior and, furthermore, one of the vertices of S is the point onto which g is projected. Now one can observe two facts: first, one can obtain an upper bound on the lattice diameter by bounding the length of the line segment $P \cap g$. Second, since p is integral, the length of the line segment $P \cap \big(p + \mathrm{lin}(e_d)\big)$ can be at most one: otherwise, there exists an integral point in the relative interior of this line segment and hence also in the interior of P. The lengths of the two line segments can be put into relation using a parameter of the simplex S with respect to p which is called the *coefficient of asymmetry*. For a d-dimensional convex set K and a point $x \in \mathrm{int}(K)$, the coefficient of asymmetry of K about x is defined as

$$\mathrm{ca}(K,x) := \max\left\{\frac{\mathrm{len}([x,a])}{\mathrm{len}([x,b])} \ : \ a,b \in \mathrm{bd}(K), x \in [a,b]\right\}.$$

Again, the reader is referred to Theorem 1.15 for a mathematically sound proof and the exact relations, but the bottom line of this paragraph is that once we have an upper bound on the coefficient of asymmetry of S about p, we obtain an upper bound on the lattice diameter of P.

As a consequence, we turned our attention to the following conjecture made by Hensley in [Hen83], for which we need the definition of the *Sylvester sequence* $(s_i)_{i\in\mathbb{N}}$ given by

$$\begin{aligned} s_1 &:= 2, \\ s_i &:= 1 + \prod_{j=1}^{i-1} s_j \qquad \text{for } i \geq 2. \end{aligned}$$

Conjecture (Hensley, 1983). Let $S \subseteq \mathbb{R}^d$ be an integral simplex with $\mathrm{int}(S) \cap \mathbb{Z}^d = \{p\}$. Then the coefficient of asymmetry of S about p is at most $s_{d+1} - 2$, which is attained for $S = \mathrm{conv}(o, s_1e_1, \dots, s_de_d)$.

In [AKN15] we prove Hensley's conjecture and also show that equality is attained if and only if S is the simplex $\mathrm{conv}(o, s_1e_1, \dots, s_de_d)$. Our proof makes use of the barycentric coordinates of p. Given a d-dimensional simplex $S \subseteq \mathbb{R}^d$ with vertices $v_1, \dots, v_{d+1}$ and a point $x \in \mathbb{R}^d$, the *barycentric coordinates* of x with respect to S are uniquely determined real numbers $\beta_1, \dots, \beta_{d+1}$ satisfying $\sum_{i=1}^{d+1} \beta_i = 1$ such that $x = \sum_{i=1}^{d+1} \beta_i v_i$. In this case, for $i \in \{1, \dots, d+1\}$, we say that β_i is the barycentric coordinate associated with v_i. One has $x \in \mathrm{int}(S)$ if and only if $\beta_i > 0$ for all $i \in \{1, \dots, d+1\}$. Note that the coefficient of asymmetry is in one-to-one-correspondence with the minimal barycentric coordinate, say β, of the interior integral point with respect to the vertices of S: one has $\mathrm{ca}(S,p) = \frac{1}{\beta} - 1$; see also [Pik01, (3)]. For our purpose of bounding the coefficient of asymmetry, we were therefore interested in providing bounds on the barycentric coordinates of p. Our main tool used to obtain these bounds was a set of inequalities derived in [Ave12, Theorem 1.1]; see Theorem 3.5 of this thesis for the precise result. However, in the process of doing so, we realized that the methods we employed could be used to answer several other questions related to the size of integral simplices (and in some cases, general integral polytopes) with one interior integral point. A more precise notion of size as well as an overview of our results is given in the following section. Note that the contributions to the analysis of lattice-free polyhedra are presented at the very end of the following section in Theorem 1.15 and Corollary 1.16.

1.4 Results on integral polytopes with one interior integral point

For $k \in \mathbb{N} \cup \{0\}$, we introduce the following two families of polytopes:

$$\mathcal{P}^d(k) := \left\{P \subseteq \mathbb{R}^d \ : \ P \in \mathcal{P}(\mathbb{Z}^d), \ \dim(P) = d, \ |\mathrm{int}(P) \cap \mathbb{Z}^d| = k\right\}$$

and

$$\mathcal{S}^d(k) := \left\{S \in \mathcal{P}^d(k) \ : \ S \text{ is a simplex}\right\}.$$

Given an integer $k \geq 1$ and a dimension $d \in \mathbb{N}$, the set $\mathcal{P}^d(k)$ is finite up to unimodular transformations. In particular, $\mathcal{S}^d(k)$ is finite as well. A natural way to prove finiteness of $\mathcal{P}^d(k)$ and $\mathcal{S}^d(k)$ is to bound the volume of their elements from above in terms of k and d. This was first done by Hensley [Hen83]. In addition to his conjecture on the coefficient of asymmetry, Hensley also conjectured that the simplex

$$S_1^d := \operatorname{conv}(o, s_1 e_1, \dots, s_{d-1} e_{d-1}, 2(s_d - 1)e_d) \in \mathcal{S}^d(1)$$

contains the maximal number of integral points among all elements of $\mathcal{S}^d(1)$. This simplex appeared in [ZPW82]. Hensley derived a bound on $|S \cap \mathbb{Z}^d|$ for $S \in \mathcal{S}^d(1)$ by applying Blichfeldt's theorem (see Theorem 3.1), which bounds $|S \cap \mathbb{Z}^d|$ in terms of $\operatorname{vol}(S)$. It is therefore natural to modify Hensley's conjecture to the following question: Does S_1^d have maximal volume among all elements of $\mathcal{S}^d(1)$? Following Hensley's results, Lagarias and Ziegler [LZ91], Pikhurko [Pik01] and Averkov [Ave12] made improvements to the upper bound on the volume of elements in $\mathcal{S}^d(1)$, but the bounds they obtained were still different from the largest known example for given d, the simplex S_1^d. For large d, the best previously known bound was due to Pikhurko: he proved that for $S \in \mathcal{S}^d(1)$, one has $\operatorname{vol}(S) \leq \frac{1}{d!} 2^{3d-2} \cdot 15^{(d-1)2^{d+1}}$. For comparison, one has $\operatorname{vol}(S_1^d) = \frac{1}{d!} 2(s_d - 1)^2 \leq \frac{1}{d!} 2^{2^d+1}$. We also point out here that qualitative arguments which show that $\max_{S \in \mathcal{S}^d(1)} \operatorname{vol}(S)$ is finite were given in [Law91] and [BB92]; see also [Bor00].

We confirm that S_1^d has indeed maximal volume in $\mathcal{S}^d(1)$. We also prove several further results on the size of the elements of $\mathcal{S}^d(1)$. In this thesis, the notions of size we will use are the maximal volume, the maximal volume of i-dimensional faces for given i and the lattice diameter. We will also give a sharp lower bound on the barycentric coordinates of the single interior integral point in an element of $\mathcal{S}^d(1)$, which gives us a bound on the coefficient of asymmetry for elements of $\mathcal{S}^d(1)$. By a theorem of Mahler (see Theorem 3.2), one can bound the volume of a simplex in $\mathcal{S}^d(1)$ in terms of the coefficient of asymmetry. The number of integral points of a simplex can then be bounded in terms of its volume. This is basically the line of argumentation used in [Hen83], [LZ91], [Pik01] and [Ave12]. For $S \in \mathcal{S}^d(1)$ and given $l \in \{1, \dots, d\}$, we give sharp upper bounds on the volume of every l-dimensional face of S, in particular for $l = d$ on the simplex S itself. We also analyze the dual of a simplex in $\mathcal{S}^d(1)$. To this end, for $l \in \{1, \dots, d\}$ we also bound the volume of l-dimensional faces of the dual S^* of $S \in \mathcal{S}^d(1)$ as well as the *Mahler volume* $\operatorname{vol}(S)\operatorname{vol}(S^*)$. We then show that the bound on the coefficient of asymmetry for elements of $\mathcal{S}^d(1)$ remains valid for the more general class $\mathcal{P}^d(1)$. This also translates into a volume bound for $\mathcal{P}^d(1)$, improving the one given in [Pik01]. For general $k \geq 1$, we determine the sharp upper bound on the lattice diameter of polytopes in $\mathcal{P}^d(k)$. Finally, we conclude the section by giving the results on lattice diameter, lattice point enumerator and volume of ℓ-maximal lattice-free polyhedra.

Before we turn to presenting the results, we give a brief overview of related results in the literature. In [Hen83], [LZ91] and [Pik01], not only elements of $\mathcal{P}^d(1)$ and $\mathcal{S}^d(1)$ were analyzed, but of $\mathcal{P}^d(k)$ and $\mathcal{S}^d(k)$, respectively, for every $k \geq 1$. The special case $k = 1$ addressed in this thesis is of interest not only for the analysis of lattice-free polyhedra, as outlined in Section 1.3, but also from a toric geometry point of view. For readers familiar with the terminology of algebraic geometry, we point out that the elements $\mathcal{S}^d(1)$ correspond one-to-one with $\mathbb{Q}$-factorial toric Fano varieties with Picard number one, so called fake weighted projective spaces, with at most canonical singularities. For background reading on toric varieties, see [CLS11]. For more information on toric varieties and their singularities, see [Nil05, Nil07] and on fake weighted projective spaces, see [Buc08, Kas09]. [AKN15, Theorems 2.11 and 2.12] provide results concerning this class of toric Fano varieties which are consequences of our result on the Mahler volume of the elements $\mathcal{S}^d(1)$. However, as the contribution of the author of this thesis did not extend to the translation of our results on $\mathcal{S}^d(1)$ into [AKN15, Theorems 2.11 and 2.12], they are not part of this thesis. Furthermore, our results on $\mathcal{S}^d(1)$ have been used to classify all 4-dimensional weighted projective spaces with canonical singularities [Kas13, Theorem 3.3].

Nonetheless, one can of course ask whether our results can be extended to the case $k \geq 1$. First, one can extend the question about the simplices with maximal volume by considering the following simplices, which were first introduced in [ZPW82]. For $d \geq 2$ and $k \geq 0$, the d-dimensional integral simplex

$$S_k^d := \operatorname{conv}(o, s_1 e_1, \dots, s_{d-1} e_{d-1}, (k+1)(s_d - 1)e_d) \tag{1.7}$$

contains exactly k interior integral points and has volume $\operatorname{vol}(S_k^d) = \frac{(k+1)}{d!}(s_d - 1)^2$. It would be interesting to know whether, analogously to the case $k = 1$ discussed in this thesis, S_k^d has maximal volume among all elements of $\mathcal{S}^d(k)$ also for general $k \geq 2$. We point out that a direct extension of our methods is not possible, because we rely on a set of inequalities relating the barycentric coordinates of the *single* interior integral point to each other (cf. Theorem 3.5). However, there is some reason to believe that for the case of several interior integral points, one could modify the arguments in [Ave12] to deduce similar inequalities for the barycentric coordinates of *one* appropriately chosen interior integral point. How to choose this point is an open question. It is also open whether it is possible to derive inequalities which lead to sharp bounds on the volume of elements of $\mathcal{S}^d(k)$ in this way.

It should also be remarked that in [LZ91] and [Pik01] the more general question of providing bounds on the volume of integral simplices containing precisely $k \in \mathbb{N}$ points of the lattice $s\mathbb{Z}^d$ for some $s \in \mathbb{N}$ was considered and bounds on the coefficient of asymmetry and the volume were given. Considering the applications motivating our research on $\mathcal{S}^d(1)$, it did not seem relevant to consider this generalization for our results. It should, however, be possible to generalize most of the results in [AKN15] to this setting without too much additional machinery.

Bounds for $\mathcal{S}^d(1)$

Our first main result gives sharp lower bounds for the sorted sequence of the barycentric coordinates. We introduce the following simplices for which those bounds are attained. For $j \in \{1, \dots, d+1\}$, we define the simplex $T_{1,j}^d \in \mathcal{S}^d(1)$ by

$$T_{1,j}^d := \operatorname{conv}(o, s_1 e_1, \dots, s_{j-1} e_{j-1}, (d-j+2)(s_j - 1)e_j, \dots, (d-j+2)(s_j - 1)e_d).$$

Note that in the degenerate cases $j \in \{1, d+1\}$, this definition should be interpreted as $T_{1,1}^d := \operatorname{conv}(o, (d+1)e_1, \dots, (d+1)e_d)$ and $T_{1,d+1}^d := \operatorname{conv}(o, s_1 e_1, \dots, s_d e_d)$, respectively. Also, note that $T_{1,d}^d = S_1^d$. A brief argument why the simplices $T_{1,j}^d$ are in $\mathcal{S}^d(1)$ is given in Remark 3.4.

Theorem 1.7 (Bounds on the barycentric coordinates). *Let $S \in \mathcal{S}^d(1)$, where $d \in \mathbb{N}$, and let $i \in \{1, \dots, d+1\}$. Let $\beta_1, \dots, \beta_{d+1}$ be the barycentric coordinates of the integral point in the interior of S such that $\beta_1 \geq \dots \geq \beta_{d+1}$. Then*

$$\beta_i \geq \frac{1}{(d-i+2)(s_i - 1)}. \tag{1.8}$$

Furthermore, the following statements hold:

(a) *For* $S \simeq T^d_{1,i}$, *the inequality* (1.8) *is attained with equality.*

(b) *Inequality* (1.8) *holds with equality if and only if*

$$(\beta_1, \dots, \beta_{d+1}) = \left(\frac{1}{s_1}, \dots, \frac{1}{s_{i-1}}, \frac{1}{(d-i+2)(s_i-1)}, \dots, \frac{1}{(d-i+2)(s_i-1)} \right).$$

(c) *For* $i = d+1$, *equality holds in* (1.8) *if and only if* $S \simeq T^d_{1,i}$.

Note that assertion (c) cannot be extended to the case $i < d+1$; see Remark 3.24.

This result confirms Hensley's conjecture regarding the coefficient of asymmetry. To see this, observe that if for some $S \in \mathcal{S}^d(1)$, we have $\operatorname{int}(S) \cap \mathbb{Z}^d = \{x\}$ and $\beta_1 \geq \ldots \geq \beta_{d+1}$ are the barycentric coordinates of x with respect to S, then as stated above, the coefficient of asymmetry can be written as

$$\operatorname{ca}(S, x) = \max_{i \in \{1,\dots,d+1\}} \frac{1-\beta_i}{\beta_i} = \frac{1-\beta_{d+1}}{\beta_{d+1}}. \tag{1.9}$$

Therefore, $\operatorname{ca}(S, x)$ is maximal when β_{d+1} is minimal and hence, in view of Theorem 1.7(c), $\operatorname{ca}(S, x)$ has maximal value over all elements of $\mathcal{S}^d(1)$ if and only if $S = \operatorname{conv}(o, s_1 e_1, \dots, s_d e_d)$. This confirms Hensley's conjecture.

Next, we present a sharp upper bound on the face volumes of simplices in $\mathcal{S}^d(1)$, including the d-dimensional face, i.e., the simplex itself.

Theorem 1.8 (Bounds on the volumes of faces). *Let* $S \in \mathcal{S}^d(1)$, *where* $d \geq 3$, *and let* $l \in \{1, \dots, d\}$. *Then*

$$\max_{F \in \mathcal{F}_l(S)} \operatorname{vol}_{\mathbb{Z}}(F) \leq \frac{2(s_d - 1)^2}{l!(s_{d-l+1} - 1)}. \tag{1.10}$$

Furthermore, the following statements hold:

(a) *For* $S \simeq S^d_1$, *inequality* (1.10) *is attained with equality.*

(b) *For* $d \geq 4$ *and* $l \in \{1, d\}$, *the equality in* (1.10) *is attained if and only if* $S \simeq S^d_1$.

In Theorem 1.8, for $l = d$ we have

$$\operatorname{vol}(S) \leq \frac{2}{d!}(s_d - 1)^2.$$

This gives us the sharp bound on the volume of the simplices in $\mathcal{S}^d(1)$. Theorem 1.8 is a generalization of Theorems A and B in [Nil07], which are concerned with reflexive simplices, i.e., integral simplices containing the origin and such that their duals are again integral. For reflexive simplices, Theorems A and B in [Nil07] cover Theorem 1.8(a) with $l = d$ and Theorem 1.8(b). Note that while Theorem 1.8(b) guarantees uniqueness for $l \in \{1, d\}$, there is nothing said about $l \in \{2, \dots, d-1\}$. We ask about a possible characterization of the simplices $S \in \mathcal{S}^d(1)$ for which (1.10) is attained with equality in the case $l \in \{2, \dots, d-1\}$. It has been conjectured that for $d \geq 4$ the inequalities in Theorem 1.8(a) remain valid for arbitrary polytopes in $\mathcal{P}^d(1)$; see [Nil07, Conjecture 1.7]. Moreover, one can ask whether in this case equality in all of the inequalities of Theorem 1.8(a) for $l \in \{1, \dots, d\}$ is only satisfied for S^d_1, up to unimodular transformation.

As a consequence of Theorem 1.8 and a well-known theorem by Blichfeldt (see Theorem 3.1 below), we derive an upper bound on the number of integral points of a simplex in $\mathcal{S}^d(1)$ and each of its l-dimensional facets.

COROLLARY 1.9 (Bounds on the number of integral points in faces). *Let $S \in \mathcal{S}^d(1)$, where $d \geq 3$, and let $l \in \{1, \dots, d\}$. Then*

$$\max_{F \in \mathcal{F}_l(S)} |F \cap \mathbb{Z}^d| \leq l + l! \operatorname{vol}_{\mathbb{Z}}(F) \leq l + \frac{2(s_d - 1)^2}{(s_{d-l+1} - 1)}.$$

Note that this corollary yields an improvement on the previously known bounds on $|S \cap \mathbb{Z}^d|$. It is, however, not fulfilled with equality for S_1^d. Thus, Hensley's conjecture that S_1^d maximizes $|S \cap \mathbb{Z}^d|$ among all elements in $\mathcal{S}^d(1)$ remains open.

Bounds for $\mathcal{S}^d(1)$ involving dualization

In the following results, we consider $S \in \mathcal{S}^d(1)$ satisfying $\operatorname{int}(S) \cap \mathbb{Z}^d = \{o\}$ and provide volume bounds for S^*. Note that the first of these results is again an extension of a result in [Nil07], namely assertion 2 of Corollary 6.1. It is a sharp estimate on the so-called Mahler volume.

THEOREM 1.10 (Bounds on the Mahler volume). *Let $d \in \mathbb{N}$ and $S \in \mathcal{S}^d(1)$ and $o \in \operatorname{int}(S)$. Then*

$$(d + 1)^{d+1} \leq (d!)^2 \operatorname{vol}(S) \operatorname{vol}(S^*) \leq (s_{d+1} - 1)^2.$$

Furthermore, the lower bound is attained with equality if and only if the unique interior integral point of S equals its centroid, while the upper bound is attained with equality if and only if $S \simeq T^d_{1,d+1}$.

The following result is about face sizes of the dual of a simplex $S \in \mathcal{S}^d(1)$.

THEOREM 1.11 (Bounds on the volume of faces of the dual). *Let $S \in \mathcal{S}^d(1)$, where $d \geq 4$. Let $o \in \operatorname{int}(S)$ and $l \in \{1, \dots, d\}$. Then*

$$\max_{F \in \mathcal{F}_l(S^*)} \operatorname{vol}_{\mathbb{Z}}(F) \leq \frac{2(s_d - 1)^2}{l!(s_{d-l+1} - 1)}. \tag{1.11}$$

Furthermore, with $T := T^{d-1}_{1,d}$, the following statements hold:

(a) Equality holds in (1.11) *if $S \simeq \operatorname{conv}\big((T \times \{0\}) \cup \{\pm e_d\}\big)$.*

(b) If $l \in \{1, d\}$, then equality holds in (1.11) *if and only if $S \simeq \operatorname{conv}\big((T \times \{0\}) \cup \{\pm e_d\}\big)$.*

We remark that for a simplex $S \in \mathcal{S}^d(1)$, where $d \geq 4$, which satisfies $o \in \operatorname{int}(S)$ and $S \simeq \operatorname{conv}\big((T \times \{0\}) \cup \{\pm e_d\}\big)$, we have $S^* \simeq S_1^d$.

Results on $\mathcal{P}^d(1)$

Using Theorem 1.7, we can give a sharp bound on the coefficient of asymmetry for polytopes containing exactly one interior integral point.

THEOREM 1.12 (Bound on the coefficient of asymmetry). *Let $P \in \mathcal{P}^d(1)$, where $d \in \mathbb{N}$, and $o \in \operatorname{int}(P)$. Then*

$$\operatorname{ca}(P, o) \leq s_{d+1} - 2.$$

Furthermore, equality holds if and only if $P \cong T^d_{1,d+1}$.

This shows that the bound on the coefficient of asymmetry conjectured by Hensley for $\mathcal{S}^d(1)$ remains valid for $\mathcal{P}^d(1)$. From Theorem 1.12, we derive a bound on the volume of an arbitrary integral polytope P which has exactly one integral point in its interior.

Theorem 1.13 (Bound on the volume of elements in $\mathcal{P}^d(1)$). *Let $P \in \mathcal{P}^d(1)$. Then*

$$\mathrm{vol}(P) \le (s_{d+1} - 1)^d.$$

Asymptotically, Theorem 1.13 improves the best known bound $\mathrm{vol}(P) = 2^{O(d4^d)}$ of Pikhurko [Pik01] to the bound $\mathrm{vol}(P) = 2^{O(d2^d)}$.

Bounds on the lattice diameter of integral polytopes

We now turn our attention to $\mathcal{P}^d(k)$ for $k \ge 1$ and deduce upper bounds on the lattice diameter $\mathrm{ld}(P)$ for $P \in \mathcal{P}^d(k)$.

Theorem 1.14 (Bound on the lattice diameter of elements in $\mathcal{P}^d(k)$). *Let $d \in \mathbb{N}$ and let $P \subseteq \mathbb{R}^d$ be a d-dimensional integral polytope such that $P' := \mathrm{conv}\left(\mathrm{int}(P) \cap \mathbb{Z}^d\right) \neq \emptyset$. Let $m := \mathrm{ld}(P')$. Then*

$$\mathrm{ld}(P) \le (m+2)(s_d - 1).$$

Furthermore, equality holds if and only if $P \simeq S^d_{m+1}$.

Let us now return to the lattice point enumerator as introduced above for a polytope as in Theorem 1.14. In view of (1.6) and Theorem 1.14, the following inequalities hold:

$$G(P)^{1/d} - 1 \le \mathrm{ld}(P) \le (\mathrm{ld}(P') + 2)(s_d - 1) \le (G(P') + 1)(s_d - 1), \tag{1.12}$$

where P' is defined as in Theorem 1.14. Thus, each of the two values $G(P)$ and $\mathrm{ld}(P)$ can be bounded in terms of each of the two values $G(P')$, $\mathrm{ld}(P')$. Note that for $m = \mathrm{ld}(P')$, the interior points of S^d_{m+1} are collinear, that is, for $P = S^d_{m+1}$ one has $\mathrm{ld}(P') + 1 = G(P')$. Hence, the equality $\mathrm{ld}(P) = (G(P')+1)(s_d-1)$ is attained if and only if $P \simeq S^d_{m+1}$, as follows from the characterization of the equality case in Theorem 1.14. In contrast to this, the inequalities linking $G(P)$ to $G(P')$ and $\mathrm{ld}(P')$, respectively, are most likely not tight.

Theorem 1.14 can be carried over to ℓ-maximal lattice-free integral polytopes. The bound we obtain is similar to the one obtained in Theorem 1.14 in the sense that $\mathrm{ld}(P') + 2 = 1$ if P does not contain any interior integral points. The following theorem and the subsequent corollary are the results for lattice-free polyhedra obtained from our analysis of integral simplices with one interior integral point.

Theorem 1.15 (Bound on the lattice diameter of ℓ-maximal lattice-free polytopes). *Let $d \in \mathbb{N}$ and let $P \in \mathcal{P}(\mathbb{Z}^d)$ be ℓ-maximal lattice-free. Then the lattice diameter of P is at most $s_d - 1$. Furthermore, the equality $\mathrm{ld}(P) = s_d - 1$ holds if and only if $P \simeq S^d_0$.*

Similarly to Theorem 1.14, we also deduce a bound on the lattice point enumerator $G(P)$ for an ℓ-maximal lattice-free polytope $P \in \mathcal{P}(\mathbb{Z}^d)$. To this, one can then apply a result from [Pik01] to deduce a bound on the volume of such a polytope.

Corollary 1.16 (Further size bounds on ℓ-maximal lattice-free polytopes). *Let $d \in \mathbb{N}$ and let $P \in \mathcal{P}(\mathbb{Z}^d)$ be ℓ-maximal lattice-free. Then*

$$G(P) \le (s_d)^d \le 2^{d2^{d-1}} \qquad \text{and} \qquad \mathrm{vol}(P) \le 2^{2^{2d+o(d)}}.$$

For $\mathbb{Z}^d$-maximal lattice-free polytopes in $\mathcal{P}(\mathbb{Z}^d)$, the above volume bound was shown in [AWW11, Remark 3.10]. One can see, however, that the corresponding proof in [AWW11] can be applied with the weaker condition of ℓ-maximality without any changes. Thus, the volume bound of Corollary 1.16 is basically a result from [AWW11]. A volume bound of the same asymptotical order for ℓ-maximal polytopes was also given in [NZ11, Theorem 2.1]; in their proof Nill and Ziegler rely on the results of Kannan and Lovász [KL88].

1.5 Definitions and notation

This section contains the background notation and definitions from convex geometry and the geometry of numbers. For further reading on those topics, the reader is referred to [Bar02], [Cas97], [GL87], [Roc97] and [Sch93].

Throughout the text, $d \in \mathbb{N}$ is the dimension of the ambient space $\mathbb{R}^d$, which is equipped with the standard Euclidian scalar product, denoted by $\langle \cdot \,, \cdot \rangle$. By o we denote the zero vector, $\mathbb{1}$ denotes the all-one vector and e_i denotes the i-th unit vector. In what follows the dimension of o, $\mathbb{1}$ and e_i is given by the context. For two points $x, y \in \mathbb{R}^d$, we denote the closed line segment connecting those points by $[x, y] := \{\lambda x + (1 - \lambda)y : 0 \leq \lambda \leq 1\}$ and its Euclidean length by $\operatorname{len}([x, y])$. Accordingly, one has the open line segment $(x, y) := \{\lambda x + (1 - \lambda)y : 0 < \lambda < 1\}$. For a subset X of $\mathbb{R}^d$, we write $Y \subseteq X$ if Y is a subset of X and $Y \subsetneq X$ if, furthermore, $Y \neq X$ holds. The cardinality of X is denoted by $|X|$. By $-X$ we denote the set $\{x : -x \in X\}$. For two subsets X, Y of $\mathbb{R}^d$, we write $X + Y := \{x + y : x \in X, y \in Y\}$ for the *Minkowski sum* of X and Y, while $X - Y$ is short for $X + (-Y)$. For $t \in \mathbb{R}$, we write $tX := \{tx : x \in X\}$ for the scalar multiple tX of X. For a set $Z \subseteq \mathbb{Z}$, we denote by $\gcd(Z)$ the *greatest common divisor* of the set Z, i.e. the largest natural number n such that n divides every element of Z. We call a vector $z \in \mathbb{Z}^d \setminus \{o\}$ *primitive* if the greatest common divisor of the components of z is one.

For a set $X \subseteq \mathbb{R}^d$, we use $\operatorname{conv}(X)$, $\operatorname{aff}(K)$ and $\operatorname{lin}(X)$ to denote the *convex hull*, *affine hull* and *linear hull* of X, respectively. By $\operatorname{bd}(K)$, $\operatorname{relbd}(K)$, $\operatorname{relint}(K)$ and $\operatorname{int}(K)$ we denote the *boundary*, the *relative boundary*, the *relative interior* and the *interior* of a convex set K, respectively. $\operatorname{vol}(K)$ denotes the *volume* of K and $\dim(K)$ denotes the *dimension* of K, which is defined as the dimension of the affine hull of K. A convex set K such that $K = -K$ is said to be o-symmetric. A compact convex set with non-empty interior is called *convex body*. For a convex body $K \subseteq \mathbb{R}^d$, the convex body $K + (-K)$ is called the *difference body* of K. If K contains the origin in its interior, we denote by K^* the *polar* (or *dual*) body of K, i.e. $K^* = \{y \in \mathbb{R}^d : \langle x, y\rangle \leq 1 \, \forall \, x \in K\}$. The product $\operatorname{vol}(K)\operatorname{vol}(K^*$ is called the *Mahler volume* of K.

For a convex set $K \subseteq \mathbb{R}^d$ and a vector $u \in \mathbb{R}^d \setminus \{o\}$, we denote by $h(K, u)$ the *support function* $h(K, u) := \sup\{\langle u\,, x\rangle : x \in K\}$ and by $\rho(K, u)$ the *radius function* $\rho(K, u) := \max\{\rho \geq 0 : \rho u \in K\}$.

Let $b_1, \ldots, b_d$ linearly independent elements of $\mathbb{R}^d$. Then we call the group $\Lambda = \{z_1 b_1 + \ldots + z_d b_d : z_1, \ldots, z_d \in \mathbb{Z}\}$ a *lattice* of rank d. The vectors $b_1, \ldots, b_d$ are said to form a *lattice basis*. The *determinant* of Λ is defined as the determinant of the matrix having columns $b_1, \ldots, b_d$. We say that a subgroup H of a lattice Λ is a *lattice hyperplane* if H spans a $(d - 1)$-dimensional affine subspace of $\mathbb{R}^d$. Two parallel lattice hyperplanes are said to be *adjacent* if there are no points of Λ properly between them.

For a subset X of $\mathbb{R}^d$ and a vector $z \in \mathbb{Z}^d \setminus \{o\}$, by

$$\mathrm{w}(X, z) \,.= \sup_{x \in X}\langle z\,, x\rangle - \inf_{y \in X}\langle z\,, y\rangle$$

we denote the *width* of X in direction of z with respect to the lattice $\mathbb{Z}^d$. Note that for a convex body K, one has 'max' and 'min' rather than 'sup' and 'inf'. The *lattice width* of a set $X \subseteq \mathbb{R}^d$ denotes the infimum of $\mathrm{w}(X, z)$ over all non-zero vectors z, i.e.

$$\mathrm{lw}(X) := \inf_{z \in \mathbb{Z}^d \setminus \{o\}} \mathrm{w}(X, z) .$$

Again, for a convex body one has 'min' instead of 'inf'. We say that the lattice width of a convex body K is *attained* for $z' \in \mathbb{Z}^d \setminus \{o\}$ if $\mathrm{lw}(K) = \mathrm{w}(K, z)$. Note that $\mathrm{lw}(K) = h(K, u) + h(K, -u)$.

The two different normalizations of volume used in this thesis are the standard i-dimensional *volume* of an i-dimensional polytope P ($i \in \{1, \ldots, d\}$), denoted by $\mathrm{vol}(P)$, and for rational polytopes also the *normalized volume*, denoted by $\mathrm{vol}_{\mathbb{Z}}(P)$, which is defined as follows: for a rational polytope P of dimension $i \in \{1, \ldots, d\}$, denote by Λ the lattice (of rank i) given as the intersection of $\mathbb{Z}^d$ with the linear hull of all vectors $x - y$ such that $x, y \in P$. Then $\mathrm{vol}_{\mathbb{Z}}(P)$ is defined as $\mathrm{vol}(P)/\det(\Lambda)$, where $\det(\Lambda)$ denotes the determinant of Λ. Clearly, if P is d-dimensional, $\mathrm{vol}_{\mathbb{Z}}(P) = \mathrm{vol}(P)$. Note that in the literature the notion normalized volume is sometimes used to denote $\dim(P)!\ \mathrm{vol}_{\mathbb{Z}}(P)$.

A *polyhedron* $P \subseteq \mathbb{R}^d$ is the intersection of finitely many closed halfspaces. A bounded polyhedron is called a *polytope* and a two-dimensional polytope is called *polygon*. A polyhedron P is called *rational* if there exists $s \in \mathbb{N}$ such that $P = \mathrm{conv}(P \cap \frac{1}{s}\mathbb{Z}^d)$. The set of vertices of P is denoted by $\mathrm{vert}(P)$. For a polytope P with $o \in \mathrm{int}(P)$, the polar body P^* is again a polytope containing o in its interior.

For a polyhedron P and a vector $u \in \mathbb{R}^d \setminus \{o\}$, we write $F(P, u) := \{x \in P : \langle x, u \rangle = h(P, u)\}$ and, if $h(P, u)$ is finite, we call $F(P, u)$ a *face* of P. We use the notation $\mathcal{F}_i(P)$ for the set of all i-dimensional faces of a d-dimensional polyhedron P, where $i \in \{1, \ldots, d\}$. If $F := F(P, u)$ has dimension $\dim(P) - 1$, we say that F is a *facet* of P and say that u is an *outer normal (facet) vector* of F. If F consists only of a single point, we call F a *vertex* of P. For a d-dimensional rational polyhedron P, we define $U(P)$ to be the set of all primitive vectors which are outer normal vectors of facets of P. Note that if P is rational, every facet of P can be given as $F(P, u)$ for some $u \in U(P)$. Let $x \in \mathrm{bd}(P)$. Then the *normal cone* of P at x is defined as $N(P, x) := \{o\} \cup \left\{u \in \mathbb{R}^d \setminus \{o\} : x \in F(P, u)\right\}$. We say that a vertex v of P is *unimodular* if there are exactly d facets of P containing v and these facets can be given as $F(P, u_1), \ldots, F(P, u_d)$, where $u_1, \ldots, u_d$ are elements of $U(P)$ forming a basis of the lattice $\mathbb{Z}^d$. A d-dimensional polytope with $d + 1$ vertices is called *simplex* of dimension d.

Chapter 2

Maximality properties of lattice-free polyhedra

In this chapter, we prove the new results of Section 1.2. All results and proofs in this chapter were obtained jointly by Gennadiy Averkov, Stefan Weltge and the author of this thesis and have not been published yet.

Structure of the chapter and main proof ideas

The main subject of this chapter is the proof of Theorem 1.3. In the proof, we will need a classification of all $\mathbb{Z}^2$-maximal polytopes in $\mathcal{P}(\frac{1}{2}\mathbb{Z}^2)$. This will be provided in Section 2.1. Every such polytope is contained in an $\mathbb{R}^2$-maximal lattice-free convex set L in the plane and its vertices then have to be contained in $L \cap \frac{1}{2}\mathbb{Z}^2$. We give a slightly extended version of the well-known classification of $\mathbb{R}^2$-maximal lattice-free convex sets L in the plane which allows us to enumerate all $\mathbb{Z}^2$-maximal lattice-free $\frac{1}{2}\mathbb{Z}^2$-polyhedra.

We then turn to integral $\mathbb{Z}^3$-maximal lattice-free polyhedra in dimension three. We can restrict ourselves to polytopes here since every unbounded $\mathbb{Z}^3$-maximal lattice-free polyhedron in $\mathcal{P}(\mathbb{Z}^3)$ is unimodularly equivalent to $[0,1]\times\mathbb{R}^2$ or $\operatorname{conv}(o, 2e_1, 2e_2)\times\mathbb{R}$ in view of Theorem 1.2(b) and the $\mathbb{R}^3$-maximality of those two sets is easy to see. Furthermore, one can easily observe that a lattice-free polytope in $\mathcal{P}(\mathbb{Z}^3)$ with lattice width one cannot be $\mathbb{Z}^3$-maximal, since any such polytope is properly contained in an unbounded lattice-free integral polyhedron formed by two adjacent parallel lattice hyperplanes of $\mathbb{Z}^3$. Therefore, it suffices to consider only the polytopes with lattice width at least two. We distinguish two cases: polytopes with lattice width two and polytopes with lattice width at least three. In the case of lattice width two, we first analyze $\mathbb{Z}^d$-maximal lattice-free integral polytopes with this lattice width in general dimension. Assuming a $\mathbb{Z}^d$-maximal lattice-free polytope P to be contained in $\mathbb{R}^{d-1} \times [-1, 1]$, we deduce properties of $P_0 = \left\{x \in \mathbb{R}^{d-1} : (x, 0) \in P\right\}$ and on the faces of P contained in $\mathbb{R}^{d-1} \times \{-1\}$ and $\mathbb{R}^{d-1} \times \{1\}$, respectively. In particular, we obtain that P_0 is a $\mathbb{Z}^{d-1}$-maximal $\frac{1}{2}\mathbb{Z}^{d-1}$-polytope. Narrowing the focus to the case of dimension three, we then make use of the fact that P_0 has to be one of the four $\mathbb{Z}^2$-maximal $\frac{1}{2}\mathbb{Z}^2$-polytopes which we enumerated in Section 2.1. Based on that, we classify all $\mathbb{Z}^3$-maximal polytopes in $\mathcal{P}(\mathbb{Z}^3)$ which have lattice width two. It turns out that every such polytope is also $\mathbb{R}^3$-maximal.

In Section 2.3, we complete the proof of Theorem 1.3 by a computer search. To this end, we develop an algorithm which finds all $\mathbb{Z}^3$-maximal polytopes in $\mathcal{P}(\mathbb{Z}^3)$ with lattice width at least three and verifies that all of them are also $\mathbb{R}^3$-maximal. To be able to enumerate all such polytopes, we establish bounds on the volume, the first successive minimum and the lattice diameter of $\mathbb{Z}^3$-maximal $\mathbb{Z}^3$-polytopes with lattice width at least three, making use of classical results from the geometry of numbers. In the last section, we give the proof of Theorem 1.5 and complete the proof of Theorem 1.6 by providing examples why (1.5) does not hold for any pairs of (d, s) other than those claimed in the theorem.

2.1 Half-integral lattice-free polyhedra in dimension two

It will turn out that in our proof of Theorem 1.3, the class of $\mathbb{Z}^2$-maximal lattice-free polytopes in $\mathcal{P}(\frac{1}{2}\mathbb{Z}^2)$ will play a particular role. Therefore, we analyze this class as a preparation for our proof of Theorem 1.3. Our results in this section also show that (1.5) holds for $d = 2, s = 2$. Since $\mathcal{P}(\mathbb{Z}^2) \subseteq \mathcal{P}(\frac{1}{2}\mathbb{Z}^2)$, the correctness of (1.5) for $d = 2, s = 1$ also follows directly from the case $s = 2$.

We make use of the following characterization of $\mathbb{R}^2$-maximal lattice-free convex sets in $\mathbb{R}^2$. Although the characterization does not seem to be available in the literature in precisely this form, it is largely known from [Hur90], [DW10, Proposition 1] and [AW12].

Theorem 2.1 (Classification of maximal lattice-free sets in dimension two). *Let L be an $\mathbb{R}^2$-maximal lattice-free convex set in $\mathbb{R}^2$. Then there exists a unimodular transformation φ such that $\varphi(L) \in \mathcal{L}_1 \cup \ldots \cup \mathcal{L}_5$, where $\mathcal{L}_1, \ldots, \mathcal{L}_5$ are the following families.*

(a) *$\mathcal{L}_1$ consists of exactly one polyhedron, namely the unbounded set* $[0, 1] \times \mathbb{R}$.

(b) *$\mathcal{L}_2$ is the set of all 'axis-aligned' triangles with vertices v_1, v_2, v_3 such that v_1 coincides with the vertex o of the square* $[0, 1]^2$, *the vertices v_2, v_3 satisfy*

$$v_2 \in (1, +\infty) \times \{0\}, \qquad v_3 \in \{0\} \times (1, +\infty)$$

and for the vertices $e_1, e_2, e_1 + e_2$ of the square $[0, 1]^2$ *one has*

$$e_1 \in (v_1, v_2), \qquad e_2 \in (v_1, v_3), \qquad e_1 + e_2 \in (v_2, v_3).$$

(c) *$\mathcal{L}_3$ is the set of triangles with vertices v_1, v_2, v_3 satisfying*

$$v_1 \in (-\infty, 0) \times \{0\}, \qquad v_2 \in (1, +\infty) \times \{0\}, \qquad v_3 \in (0, 1) \times (1, +\infty)$$

and such that for the vertices $o, e_1, e_2, e_1 + e_2$ of the square $[0, 1]^2$ *one has*

$$o, e_1 \in (v_1, v_2), \qquad e_2 \in (v_1, v_3), \qquad e_1 + e_2 \in (v_2, v_3).$$

(d) *$\mathcal{L}_4$ is the set of triangles with vertices v_1, v_2, v_3 satisfying*

$$v_1 \in \left\{(x_1, x_2) \in \mathbb{R}^2 \,:\, x_2 > 1,\, 0 < x_1 + x_2 < 1\right\},$$
$$v_2 \in \left\{(x_1, x_2) \in \mathbb{R}^2 \,:\, 0 < x_1 < 1,\, x_1 + x_2 < 0\right\},$$
$$v_3 \in \left\{(x_1, x_2) \in \mathbb{R}^2 \,:\, x_1 > 1,\, 0 < x_2 < 1\right\}$$

and such that for the vertices o, e_1, e_2 of the triangle $\operatorname{conv}(o, e_1, e_2)$ *one has*

$$o \in (v_1, v_2), \qquad e_1 \in (v_2, v_3), \qquad e_2 \in (v_3, v_1).$$

(e) $\mathcal{L}_5$ *is the set of quadrilaterals with vertices* v_1, v_2, v_3, v_4 *satisfying*

$$v_1 \in (-\infty, 0) \times (0,1), \qquad v_2 \in (0,1) \times (-\infty, 0),$$
$$v_3 \in (1, +\infty) \times (0,1), \qquad v_4 \in (0,1) \times (1, +\infty),$$

and such that for the vertices $o, e_1, e_2, e_1 + e_2$ *of the square* $[0,1]^2$ *one has*

$$o \in (v_1, v_2), \qquad e_1 \in (v_2, v_3), \qquad e_1 + e_2 \in (v_3, v_4), \qquad e_2 \in (v_4, v_1).$$

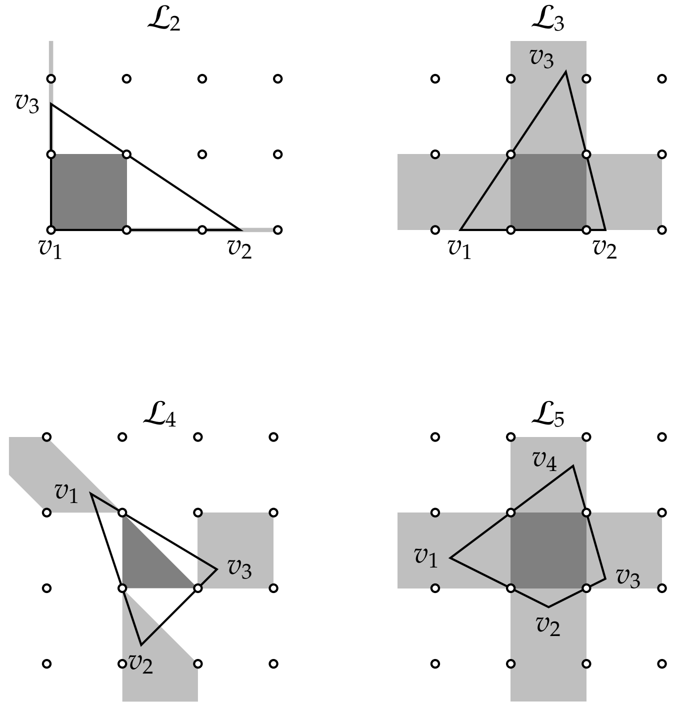

Figure 2.1: Illustration of the classes $\mathcal{L}_2, \ldots, \mathcal{L}_5$ of Theorem 2.1. The area shaded in darker grey is $[0,1]^2$ for $\mathcal{L}_2$, $\mathcal{L}_3$, $\mathcal{L}_5$ and $\mathrm{conv}(o, e_1, e_2)$ for $\mathcal{L}_4$. The areas shaded in light grey are the regions containing the vertices of $\varphi(L)$.

Proof. If L is unbounded, then in view of Theorem 1.1(b), it is unimodularly equivalent to $[0,1] \times \mathbb{R} \in \mathcal{L}_1$. If L is bounded, Theorem 1.1(a) yields that L is either a triangle or a quadrilateral and by Theorem 1.1(c) each edge of L is blocked. In what follows, we will need the following well-known assertion.

Claim 2.1.1. Let $P \in \mathcal{P}(\mathbb{Z}^2)$ be such that $\mathrm{vert}(P) = P \cap \mathbb{Z}^2$. Then $P \simeq [0,1]^2$ or $P \simeq \mathrm{conv}(o, e_1, e_2)$.

Proof of Claim. First, we claim that P has at most four vertices. Otherwise, two vertices of P, say x and y, have to be congruent modulo 2 in each coordinate and hence, $\frac{1}{2}(x+y)$ is in $P \cap \mathbb{Z}^2$ but not a vertex, a contradiction. Hence, P is either a triangle or a quadrilateral. If P is a triangle, then by Pick's formula (see [Pic99]) it has area 1/2. Since we can assume w.l.o.g. that one vertex of the triangle is o, we can denote the remaining two vertices by v_1, v_2 and compute the area of P as $1/2 \cdot \det(v_1, v_2)$. Hence, $\det(v_1, v_2) = 1$, i.e., v_1, v_2

form a basis of $\mathbb{Z}^2$ and can be mapped to e_1, e_2 using a unimodular transformation. If P is a quadrilateral, we can again employ Pick's formula to obtain that the area of P is one. Again, we assume that one vertex of P is o. Let v_1, v_2 be the two vertices of P adjacent to o. By our previous arguments, we can apply a unimodular transformation mapping v_1, v_2 to e_1, e_2. Since in the resulting integral quadrilateral, the fourth vertex is not adjacent to o, it has to be contained in $(0, \infty) \times (0, \infty)$. Since the area of the quadrilateral is one, we obtain that this vertex has to be $e_1 + e_2$, which proves the claim.

Furthermore, let v be a vertex of P and v_1, v_2 the vertices of P adjacent to v. By our previous argument, we can apply a unimodular transformation which maps the triangle $\operatorname{conv}(o, v_1, v_2)$ onto $\operatorname{conv}(o, e_1, e_2)$ such that v is mapped onto o. Let v_3 be the remaining vertex of P. Then $\varphi(v_3)$ is not adjacent to o in $\varphi(P)$ and hence, it is contained in the positive orthant. Furthermore, since $\varphi(P)$ is an integral quadrilateral, $\varphi(v_3)$ cannot be included in $(0, \infty) \times \{0\}$ or $\{0\} \times \infty$. Hence, $[0, 1]^2 \subseteq \varphi(P)$. Since $\varphi(P)$ has area one, we have the equality $[0, 1]^2 = \varphi(P)$. ∎

In the case that L is a quadrilateral, we have that each of the four edges contains precisely one integral point in its relative interior: suppose that one edge contains two integral points u_1, u_2 in its relative interior such that $(u_1, u_2) \cap \mathbb{Z}^2 = \emptyset$. Then one of the two points, say, u_1, has to be congruent modulo two to a point u blocking one of the remaining edges and hence $\frac{1}{2}(u_1 + u) \in \operatorname{int}(L)$ is integral, a contradiction. Hence, we can use the claim to see that there exists a unimodular transformation φ mapping the four integral points blocking the edges of L onto $\{0, 1\}^2$. It is then straightforward to see that φ maps the vertices of L on points v_1, v_2, v_3, v_4 as specified in (e) and hence, $\varphi(L) \in \mathcal{L}_5$.

This leaves the case that L is a triangle. Assume first that L has an integral vertex v. Then we can choose an integral point in the relative interior of each of the three edges of L such that those three points together with v form an integral quadrilateral not containing any other integral points. Hence, in view of the claim, by applying a suitable unimodular transformation φ, we can map v onto o and the three integral points we chose onto $e_1, e_2, e_1 + e_2$. Thus, $\varphi(L) \in \mathcal{L}_2$. We now switch to the case that L does not have integral vertices. If L contains at least four integral points, then the relative interior of some edge of L contains at least two integral points u_1, u_2 such that $(u_1, u_2) \cap \mathbb{Z}^2 = \emptyset$. Together with one point from the relative interior of each of the two remaining edges, they form an integral quadrilateral not containing any other integral points. Then applying the claim again, we can map this quadrilateral onto $[0, 1]^2$ using a unimodular transformation φ which maps $\{u_1, u_2\}$ onto $\{o, e_1\}$. It is then straightforward to see that $\varphi(L) \in \mathcal{L}_3$.

This leaves the case that L has precisely three integral points. Again in view of the claim, we can apply a unimodular transformation φ such that $\varphi(L) \cap \mathbb{Z}^2 = \{o, e_1, e_2\}$ and $\varphi(L)$ has vertices v_1, v_2, v_3 with $o \in (v_1, v_2)$, $e_1 \in (v_2, v_3)$ and $e_2 \in (v_3, v_1)$. We prove $\varphi(L) \in \mathcal{L}_4$, for which it remains to show that v_1, v_2, v_3 are situated as claimed in (d). We can express o, e_1, e_2 with respect to v_1, v_2, v_3 as follows: there exist $0 < \alpha_1, \alpha_2, \alpha_3 < 1$ such that

$$\begin{aligned} o &= \alpha_1 v_1 + (1 - \alpha_1) v_2, \\ e_1 &= \alpha_2 v_2 + (1 - \alpha_2) v_3, \\ e_2 &= \alpha_3 v_3 + (1 - \alpha_3) v_1. \end{aligned} \tag{2.1}$$

We now want to express v_1, v_2, v_3 with respect to o, e_1, e_2. We follow the argumentation in [AW12, Proof of Lemma 4.2] and [Hur90, (7)] and translate (2.1) into the following matrix representation:

$$\begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ v_1 & v_2 & v_3 \end{pmatrix} \begin{pmatrix} \alpha_1 & 0 & 1-\alpha_3 \\ 1-\alpha_1 & \alpha_2 & 0 \\ 0 & 1-\alpha_2 & \alpha_3 \end{pmatrix}.$$

The determinant of the matrix involving $\alpha_1, \alpha_2, \alpha_3$ is $D := \alpha_1\alpha_2\alpha_3 + (1-\alpha_1)(1-\alpha_2)(1-\alpha_3) > 0$. Hence, this matrix is invertible and we can directly compute the components of v_1, v_2, v_3 via Cramer's rule:

$$\begin{aligned} v_1 &= \frac{1}{D}\Big(-(1-\alpha_1)\alpha_3,\ (1-\alpha_1)(1-\alpha_2)\Big), \\ v_2 &= \frac{1}{D}\Big(\alpha_1\alpha_3,\ -\alpha_1(1-\alpha_2)\Big), \\ v_3 &= \frac{1}{D}\Big((1-\alpha_1)(1-\alpha_3),\ \alpha_1\alpha_2\Big). \end{aligned} \tag{2.2}$$

In [AW12, Lemma 5.1] it was shown that either

$$\alpha_i + \alpha_j < 1 \text{ for every } 1 \le i < j \le 3 \tag{2.3}$$

or $\alpha_i + \alpha_j > 1$ for every $1 \le i < j \le 3$. In the case that (2.3) holds, it is straightforward to verify that the vertices v_1, v_2, v_3 are situated as claimed. If $\alpha_i + \alpha_j > 1$ for every $i, j \in \{1, 2, 3\}$ holds instead of (2.3), one can instead prove in a straightforward way that this yields the following regions for the vertices v_1, v_2, v_3:

$$\begin{aligned} v_1 &\in \Big\{(x_1, x_2) \in \mathbb{R}^2 \ :\ x_1 + x_2 < 0,\ 0 < x_2 < 1\Big\}, \\ v_2 &\in \Big\{(x_1, x_2) \in \mathbb{R}^2 \ :\ x_1 > 1,\ 0 < x_1 + x_2 < 1\Big\} \\ v_3 &\in \Big\{(x_1, x_2) \in \mathbb{R}^2 \ :\ 0 < x_1 < 1,\ x_2 > 1\Big\}. \end{aligned}$$

Applying a unimodular transformation swapping e_1 and e_2 (i.e. the reflection with respect to the line $\Big\{(x_1, x_2) \in \mathbb{R}^2 \ :\ x_1 = x_2\Big\}$) and appropriately re-indexing the vertices yields a triangle in $\mathcal{L}_4$. This is again straightforward to verify. □

Based on the previous theorem, we now enumerate all $\mathbb{Z}^2$-maximal lattice-free half-integral polygons up to unimodular equivalence. The polygons Q_2, Q_3, Q_4, Q_5 of the following theorem are depicted in Figure 1.5 on page 10.

Theorem 2.2 ($\mathbb{Z}^2$-maximal polyhedra in $\mathcal{P}(\frac{1}{2}\mathbb{Z}^2)$). *Let $Q \in \mathcal{P}(\frac{1}{2}\mathbb{Z}^2)$. Then Q is $\mathbb{Z}^2$-maximal lattice-free if and only if $Q \simeq Q_i$ for some $i \in \{1, \ldots, 5\}$, where*

Q_1 is the unbounded polyhedron $[0, 1] \times \mathbb{R}$,

Q_2 is the triangle with vertices $(0, 0), (2, 0), (0, 2)$,

Q_3 is the triangle with vertices $(\frac{1}{2} \pm \frac{3}{2}, 0), (\frac{1}{2}, \frac{3}{2})$,

Q_4 is the triangle with vertices $(\frac{1}{2} \pm 1, 0), (\frac{1}{2}, 2)$,

Q_5 is the quadrilateral with vertices $(-\frac{1}{2}, \frac{1}{2}), (\frac{1}{2}, \frac{3}{2}), (\frac{3}{2}, \frac{1}{2}), (\frac{1}{2}, -\frac{1}{2})$.

In particular, Q is $\mathbb{Z}^2$-maximal lattice-free if and only if Q is $\mathbb{R}^2$-maximal lattice-free.

Proof. We first remark that in order to prove the statement that Q is $\mathbb{Z}^2$-maximal if and only if Q is $\mathbb{R}^2$-maximal, it suffices to prove that Q is $\mathbb{Z}^2$-maximal lattice-free if and only if $Q \simeq Q_i$ for some $i \in \{1, \dots, 5\}$. To see this, observe that every $\mathbb{R}^2$-maximal polygon is $\mathbb{Z}^2$-maximal by definition. On the other hand, assume that we have shown that if Q is $\mathbb{Z}^2$-maximal, we have $Q \simeq Q_i$ for some $i \in \{1, \dots, 5\}$. Then from the fact that for every $i \in \{1, \dots, 5\}$ each facet of Q_i is blocked (see also Figure 1.5), we have that Q is also $\mathbb{R}^2$-maximal.

As we have just observed, Q_i is $\mathbb{R}^2$-maximal and thus, in particular, $\mathbb{Z}^2$-maximal for every $i \in \{1, \dots, 5\}$. Hence, it follows that if Q is unimodularly equivalent to Q_i for some $i \in \{1, \dots, 5\}$, it is $\mathbb{Z}^2$-maximal. Conversely, let $Q \in \mathcal{P}(\frac{1}{2}\mathbb{Z}^2)$ be $\mathbb{Z}^2$-maximal lattice-free. We show that then, $Q \simeq Q_i$ for some $i \in \{1, \dots, 5\}$.

It is known, see for example [AW12, Proposition 3.1], that every lattice-free set in $\mathbb{R}^2$ is a subset of an $\mathbb{R}^2$-maximal lattice-free set L. In particular, there exists an $\mathbb{R}^2$-maximal lattice-free set L such that $Q \subseteq L$. By applying a suitable unimodular transformation, we can assume $L \in \mathcal{L}_i$ with $i \in \{1, \dots, 5\}$, where $\mathcal{L}_1, \dots, \mathcal{L}_5$ are defined as in Theorem 2.1. We observe that one has

$$\operatorname{conv}(L \cap \mathbb{Z}^2) \subseteq Q \tag{2.4}$$

and

$$Q \subseteq \operatorname{conv}\left(L \cap \frac{1}{2}\mathbb{Z}^2\right), \tag{2.5}$$

where (2.4) holds since Q is $\mathbb{Z}^2$-maximal and (2.5) holds since $Q \in \mathcal{P}(\frac{1}{2}\mathbb{Z}^2)$ and $Q \subseteq L$.

Case 1: $L \in \mathcal{L}_1$. Then $L = [0,1] \times \mathbb{R}$ and hence, (2.4) together with (2.5) yields $Q = L$.

Case 2: $L \in \mathcal{L}_2$. In view of (2.4), we have $[0,1]^2 \subseteq Q$. From the definition of $\mathcal{L}_2$, we have that every point of $L \cap \left(\frac{1}{2}\mathbb{Z}^2 \setminus [0,1]^2\right)$ has one of the following forms:

$$\begin{aligned} &(3/2, 0) + k\,(1/2, 0)\,, && (0, 3/2) + k\,(0, 1/2)\,, \\ &(3/2, 1/2) + k\,(1/2, 0)\,, && (1/2, 3/2) + k\,(0, 1/2)\,, \end{aligned}$$

where k is some non-negative integer; see also Figure 2.2.

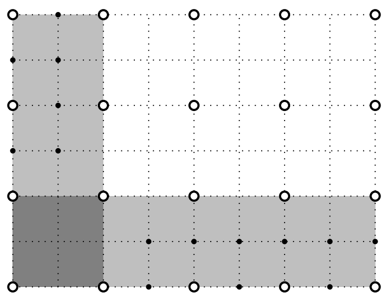

Figure 2.2: Illustration of Case 2 in the proof of Theorem 2.2: Q is contained in the shaded area, the white dots are the elements of $\mathbb{Z}^2$ and the black dots are the elements of $\frac{1}{2}\mathbb{Z}^2$ involved in the proof.

Let us first assume $(\frac{3}{2}, \frac{1}{2})$ and $(\frac{1}{2}, \frac{3}{2})$ are both in Q. Since $(1,1)$ is contained in the relative interior of the line segment between these two points, $\left[(\frac{3}{2}, \frac{1}{2}), (\frac{1}{2}, \frac{3}{2})\right]$ is contained in an edge of Q. Consequently, $Q \subseteq \operatorname{conv}\big((0,0),(2,0),(0,2)\big) = Q_2$ and since Q is $\mathbb{Z}^2$-maximal, this implies the equality $Q = Q_2$. Let us now assume that $(\frac{1}{2}, \frac{3}{2})$ or $(\frac{3}{2}, \frac{1}{2})$ is not in Q. By applying a linear unimodular transformation swapping e_1 and e_2 if necessary, we can assume $(\frac{1}{2}, \frac{3}{2}) \notin Q$. This implies that no point of the form $\left(\frac{1}{2}, \frac{3}{2}\right) + k\left(0, \frac{1}{2}\right)$ is in Q. Likewise, since $(1,1) \in Q$ and $(\frac{1}{2}, \frac{3}{2}) \in [(1,1),(0,2)]$, we have $(0,2) \notin Q$ and consequently, $\left(0, \frac{3}{2}\right) + k\left(0, \frac{1}{2}\right) \notin Q$ for every $k \geq 1$. Hence, either $(0, 3/2) \in Q$ or $Q \subseteq [0, +\infty) \times [0,1]$. If $(0,3/2) \in Q$, we have $Q \subseteq \operatorname{conv}\big((0,0),(0,3/2),(3,0)\big) \simeq Q_3$ and the $\mathbb{Z}^2$-maximality of Q implies the equality $Q \simeq Q_3$. Otherwise, we then have $Q \subseteq [0,+\infty) \times [0,1] \subsetneq \mathbb{R} \times [0,1]$, a contradiction to the $\mathbb{Z}^2$-maximality of Q.

Case 3: $L \in \mathcal{L}_3$. In view of (2.4), we have $[0,1]^2 \subseteq Q$. From the definition of $\mathcal{L}_3$, we have that every point in $L \cap \left(\frac{1}{2}\mathbb{Z}^2 \setminus [0,1]^2\right)$ has one of the following forms:

$$\begin{array}{lll} (3/2,0) + k\,(1/2,0)\,, & (-1/2,0) + k\,(-1/2,0)\,, & (1/2,3/2) + k\,(0,1/2)\,, \\ (3/2,1/2) + k\,(1/2,0)\,, & (-1/2,1/2) + k\,(-1/2,0)\,, & \end{array}$$

where k is some non-negative integer; see also Figure 2.3.

Analogously to Case 2, we can now restrict the values of k for each of the five forms: if a point of any of the forms is in L for which the value of k is too large, then, because $(0,1)$ and $(1,1)$ are in the boundary of L, we have that $L \cap \frac{1}{2}\mathbb{Z}^2$ is contained in $\mathbb{R} \times [0,1]$ or $[0,1] \times \mathbb{R}$. In those cases, in view of (2.5), Q is contained in a lattice-free unbounded polyhedron in $\mathcal{P}(\mathbb{Z}^2)$. Since Q is bounded, this inclusion is strict, a contradiction to the $\mathbb{Z}^2$-maximality of Q. This leaves a finite number of points in $\frac{1}{2}\mathbb{Z}^2$ which can be in Q and from (2.5), we obtain that the vertices of Q which are not in $\{0,1\}^2$ are among the points

$$\big(-1,0\big), \big(-\frac{1}{2},0\big), \big(-\frac{1}{2},\frac{1}{2}\big), \big(\frac{1}{2},\frac{3}{2}\big), \big(\frac{1}{2},1\big), \big(\frac{3}{2},0\big), \big(\frac{3}{2},\frac{1}{2}\big), \big(2,0\big).$$

It can be checked in a straightforward way that the only $\mathbb{Z}^2$-maximal lattice-free polygons in $\mathcal{P}(\frac{1}{2}\mathbb{Z}^2)$ with vertices in this set are Q_3 and Q_4.

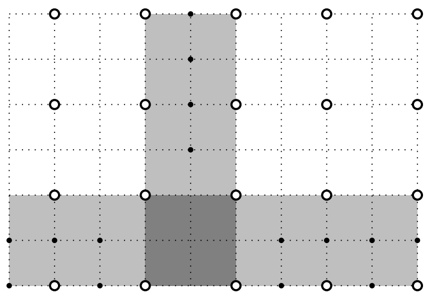

Figure 2.3: Illustration of Case 3 in the proof of Theorem 2.2: Q is contained in the shaded area, the white dots are the elements of $\mathbb{Z}^2$ and the black dots are the elements of $\frac{1}{2}\mathbb{Z}^2$ involved in the proof.

Case 4: $L \in \mathcal{L}_4$. Here, we deduce $\Delta := \operatorname{conv}\big((0,0),(0,1),(1,0)\big) \subseteq Q$ from (2.4). From the definition of $\mathcal{L}_4$, we have that every point of $L \cap \left(\frac{1}{2}\mathbb{Z}^2 \setminus \Delta\right)$ has one of the following forms:

$$(1,1/2) + k\,(1/2,0)\,, \qquad (1/2,-1/2) + k\,(0,-1/2)\,, \qquad (-1/2,1) + k\,(-1/2,1/2)\,,$$

where k is some non-negative integer; see also Figure 2.4. As in the previous cases, we exploit the fact that $(0,0),(0,1),(1,0)$ lie in the boundary of L to obtain bounds on k

for each of the three forms: if k is too large, we again deduce that Q is contained in an unbounded set unimodularly equivalent to $\mathbb{R}\times[0,1]$. Since Q is bounded, this contradicts the $\mathbb{Z}^2$-maximality of Q. In fact, we have $k < 2$ for each of the three forms. In view of (2.5), this yields a set of points of $\frac{1}{2}\mathbb{Z}^2$ which can be vertices of Q. The verification that no lattice-free half-integral polygon with vertices in this set is $\mathbb{Z}^2$-maximal is left to the reader.

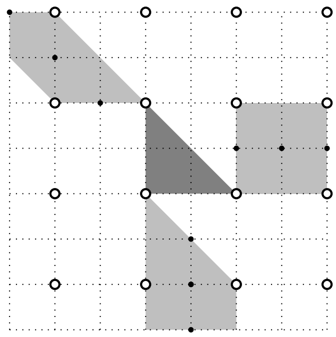

Figure 2.4: Illustration of Case 4 in the proof of Theorem 2.2: the vertices of Q are contained in the shaded area, the white dots are the elements of $\mathbb{Z}^2$ and the black dots are the elements of $\frac{1}{2}\mathbb{Z}^2$ involved in the proof.

Case 5: $L \in \mathcal{L}_5$. In view of (2.4), we have $[0,1]^2 \subseteq L$. Furthermore, it is easy to see that every point of $(L \cap \frac{1}{2}\mathbb{Z}^2) \setminus \{0,1\}^2$ has one of the following forms:

$$\left(\frac{1}{2},\frac{1}{2}\right) \pm k\left(\frac{1}{2},0\right), \qquad \left(\frac{1}{2},\frac{1}{2}\right) \pm k\left(0,\frac{1}{2}\right),$$

where k is an integer and $k \geq 2$; see also Figure 2.5. One can observe that, since the points of $\{0,1\}^2$ are in the boundary of Q, if there exists a point of any of the four forms with $k > 2$ we have that $Q \subseteq L \cap \frac{1}{2}\mathbb{Z}^2$ is contained in $\mathbb{R} \times [0,1]$ or $[0,1] \times \mathbb{R}$. Since Q is bounded, this contradicts the $\mathbb{Z}^2$-maximality of Q. This yields $Q \subseteq Q_5$. It is straightforward to check that every $\frac{1}{2}\mathbb{Z}^2$-maximal integral polygon properly contained in Q_5 is not $\mathbb{Z}^2$-maximal, which implies $Q = Q_5$. □

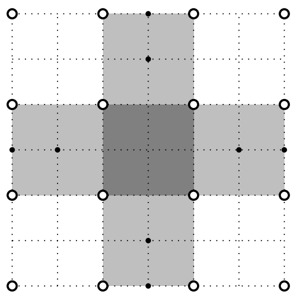

Figure 2.5: Illustration of Case 5 in the proof of Theorem 2.2: Q is contained in the shaded area, the white dots are the elements of $\mathbb{Z}^2$ and the black dots are the elements of $\frac{1}{2}\mathbb{Z}^2$ involved in the proof.

2.2 $\mathbb{Z}^d$-maximal lattice-free integral polytopes with lattice width two

As explained in the proof strategy section, we need to prove the equivalence of $\mathbb{Z}^3$-maximality and $\mathbb{R}^3$-maximality only for polytopes in $\mathcal{P}(\mathbb{Z}^3)$, because for unbounded polyhedra in $\mathcal{P}(\mathbb{Z}^3)$ this equivalence is straightforward to see in view of Theorem 1.2(b).

In the beginning of the previous section, we remarked that $\mathbb{Z}^2$-maximal lattice-free polytopes in $\mathcal{P}(\frac{1}{2}\mathbb{Z}^2)$ appear naturally when considering $\mathbb{Z}^3$-maximal lattice-free polytopes in $\mathcal{P}(\mathbb{Z}^3)$. More precisely, they appear as intersections of $\mathbb{Z}^3$-maximal lattice-free polytopes in $\mathcal{P}(\mathbb{Z}^3)$ with lattice hyperplanes, as we will explain in detail in this section. However, where possible, we do not restrict ourselves to dimension three but instead present the results in arbitrary dimension $d \geq 3$. Our general setting is the following: let $P \in \mathcal{P}(\mathbb{Z}^d)$ be a $\mathbb{Z}^d$-maximal lattice-free polytope with lattice width two, i.e, there exists a primitive vector $u \in \mathbb{Z}^d \setminus \{o\}$ such that $\mathrm{w}(P, u) = 2$. Let A be a unimodular matrix and let b be an integral vector. Then $\varphi\colon \mathbb{R}^d \to \mathbb{R}^d$ given by $\varphi(x) = (A^{-1})^\top x + b$ is a unimodular transformation. Note that $\mathrm{w}(\varphi(P), A(u)) = \mathrm{w}(P, u) = 2$. In the following, by applying a linear unimodular transformation mapping u to e_d and translating by a suitable integral vector, we can therefore always assume that the lattice width of P is attained for e_d and that $P \subseteq \mathbb{R}^{d-1} \times [-1, 1]$.

Properties of faces and cross-sections

If $P \in \mathcal{P}(\mathbb{Z}^d)$ is contained in $\mathbb{R}^{d-1} \times [-1, 1]$ and has lattice width two, then the integral points of P are contained in $\mathbb{R}^{d-1} \times \{-1, 0, 1\}$ and in particular, the latter set contains all vertices of P. Note that $\mathbb{R}^{d-1} \times \{0\}$ meets the interior of P and since P is lattice-free, this allows us to derive a characterization of $P \cap \mathbb{R}^{d-1} \times \{0\}$ in the beginning of this section. We then provide relations between $P \cap \mathbb{R}^{d-1} \times \{0\}$ and $F(P, e_d), F(P, -e_d)$. To characterize $P \cap \mathbb{R}^{d-1} \times \{0\}$, we first need the following lemmas, where H plays the role of $\mathbb{R}^{d-1} \times \{0\}$.

Lemma 2.3. *Let H be an affine subspace of $\mathbb{R}^d$. Let A, B be convex subsets of $\mathbb{R}^d$. Then the following statements hold:*

(a) If $A \subseteq H$, then $H \cap \mathrm{conv}(A \cup B) = \mathrm{conv}\big(A \cup (H \cap B)\big)$.

(b) If $A \not\subseteq H$, $B \not\subseteq H$ and $(1 - \lambda)A + \lambda B \subseteq H$ for some $0 < \lambda < 1$, then

$$H \cap \mathrm{conv}(A \cup B) = (1 - \lambda)A + \lambda B.$$

Proof. (a): Let $A \subseteq H$. It suffices to verify the inclusion $H \cap \mathrm{conv}(A \cup B) \subseteq \mathrm{conv}\big(A \cup (H \cap B)\big)$; the reverse inclusion is trivial, as both A and $H \cap B$ are subsets of $H \cap \mathrm{conv}(A \cup B)$. Consider an arbitrary $x \in H \cap \mathrm{conv}(A \cup B)$. That is, x is a point of H that can be written as a convex combination of some $a \in A$ and $b \in B$. If $x = a$, then in particular $x \in A$ and we are done. If not, then b lies on the line passing through x and a. Since $x, a \in H$, this line lies in H and therefore, we also have $b \in H$.

(b): Let $A \not\subseteq H$ and $B \not\subseteq H$. It suffices to verify the inclusion $H \cap \mathrm{conv}(A \cup B) \subseteq (1 - \lambda)A + \lambda B$, as the reverse inclusion is trivial. Fix an affine function $f : \mathbb{R}^d \to \mathbb{R}$ such that $H = \big\{x \in \mathbb{R}^d \,:\, f(x) = 0\big\}$. Since $H \neq \mathbb{R}^d$, the function f is not identically equal to zero. Applying f to $(1 - \lambda)A + \lambda B \subseteq H$, we arrive at $(1 - \lambda)f(A) + \lambda f(B) \subseteq f(H)$, where by the choice of f, one has $f(H) = \{0\}$. The latter shows that $f(A)$ and $f(B)$ must be singletons. We interpret the singletons $f(A), f(B), f(H)$ as real values, where $f(H) = 0$. Let $f(A) = \alpha$

and $f(B) = \beta$. Since A and B are not subsets of H, we have $\alpha, \beta \neq 0$. Since $(1-\lambda)\alpha + \lambda\beta = 0$, we have $\alpha \neq \beta$. Let μ be a parameter in the range $[0, 1]$. By our previous arguments, we have shown that $(1-\mu)\alpha + \mu\beta = 0$ if and only if $\mu = \lambda$. Thus, we have shown that $(1-\mu)A + \mu B$ is disjoint with H unless $\mu = \lambda$. Consequently,

$$H \cap \operatorname{conv}(A \cup B) = H \cap \bigcup_{\mu \in [0,1]} \Big((1-\mu)A + \mu B)\Big) = H \cap \Big((1-\lambda)A + \lambda B\Big) = (1-\lambda)A + \lambda B$$

and hence we obtain (b). □

Theorem 2.4. *Let $P \in \mathcal{P}(\mathbb{Z}^d)$ be a $\mathbb{Z}^d$-maximal lattice-free polytope such that $P \subseteq \mathbb{R}^{d-1} \times [-1, 1]$ and $\mathrm{w}(P, e_d) = 2$. For $i \in \{-1, 0, 1\}$, let $P_i := \Big\{x \in \mathbb{R}^{d-1} : (x, i) \in P\Big\}$. Then the following statements hold:*

(a) P_0 belongs to $\mathcal{P}(\frac{1}{2}\mathbb{Z}^{d-1})$ and is $\mathbb{Z}^{d-1}$-maximal lattice-free.

(b) P_{-1} and P_1 belong to $\mathcal{P}(\mathbb{Z}^{d-1})$ and have the following properties relative to P_0:

(b1) P_1 and P_{-1} are integral polytopes satisfying

$$P_1 + P_{-1} \subseteq 2P_0. \tag{2.6}$$

(b2) The pair (P_1, P_{-1}) satisfies the following maximality condition: For all polytopes $R_{-1}, R_1 \in \mathcal{P}(\mathbb{Z}^{d-1})$ satisfying $P_1 \subseteq R_1$, $P_{-1} \subseteq R_{-1}$ and $R_1 + R_{-1} \subseteq 2P_0$, one has $R_1 = P_1$ and $R_{-1} = P_{-1}$.

(b3) P_1 and P_{-1} satisfy

$$2\operatorname{conv}(\operatorname{vert}(P_0) \setminus \mathbb{Z}^{d-1}) \subseteq P_1 + P_{-1}. \tag{2.7}$$

Proof. Throughout the proof, we will use the following notation: H denotes the hyperplane $\mathbb{R}^{d-1} \times \{0\}$ and for $i \in \{-1, 0, 1\}$, we write $\overline{P}_i := P_i \times \{i\}$. We will repeatedly make use of the fact that $P \subseteq \mathbb{R}^{d-1} \times [-1, 1]$ and hence, $P \cap \mathbb{Z}^d \subseteq \mathbb{Z}^{d-1} \times \{-1, 0, 1\}$. In particular, taking into account $P \in \mathcal{P}(\mathbb{Z}^d)$, we have

$$\operatorname{vert}(P) \subseteq \overline{P}_{-1} \cup \overline{P}_0 \cup \overline{P}_1. \tag{2.8}$$

The assumption $\mathrm{w}(P, e_d) = 2$ implies $P_1 \neq \emptyset$ and $P_{-1} \neq \emptyset$.

We use the representation $P = \operatorname{conv}(A \cup B)$ with

$$A := \operatorname{conv}(H \cap \operatorname{vert}(P)) \qquad \text{and} \qquad B := \operatorname{conv}\Big(\overline{P}_{-1} \cup \overline{P}_1\Big).$$

From (2.8), it is obvious that $\operatorname{conv}(A \cup B)$ is indeed P. Hence

$$\overline{P}_0 = H \cap \operatorname{conv}(A \cup B) = \operatorname{conv}\Big(A \cup (H \cap B)\Big), \tag{2.9}$$

where the second equality is a consequence of Lemma 2.3(a).

Assertion (a): We first prove that P_0 belongs to $\mathcal{P}(\frac{1}{2}\mathbb{Z}^d)$, which is equivalent to $\operatorname{vert}(\overline{P}_0) \subseteq \frac{1}{2}\mathbb{Z}^{d-1} \times \{0\}$. In (2.9), the set A is an integral polytope, possibly empty. Thus, it suffices to verify that the vertices of $H \cap B$ belong to $\frac{1}{2}\mathbb{Z}^{d-1} \times \{0\}$. In fact, Lemma 2.3(b) yields

$$H \cap B = H \cap \operatorname{conv}\Big(\overline{P}_{-1} \cup \overline{P}_1\Big) = \frac{1}{2}\overline{P}_{-1} + \frac{1}{2}\overline{P}_1. \tag{2.10}$$

Thus, since $\overline{P}_{-1}$ and $\overline{P}_1$ are integral polytopes, $H \cap B$ is half-integral and so is P_0.

Next, we show that P_0 is lattice-free. Indeed, by [Roc97, Corollary 6.5.1] we have

$$\operatorname{relint}(\overline{P}_0) \cap \mathbb{Z}^d = \operatorname{relint}(P \cap H) \cap \mathbb{Z}^d = \operatorname{relint}(P) \cap H \cap \mathbb{Z}^d \subseteq \operatorname{relint}(P) \cap \mathbb{Z}^d,$$

which is empty since P is lattice-free. Hence, $\operatorname{relint}(\overline{P}_0)$ does not contain points of $\mathbb{Z}^{d-1} \times \{0\}$ and thus, P_0 is lattice-free.

To complete the proof of (a), it remains to show that P_0 is $\mathbb{Z}^{d-1}$-maximal. Let $p \in \mathbb{Z}^{d-1} \times \{0\} \setminus \overline{P}_0$. As $p \notin P$ and P is $\mathbb{Z}^d$-maximal lattice-free, there exists some $z \in \mathbb{Z}^d$ in $\operatorname{int}\Big(\operatorname{conv}(P \cup \{p\})\Big)$. Since P is lattice-free, we have $z = \lambda p + (1-\lambda)x$ for some $0 < \lambda < 1$ and $x \in P$. Let x_d, p_d, z_d denote the d-th component of x, p, z, respectively. Because $x_d \in [-1, 1]$ and $p_d = 0$, we obtain $-1 < z_d < 1$ and hence $z_d = 0$. Together with [Roc97, Corollary 6.5.1], this implies

$$\begin{aligned} z \in \operatorname{relint}\Big(\operatorname{conv}(P \cup \{p\})\Big) \cap H &= \operatorname{relint}\Big(\operatorname{conv}(P \cup \{p\}) \cap H\Big) \\ &= \operatorname{relint}\Big(\operatorname{conv}(\overline{P}_0 \cup \{p\})\Big). \end{aligned}$$

Hence, P_0 is $\mathbb{Z}^{d-1}$-maximal lattice-free.

Assertion (b): Obviously, P_{-1}, P_1 are integral polytopes because $\overline{P}_{-1}, \overline{P}_1$ are faces of the integral polytope P.

(b1): We have $\frac{1}{2}\overline{P}_{-1} + \frac{1}{2}\overline{P}_1 \subseteq P$. From (2.10), we have $\frac{1}{2}\overline{P}_{-1} + \frac{1}{2}\overline{P}_1 \subseteq H$. Combining both observations leads to $\frac{1}{2}\overline{P}_{-1} + \frac{1}{2}\overline{P}_1 \subseteq H \cap P = \overline{P}_0$. This implies $\frac{1}{2}P_1 + \frac{1}{2}P_{-1} \subseteq P_0$ and hence assertion (b1) follows.

(b2): Let $R_1, R_{-1} \subseteq \mathbb{R}^{d-1}$ be integral polytopes such that $R_1 + R_{-1} \subseteq 2P_0$ and $P_1 \subseteq R_1$, $P_{-1} \subseteq R_{-1}$. Consider the integral polytope

$$R := \operatorname{conv}\Big((R_1 \times \{1\}) \cup (R_{-1} \times \{-1\}) \cup \overline{P}_0\Big),$$

which is contained in $\mathbb{R}^{d-1} \times [-1, 1]$ and contains P. We write $\overline{R}_i = R_i \times \{i\}$ for $i \in \{-1, 1\}$. Using this notation, we have

$$R \cap H = \operatorname{conv}\Big(\overline{R}_1 \cup \overline{R}_{-1} \cup \overline{P}_0\Big) \cap H = \operatorname{conv}\Big(\overline{P}_0 \cup \Big(\operatorname{conv}\Big(\overline{R}_1 \cup \overline{R}_{-1}\Big) \cap H\Big)\Big),$$

where the second equality follows from Lemma 2.3(a). Applying Lemma 2.3(b) yields

$$\operatorname{conv}\Big(\overline{R}_1 \cup \overline{R}_{-1}\Big) \cap H = \Big(\frac{1}{2}R_1 + \frac{1}{2}R_{-1}\Big) \times \{0\} \subseteq \overline{P}_0,$$

where the second equality follows from $R_1 + R_{-1} \subseteq 2P_0$. Hence, $R \cap H = \overline{P}_0$. Therefore, one has $\operatorname{relint}(H \cap R) \cap \mathbb{Z}^d = \operatorname{relint}(\overline{P}_0) \cap \mathbb{Z}^d$. By (a), P_0 is lattice-free and hence, we have $\operatorname{relint}(\overline{P}_0) \cap \mathbb{Z}^d = \emptyset$. Since $R \cap \mathbb{Z}^d \subseteq \mathbb{Z}^{d-1} \times \{-1, 0, 1\}$, where $R \cap \mathbb{Z}^{d-1} \times \{-1, 1\}$ is contained in the boundary of R, this shows that R is a lattice-free integral polytope containing P. Since P is $\mathbb{Z}^d$-maximal, we have $P = R$ and in particular, $R_1 = P_1$ and $R_{-1} = P_{-1}$.

Assertion (b3): Let $v \in \mathbb{R}^{d-1}$ be a non-integral vertex of P_0 and let $\overline{v} := (v, 0) \in \mathbb{R}^d$. Then $\overline{v}$ is not integral and since P is an integral polytope, $\overline{v} \notin \operatorname{vert}(P)$. On the other hand, since v is a vertex of P_0, $\overline{v}$ cannot be written as convex combination of any points of $P \cap H$. Thus, we have $v \notin A$ and consequently, $v \in H \cap B$. By (2.10), there exist $x_1 \in \overline{P}_1$, $x_{-1} \in \overline{P}_{-1}$ such that $\overline{v} = \frac{1}{2}x_1 + \frac{1}{2}x_{-1}$. Accordingly, $2v \in P_1 + P_{-1}$. This proves the assertion. □

Analysis of special cross-sections

From Figure 1.5 on page 10, one can make the following observation: three of the four $\mathbb{Z}^2$-maximal half-integral polytopes are simplices with the property that all of their integral vertices are unimodular. It turns out that if P_0 in the setting of Theorem 2.4 is a simplex with this property, one can extend the results about the relation between P_1, P_{-1} and P_0 presented in Theorem 2.4. In particular, to prove Theorem 1.3, this will be very useful. In what follows, we will make use of the following terminology: for a convex set $K \subseteq \mathbb{R}^d$, we say that K' is a *homothetic copy* of K if $K' = \lambda K + v$ for some $\lambda \in \mathbb{R}$ and $v \in \mathbb{R}^d$. We call K' a positive (non-negative) homothetic copy of K if λ is a positive (non-negative) number.

Lemma 2.5. *Let $Q \in \mathcal{P}(\mathbb{Z}^d)$ be a polytope such that Q is not a singleton and let v be a vertex of Q. Let $g := \gcd\Big(\{\langle w\,,\,e_i\rangle \,:\, w \in \operatorname{vert}(Q-v),\, i \in \{1,\dots,d\}\}\Big)$, i.e., g is the greatest common divisor of all the components of the vertices of $Q - v$. Let $\widetilde{Q} := \frac{1}{g}(Q-v) \in \mathcal{P}(\mathbb{Z}^d)$. Then every non-negative homothetic copy Q' of Q belonging to $\mathcal{P}(\mathbb{Z}^d)$ has the form $Q' = a\widetilde{Q} + b$, where $a \in \mathbb{N} \cup \{0\}$ and $b \in \mathbb{Z}^d$.*

Proof. Let $Q' \in \mathcal{P}(\mathbb{Z}^d)$ be a non-negative homothetic copy of Q. Since obviously Q' is then also a non-negative homothetic copy of $\widetilde{Q}$, there exist $a \geq 0$ and $b \in \mathbb{R}^d$ such that $Q' = a\widetilde{Q} + b$. By definition of $\widetilde{Q}$, one of its vertices is o. Hence, $b \in \operatorname{vert}(Q')$ and therefore, in view of $Q' \in \mathcal{P}(\mathbb{Z}^d)$, we have $b \in \mathbb{Z}^d$. Furthermore, for every vertex w' of Q, there exists a $w'' \in \operatorname{vert}(Q') \subseteq \mathbb{Z}^d$ such that $w'' = \frac{a}{g}w' - \frac{a}{g}v + b$. Since $w'' - b \in \mathbb{Z}^d$, we also have $\frac{a}{g}(w' - v) \in \mathbb{Z}^d$. In other words, we have $a \cdot \frac{\langle w'-v\,,\,e_i\rangle}{g} \in \mathbb{Z}$ for every $w' \in \operatorname{vert}(Q)$ and every $i \in \{1,\dots,d\}$. Suppose now that a is not an integer, i.e. a has a representation as p/q with $p \in \mathbb{N}$ and $q \in \mathbb{N} \setminus \{1\}$ having no common divisor. Then q divides $\frac{\langle w'-v\,,\,e_i\rangle}{g}$ for every $w' \in \operatorname{vert}(Q)$ and every $i \in \{1,\dots,d\}$ and hence, qg divides $\langle w\,,\,e_i\rangle$ for every $w \in \operatorname{vert}(Q-v)$ and every $i \in \{1,\dots,d\}$, which contradicts the definition of g. □

Theorem 2.6. *Let P, P_0, P_1, P_{-1} be as in Theorem 2.4. If P_0 is a $(d-1)$-dimensional simplex such that all integral vertices of P_0 are unimodular, the following statements hold:*

(a) P_1 and P_{-1} are non-negative homothetic copies of P_0,

(b) $P_1 + P_{-1} = 2P_0$.

Proof. Assertion (a). Let $u_1, \dots, u_d \in \mathbb{Z}^{d-1} \setminus \{o\}$ be primitive vectors such that $U(P_0) = \{u_1, \dots, u_d\}$. We circumscribe a non-negative homothetic copy of P_0 around P_1. More precisely, we consider the polytope

$$P_1' := \Big\{x \in \mathbb{R}^{d-1} \,:\, \langle x\,,\,u_j\rangle \leq h(P_1, u_j) \text{ for every } j \in \{1,\dots,d\}\Big\},$$

which contains P_1 and is a non-negative homothetic copy of P_0 since it is a simplex having the same set of outer normal facet vectors as P_0. We will now prove that $P_1' = P_1$, which implies that P_1 is a non-negative homothetic copy of P_0.

Let $v \in \operatorname{vert}(P_1')$. Appropriately reindexing $u_1, \dots, u_d$, we assume $v \in F(P_1', u_i)$ for every $i \in \{1,\dots,d-1\}$ and denote by v_0 the vertex of $2P_0$ with the property $v_0 \in F(2P_0, u_i)$ for every $i \in \{1,\dots,d-1\}$. We now distinguish two cases: $\frac{v_0}{2} \in \mathbb{Z}^{d-1}$ and $\frac{v_0}{2} \notin \mathbb{Z}^{d-1}$. Let us first deal with the latter case. Then in view of (2.7), we have $v_0 \in P_1 + P_{-1}$. Since v_0 is a vertex of $2P_0$ and $P_1 + P_{-1} \subseteq 2P_0$, we have that v_0 is a vertex of $P_1 + P_{-1}$. Note that $P_1 + P_{-1} = \operatorname{conv}(\operatorname{vert}(P_1)) + \operatorname{conv}(\operatorname{vert}(P_{-1})) = \operatorname{conv}(\operatorname{vert}(P_1) + \operatorname{vert}(P_{-1}))$ (see [Sch93, Theorem 1.1.2]) and hence, $\operatorname{vert}(P_1 + P_{-1}) \subseteq \operatorname{vert}(P_1) + \operatorname{vert}(P_{-1})$. Therefore, there exist $v_1 \in \operatorname{vert}(P_1)$, $v_{-1} \in \operatorname{vert}(P_{-1})$ with $v_0 = v_1 + v_{-1}$. In view of $P_1 + P_{-1} \subseteq 2P_0$, we have $\operatorname{cone}(u_1, \ldots, u_{d-1}) = N(2P_0, v_0) \subseteq N(P_1 + P_{-1}, v_0)$. Furthermore, we have $N(P_1 + P_{-1}, v_0) = N(P_1, v_1) \cap N(P_{-1}, v_{-1})$; see [Sch93, Theorem 2.2.1]. Together, this yields $\operatorname{cone}(u_1, \ldots, u_{d-1}) \subseteq N(P_1, v_1)$. In other words, $u_1, \ldots, u_{d-1}$ are outer normal vectors of P_1 at v_1. Hence, we have that

$$\langle v_1 \, , \, u_j \rangle = h(P_1, u_j) \text{ for every } j \in \{1, \ldots, d-1\},$$

and thus, $v = v_1$. In particular, v is integral.

We now treat the case that $\frac{v_0}{2} \in \mathbb{Z}^{d-1}$, i.e., $\frac{v_0}{2}$ is a vertex of P_0. In this case, since all integral vertices of P_0 are unimodular, $u_1, \ldots, u_{d-1}$ form a basis of $\mathbb{Z}^{d-1}$, i.e., the matrix with rows $u_1, \ldots, u_{d-1}$ has determinant one. Since the vertex v of P'_1 is given by

$$\langle u_j \, , \, v \rangle = h(P_1, u_j) \text{ for every } j \in \{1, \ldots, d-1\},$$

and $h(P_1, u_j)$ is integral for every $j \in \{1, \ldots, d-1\}$, it thus follows from Cramer's rule that v is integral.

We have now shown that all vertices of P'_1 are integral and hence, P'_1 is an integral polytope containing P_1. Observe now that $P'_1 + P_{-1} \subseteq 2P_0$, since for $x \in P'_1$ and $y \in P_{-1}$ and every $j \in \{1, \ldots, d\}$, one has

$$\langle x + y \, , \, u_j \rangle = \langle x \, , \, u_j \rangle + \langle y \, , \, u_j \rangle \leq h(P_1, u_j) + h(P_{-1}, u_j) \leq h(P_1 + P_{-1}, u_j) \leq h(2P_0, u_j).$$

Here, the last inequality follows from $P_1 + P_{-1} \subseteq 2P_0$. In view of Theorem 2.4 (b2) with $R_1 = P'_1$ and $R_{-1} = P_{-1}$, we then immediately obtain $P_1 = P'_1$. This proves that P_1 is a non-negative homothetic copy of P_0. To show that P_{-1} is a non-negative homothetic copy of P_0, one can argue in exactly the same way by interchanging the roles of P_1 and P_{-1}.

Assertion (b). Note that if P_0 does not have any integral vertices, then in view of (2.6) and (2.7) we have $2P_0 = P_1 + P_{-1}$ and hence we are done. Let us now assume that P_0 has at least one integral vertex. By applying an integral translation to P if necessary, we may assume this vertex to be o and hence, $o \in \operatorname{vert}(2P_0)$. Let $\widetilde{P_0} := \frac{1}{g}(2P_0)$, where g is defined as in Lemma 2.5. In view of assertion (a) and Lemma 2.5, we can write $P_1 = a\widetilde{P_0} + b$ and $P_{-1} = a'\widetilde{P_0} + b'$, where $a, a' \in \mathbb{N} \cup \{0\}$ and $b, b' \in \mathbb{Z}^{d-1}$. Furthermore, we have $P_1 + P_{-1} \subseteq 2P_0$ by Theorem 2.4 (b1). In other words, we have

$$a\widetilde{P_0} + a'\widetilde{P_0} + (b + b') \subseteq 2P_0 = g\widetilde{P_0}.$$

Since $g, a, a' \geq 0$ and since $\widetilde{P_0}$ is neither empty nor a singleton, we have $a + a' \leq g$, i.e. $0 \leq a' \leq g - a$. Then since $g, a \in \mathbb{N} \cup \{0\}$, the polytope $R_{-1} := (g - a)\widetilde{P_0} + b'$ is in $\mathcal{P}(\mathbb{Z}^{d-1})$ and contains P_{-1}. In view of $P_1 + R_{-1} \subseteq 2P_0$ and Theorem 2.4 (b2), we obtain $a' = g - a$. Thus, $P_1 + P_{-1} = 2P_0 + (b + b') \subseteq 2P_0$, which implies $b + b' = o$ and hence proves assertion (b). □

Enumeration for lattice width two and dimension three

In view of the results of this section, all possible choices for P_0 are contained in the list of polygons given in Theorem 2.2. From this list, we can now construct all $\mathbb{Z}^3$-maximal lattice-free polytopes P in $\mathcal{P}(\mathbb{Z}^3)$. For every such P, we will see that each of its facets is blocked, which yields that P is also $\mathbb{R}^3$-maximal.

Proposition 2.7. *Let $P \in \mathcal{P}(\mathbb{Z}^3)$ be a lattice-free polytope with $\operatorname{lw}(P) = 2$. Then, P is $\mathbb{Z}^3$-maximal if and only if P is unimodularly equivalent to one of the following polytopes:*

the simplex $M_{4,6} := \operatorname{conv}(-2e_1, 4e_1, e_1 + 3e_2, 2e_3)$*,*

the simplex $M_{4,4} := \operatorname{conv}(o, 4e_1, 4e_2, 2e_3)$*,*

the simplex $M'_{4,4} := \operatorname{conv}(-e_1, 3e_1, e_1 + 4e_2, 2e_3)$*,*

the prism $M_{5,2} := \operatorname{conv}(-e_1, e_1, 2e_2, 2e_3, 2e_1 + 2e_3, e_1 + 2e_2 + 2e_3)$*,*

the pyramid $M_{5,4} := \operatorname{conv}(\pm 2e_1, \pm 2e_2, 2e_3)$*,*

the simplex $M_{4,2} := \operatorname{conv}(-e_1 + e_2, e_1 + 3e_2, 2e_3, 2e_1 - 2e_2 + 2e_3)$*,*

the parallelepiped $M_{6,2} := \operatorname{conv}(o, -e_1+e_2, 2e_2, e_1+e_2, 2e_3, e_1+e_2+2e_3, 2e_1+2e_3, e_1-e_2+2e_3)$.

In particular, P is $\mathbb{Z}^3$*-maximal if and only if P is* $\mathbb{R}^3$*-maximal.*

Proof. Let P be $\mathbb{Z}^3$-maximal.

By applying a unimodular transformation, we can assume $P \subseteq \mathbb{R}^2 \times [-1, 1]$ and $\mathrm{w}(P, e_3) = 2$. For $i \in \{-1, 0, 1\}$, let $P_i := \{x \in \mathbb{R}^2 : (x, i) \in P\}$. In view of Theorem 2.2 and Theorem 2.4 (a), we have that P_0 is unimodularly equivalent to one of the polygons Q_2, Q_3, Q_4, Q_5 as in Theorem 2.2. In other words, we can (by applying another unimodular transformation) assume that $P_0 = Q_i$ for some $i \in \{2, 3, 4, 5\}$. Furthermore, P_1 and P_{-1} satisfy the conditions of Theorem 2.4 (b).

Case 1: P_0 is a simplex. Note that Q_2, Q_3, Q_4 are simplices. One can easily check that all three simplices have the property that each of their integral vertices is unimodular. In view of Theorem 2.6, we obtain that if $P_0 \in \{Q_2, Q_3, Q_4\}$, then $P_1, P_{-1} \in \mathcal{P}(\mathbb{Z}^2)$ are non-negative homothetic copies of P_0 such that $P_1 + P_{-1} = 2P_0$. In order to apply Lemma 2.5, we fix a vertex $v \in \mathcal{P}(\mathbb{Z}^2)$ of $2P_0$ and consider $\widetilde{P_0} := \frac{1}{g}(2P_0 - v)$, where $g := \gcd(\{w_1, w_2, w_3, w_4\})$ with (w_1, w_2) and (w_3, w_4) being the elements of $\operatorname{vert}(2P_0 - v) \setminus \{o\}$. Then there exist $a, a' \in \mathbb{N} \cup \{0\}$ and $b, b' \in \mathbb{Z}^2$ such that $P_1 = a\widetilde{P_0} + b$, $P_{-1} = a'\widetilde{P_0} + b'$ and $2P_0 = g\widetilde{P_0} + v = (a + a')\widetilde{P_0} + (b + b')$. Clearly, we have $b + b' = v$, i.e. $b' = v - b$, and $a + a' = g$. It is also obvious that reversing the roles of P_1 and P_{-1} corresponds to reflecting P with respect to $\mathbb{R}^2 \times \{0\}$, which is a unimodular transformation. Without loss of generality, we can therefore assume $a \le a'$. Moreover, observe that we can also assume $b = o$ (and hence, $b' = v$). To see this, let $b = (b_1, b_2)$ and let $\varphi\colon \mathbb{R}^3 \to \mathbb{R}^3$ be the linear mapping given by $\varphi(e_1) = e_1$, $\varphi(e_2) = e_2$ and $\varphi(e_3) = e_3 - b_1 e_1 - b_2 e_2$. Then φ is indeed a unimodular transformation mapping $(a\widetilde{P_0} + b) \times \{1\}$ onto $a\widetilde{P_0} \times \{1\}$ and $(a'\widetilde{P_0} + v - b) \times \{-1\}$ onto $(a'\widetilde{P_0} + v) \times \{-1\}$ while leaving $g\widetilde{P_0} \times \{0\}$ unchanged.

We now proceed as follows: for given P_0, we select a vertex v and determine g and $\widetilde{P_0}$. Then for every pair of non-negative integers a, a' with $a \le a'$ and $a + a' = g$, we check the polytope $P = \operatorname{conv}\left((a'\widetilde{P_0} + v) \times \{-1\} \cup a\widetilde{P_0} \times \{1\}\right)$ for $\mathbb{Z}^3$-maximality. If P is $\mathbb{Z}^3$-maximal, we show that it is unimodularly equivalent to one of the seven polytopes given in the formulation of the theorem.

For the three cases, we select the vertex v and obtain $\widetilde{P_0}$ as follows:

Case 1.1:	$P_0 = Q_2$,	$v = (0, 0)$,	$\widetilde{P_0} := \operatorname{conv}\left((0, 0), (1, 0), (0, 1)\right)$;
Case 1.2:	$P_0 = Q_3$,	$v = (-2, 0)$,	$\widetilde{P_0} = \operatorname{conv}\left((0, 0), (2, 0), (1, 1)\right)$;
Case 1.3:	$P_0 = Q_4$,	$v = (-1, 0)$,	$\widetilde{P_0} = \operatorname{conv}\left((0, 0), (2, 0), (1, 2)\right)$.

Case 1.1: $P_0 = Q_2 = \operatorname{conv}\left((0, 0), (2, 0), (0, 2)\right)$. Since $o \in P_0$, we can choose $v = o$ and obtain $\widetilde{P_0} := \operatorname{conv}\left((0, 0), (1, 0), (0, 1)\right)$. Then $2P_0 = 4\widetilde{P_0}$. In view of $a \le a'$, we have three

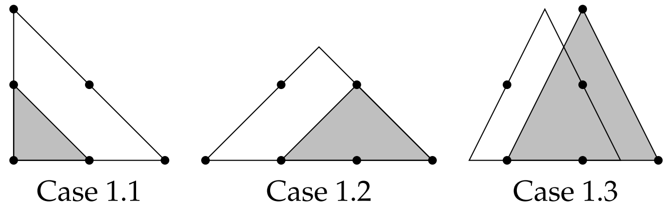

Figure 2.6: Illustration of P_0 and $\widetilde{P_0}$ (shaded) in the Cases 1.1-1.3 of the proof of Proposition 2.7.

cases to distinguish: first, $a = 0$ and $a' = 4$, second, $a = 1$ and $a' = 3$, and third, $a = a' = 2$. In the first case, P is the simplex $M_{4,4} - e_3$. In the second case, P is $\operatorname{conv}\big((3\widetilde{P_0} - e_3) \cup (\widetilde{P_0} + e_3)\big)$, which is properly contained in the integral lattice-free polytope $\operatorname{conv}(o, 3e_1, 3e_2, 3e_3) - e_3$ and is thus not $\mathbb{Z}^3$-maximal. If $a = 2$, then $P = \operatorname{conv}(o, 2e_1, 2e_2) \times [-1, 1]$, which is properly contained in the integral lattice-free polyhedron $\operatorname{conv}(o, 2e_1, 2e_2) \times \mathbb{R}$ and thus not $\mathbb{Z}^3$-maximal.

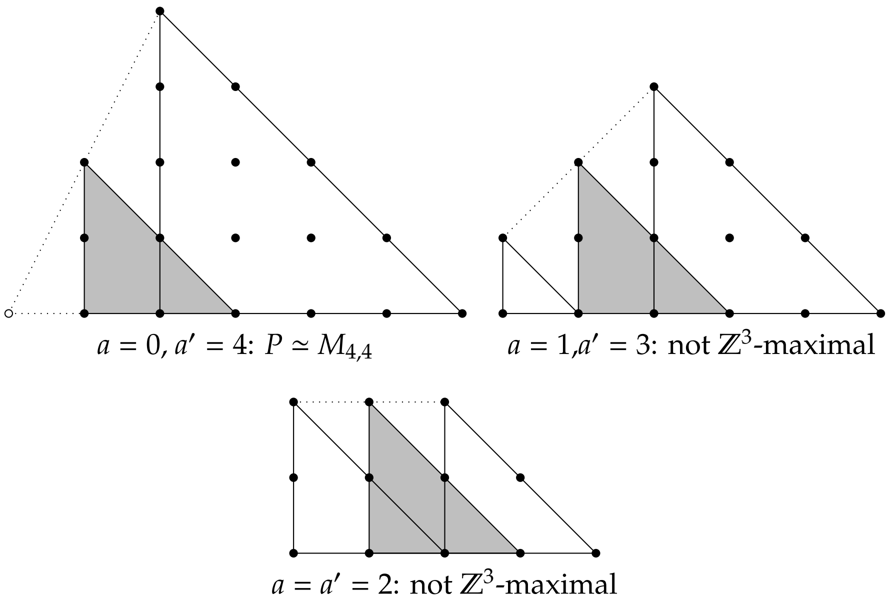

Figure 2.7: Illustration of Case 1.1 in the proof of Proposition 2.7, where $P_0 = \operatorname{conv}\big((0,0),(2,0),(0,2)\big)$ is shaded in grey.

Case 1.2: $P_0 = Q_3 = \operatorname{conv}\big((-1,0),(2,0),(\frac{1}{2},\frac{3}{2})\big)$. We set $v = (-2,0)$ and obtain $\widetilde{P_0} = \operatorname{conv}\big((0,0),(2,0),(1,1)\big)$, which yields $2P_0 = 3\widetilde{P_0} - (2,0)$. There are two cases to distinguish: $a = 0$, $a' = 3$ and $a = 1$, $a' = 2$. In the former case, P is the simplex $M_{4,6} - e_3$. In the latter case,

$$P = \operatorname{conv}\big((-2,0,-1),(0,0,-1),(-1,1,-1),(0,0,1),(2,0,1),(1,1,1)\big),$$

which is properly contained in $\operatorname{conv}\big((-2,0,-1),(0,0,-1),(-1,1,-1),(0,0,2)\big)$. This implies that P is not $\mathbb{Z}^3$-maximal.

Case 1.3: $P_0 = Q_4 = \operatorname{conv}\big((-\frac{1}{2},0),(\frac{3}{2},0),(\frac{1}{2},2)\big)$. We set $v = (-1,0)$ and obtain $\widetilde{P_0} = \operatorname{conv}\big((0,0),(2,0),(1,2)\big)$, which yields $2P_0 = 2\widetilde{P_0} - (1,0)$. There are two cases to distinguish:

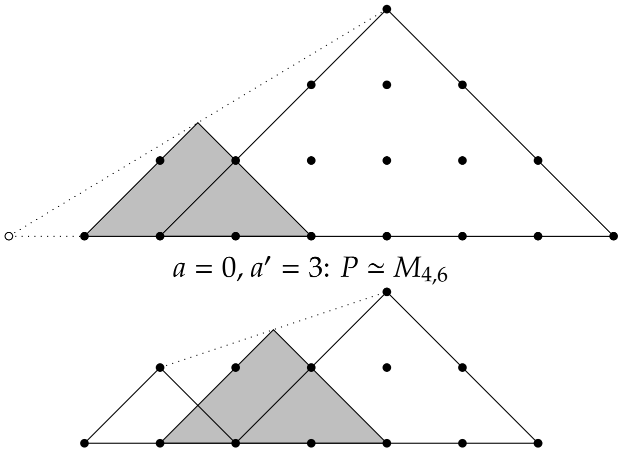

Figure 2.8: Illustration of Case 1.2 in the proof of Proposition 2.7, where $P_0 = \operatorname{conv}\big((-1,0),(2,0),(\frac{1}{2},\frac{3}{2})\big)$ is shaded in grey.

$a = 0, a' = 2$ and $a = a' = 1$. In the former case, P is the simplex $M'_{4,4} - e_3$. If $a = a' = 1$, then $P = \operatorname{conv}\big((\widetilde{P_0} - (1,0)) \times \{-1\} \cup \widetilde{P_0} \times \{1\}\big) = M_{5,2} - e_3$.

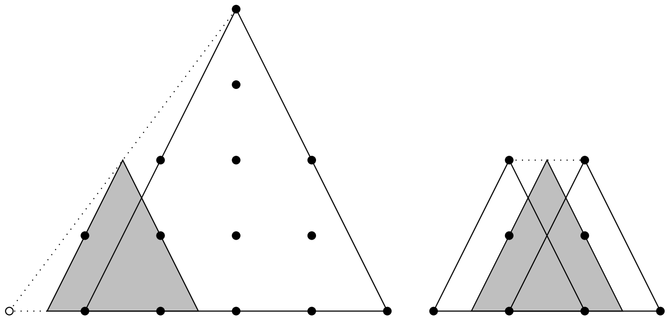

Figure 2.9: Illustration of Case 1.3 in the proof of Proposition 2.7,where $P_0 = \operatorname{conv}\big((-\frac{1}{2},0),(\frac{3}{2},0),(\frac{1}{2},2)\big)$ is shaded in grey.

Case 2: P_0 is not a simplex. Then by Theorem 2.2, P_0 is the quadrilateral $Q_5 = \big(\frac{1}{2},\frac{1}{2}\big) + \operatorname{conv}\big(\pm(1,0),\pm(0,1)\big)$ and we have $2P_0 = \operatorname{conv}(\pm(2,0),\pm(0,2)) + (1,1)$. Since P_0 does not have integral vertices, we have $2\operatorname{conv}(\operatorname{vert}(P_0) \setminus \mathbb{Z}^2) = 2P_0$ and hence, combining (2.6) and (2.7), we obtain $P_1 + P_{-1} = 2P_0$. Furthermore, for every $u \in \mathbb{Z}^2 \setminus \{o\}$, one has $F(2P_0,u) = F(P_1 + P_{-1},u) = F(P_1,u) + F(P_{-1},u)$; see [Sch93, Theorem 1.7.5(c)]. Therefore, if $F(P_1,u)$ is an edge of P_1 or $F(P_{-1},u)$ is an edge of P_{-1}, then $F(2P_0,u)$ is an edge of $2P_0$. In other words, if P_1 or P_{-1} is not a singleton, each of its facets is parallel to one of the line segments $S_1 := [(0,0),(1,1)]$ and $S_2 := [(0,0),(1,-1)]$ and thus, there exist non-negative integers k_1,k_2,l_1,l_2 and vectors $v,w \in \mathbb{Z}^2$ such that

$$P_1 = k_1S_1 + k_2S_2 + v \text{ and } P_{-1} = l_1S_1 + l_2S_2 + w.$$

Observe also that one has $2P_0 = 2S_1 + 2S_2 + (-1,1)$, which in view of $P_1 + P_{-1} = 2P_0$ implies $v + w = (-1,1)$ and $k_1 + l_1 = k_2 + l_2 = 2$. As argued in Case 1, reversing the roles of P_1

and P_{-1} results in reflecting P with respect to $\mathbb{R}^2 \times \{0\}$ and hence, we can assume $k_1 \leq l_1$. Likewise, we have shown in Case 1 that we can assume $v = (0,0)$ up to unimodular equivalence, which implies $w = (-1,1)$. Since l_1 and l_2 are determined by the choice of k_1 and k_2, respectively, this yields the following six cases: $(k_1,k_2) \in \{0,1\} \times \{0,1,2\}$.

- If $(k_1,k_2) = (0,0)$, then $P = \operatorname{conv}(2P_0 \times \{-1\} \cup \{e_3\}) = M_{5,4} - e_3$.
- If $(k_1,k_2) = (0,1)$, then $P = \operatorname{conv}\left((2S_1 + S_2 + (-1,1)\right) \times \{-1\} \cup S_2 \times \{1\})$. Here, P is a prism unimodularly equivalent to $M_{5,2}$.
- If $(k_1,k_2) = (0,2)$, then $P = \operatorname{conv}\left((2S_1 + (-1,1)\right) \times \{-1\} \cup 2S_2 \times \{1\} = M_{4,2} - e_3$.
- If $(k_1,k_2) = (1,0)$, then P is a prism unimodularly equivalent to the case $(k_1,k_2) = (0,1)$ and hence to $M_{5,2}$.
- If $(k_1,k_2) = (1,1)$, then $P = \operatorname{conv}\left((S_1 + S_2 + (-1,1)\right) \times \{-1\} \cup (S_1 + S_2) \times \{1\}) = M_{6,2} - e_3$.
- If $(k_1,k_2) = (1,2)$, then P is a prism unimodularly equivalent to the case $(k_1,k_2) = (0,1)$ and hence to $M_{5,2}$.

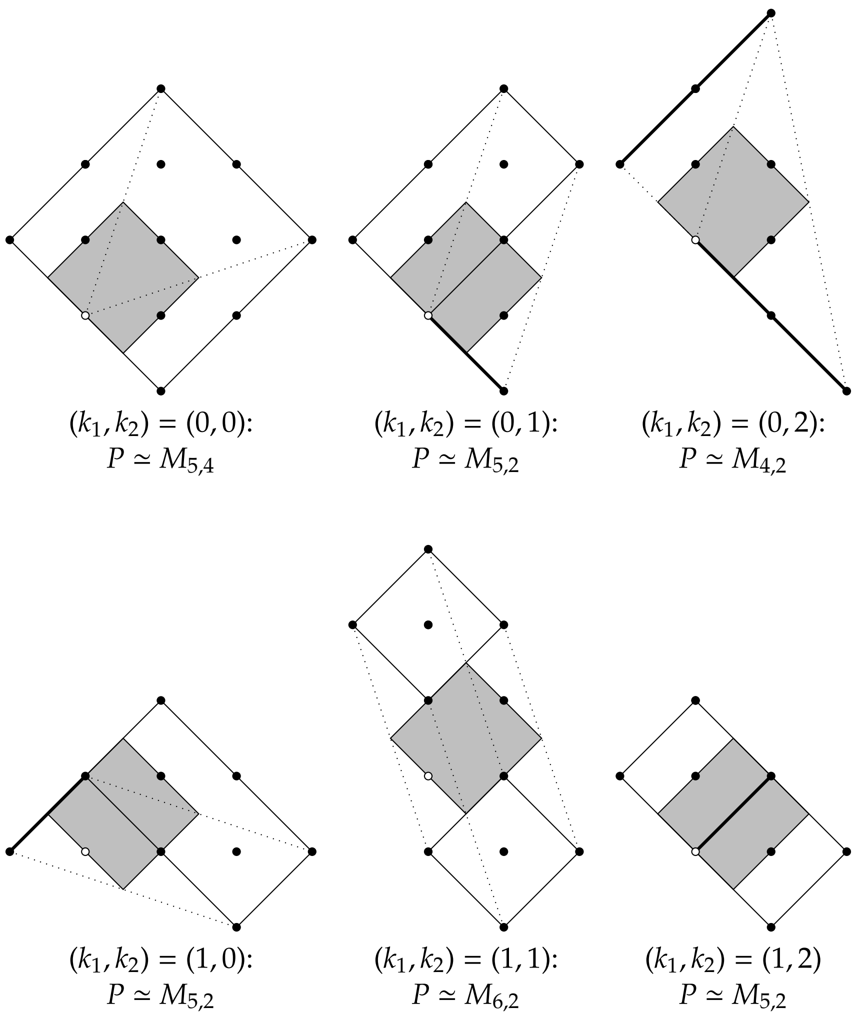

Figure 2.10: Illustration of Case 2 in the proof of Proposition 2.7.

This completes the proof that if P is $\mathbb{Z}^3$-maximal, it is unimodularly equivalent to one of the seven polytopes specified in the proposition. Conversely, it is straightforward to check that if P is unimodularly equivalent to one of the seven polytopes listed, it is indeed $\mathbb{Z}^3$-maximal, because each of them has the property that all of its facets are blocked.

The latter fact implies that all seven polytopes listed are also $\mathbb{R}^3$-maximal. Hence, by our previous arguments, if P is $\mathbb{Z}^3$-maximal, it is unimodularly equivalent to one of those seven $\mathbb{R}^3$-maximal polytopes and hence is $\mathbb{R}^3$-maximal. On the other hand, if P is $\mathbb{R}^3$-maximal, it is also $\mathbb{Z}^3$-maximal by the definition of $\mathbb{Z}^d$-maximality. □

2.3 The case of lattice width at least three

In view of Proposition 2.7, to complete the proof of Theorem 1.3 it remains to show that every $\mathbb{Z}^3$-maximal lattice-free polytope $P \in \mathcal{P}(\mathbb{Z}^3)$ with lattice width at least three is also $\mathbb{R}^3$-maximal. Our goal is to derive an algorithm for a computer search which finds all such polytopes and verifies the claim. To be able to do so, we first need reasonably good bounds on the (suitably defined) size of P.

Bounds on the size of lattice-free polytopes in $\mathcal{P}(\mathbb{Z}^3)$ with lattice width at least three

Let us start this section by introducing the parameters we use to quantify the size of a $\mathbb{Z}^3$-maximal lattice-free polytope $P \in \mathcal{P}(\mathbb{Z}^3)$. We use the volume of both P and its difference body $P-P$. We will also use the lattice diameter of P. Finally, we use the reciprocal of the first successive minimum of $P-P$: for a convex body $C \subseteq \mathbb{R}^d$ centrally symmetric with respect to the origin, $i \in \{1, \ldots, d\}$, the minimal value $\lambda > 0$ such that λC contains i linearly independent points of $\mathbb{Z}^d \setminus \{o\}$ is denoted by $\lambda_i(C)$ and called the i-th *successive minimum* of C. We remark that clearly, $0 < \lambda_1(C) \leq \ldots \leq \lambda_d(C)$ and also $\lambda_1(tC) = \frac{1}{t}\lambda_1(C)$ for every positive number t.

In order to bound the volume from above, we make use of the first and second theorem of Minkowski; see [Gru93, Theorems 4 and 12], which link the volume of an o-symmetric body to its successive minima. For a convex body $C \subseteq \mathbb{R}^d$ symmetric with respect to the origin, one has

$$\operatorname{vol}(C) \leq \frac{2^d}{\prod_{i=1}^d \lambda_i(C)} \leq \frac{2^d}{\lambda_1(C)^d}. \tag{2.11}$$

Consequently, lower bounds on the first successive minimum imply upper bounds on the volume. Let K be a convex body in $\mathbb{R}^d$, not necessarily a centrally symmetric one. The volume of K and the volume of its difference body $K-K$ are related by the well-known inequality $2^d \operatorname{vol}(K) \leq \operatorname{vol}(K-K)$; see for example [Sch93, Theorem 7.3.1]. Since $K-K$ is o-symmetric, one can apply (2.11) to obtain

$$\operatorname{vol}(K) \leq \frac{1}{\prod_{i=1}^d \lambda_i(K-K)} \leq \frac{1}{\lambda_1(K-K)^d}. \tag{2.12}$$

In the following, we will derive a lower bound on $\lambda_1(P-P)$ for a lattice-free polytope P with $\operatorname{lw}(P) \geq 3$.

To establish a connection between the lattice width of a convex body and the successive minima of its difference body, we use another sequence of parameters connected to a convex body K. For $i \in \{1, \ldots, d\}$, we denote by $\mu_i(K)$ the *i-th covering minimum* of K, defined to be the minimum over all $\mu > 0$ for which $\mu K + \mathbb{Z}^d$ meets every $(d-i)$-dimensional affine subspace of $\mathbb{R}^d$ (see [KL88]). Clearly, $0 < \mu_1(K) \leq \cdots \leq \mu_d(K)$. Kannan and Lovász [KL88, Lemmas 2.3 and 2.5] provided a link between covering minima and successive minima by showing that

$$\mu_{i+1}(K) \leq \mu_i(K) + \lambda_{d-i}(K-K) \tag{2.13}$$

holds for every $i \in \{1, \ldots, d-1\}$. Furthermore, they observed $\operatorname{lw}(K) = 1/\mu_1(K)$. Note that the value $\mu_d(K)$ is the standard *covering radius* (also called *inhomogenious minimum*) of K and that $\mu_d(K) \geq 1$ if and only if some translation of K is lattice-free.

For the case of $d = 2$, Hurkens [Hur90] proved the following relation between μ_2 and μ_1 for $K \subseteq \mathbb{R}^2$:

$$\mu_2(K) \leq \left(1 + \frac{2}{\sqrt{3}}\right)\mu_1(K). \tag{2.14}$$

Kannan and Lovász [KL88] observed that this also implies that (2.14) holds for $K \subseteq \mathbb{R}^d$ with general $d \geq 2$. For the case of $d = 3$ and a lattice-free convex body $K \subseteq \mathbb{R}^3$, we can therefore combine (2.14) with (2.13) for $i = 2$ and the fact that $\mu_3(K) \geq 1$ to obtain the following chain of inequalities:

$$1 \leq \mu_3(K) \leq \mu_2(K) + \lambda_1(K - K) \leq \left(1 + \frac{2}{\sqrt{3}}\right)\mu_1(K) + \lambda_1(K - K).$$

Consequently, one has

$$\lambda_1(K - K) \geq 1 - \left(1 + \frac{2}{\sqrt{3}}\right)\mu_1(K). \tag{2.15}$$

Recall that $\mu_1(K)$ is the reciprocal of $\operatorname{lw}(K)$. Hence, the right hand side of (2.15) is positive whenever $\operatorname{lw}(K) > 1 + \frac{2}{\sqrt{3}}$. Applying these observations to the case of a lattice-free polytope $P \in \mathcal{P}(\mathbb{Z}^3)$ with lattice width at least three, and noting that $1 + \frac{2}{\sqrt{3}} = 2.154\cdots$, we obtain a positive lower bound on $\lambda_1(P - P)$ from (2.15):

$$\lambda_1(P - P) \geq \frac{2}{3}\left(1 - \frac{1}{\sqrt{3}}\right) > \frac{1}{4}. \tag{2.16}$$

The following proposition contains the statements of this section which are needed for our proof of Theorem 1.3.

Proposition 2.8 (Size bounds for lattice-free polytopes in $\mathcal{P}(\mathbb{Z}^3)$ with lattice width at least three). *Let $P \in \mathcal{P}(\mathbb{Z}^3)$ be a lattice-free polytope with $\operatorname{lw}(P) \geq 3$. Then, the following statements hold:*

(a) $\operatorname{vol}(P) \leq 27$,

(b) $\operatorname{vol}(P - P) \leq 8 \cdot 27$,

(c) $\lambda_1(P - P) > \frac{1}{4}$,

(d) $\operatorname{ld}(P) \leq 3$.

Proof of Proposition 2.8. Let $\lambda_i := \lambda_i(P - P)$ and $\mu_i := \mu_i(P)$ for $i \in \{1, 2, 3\}$. Assertion (c) follows immediately from (2.16).

We now prove (a) and (b). By (2.12), it suffices to prove that the product $\lambda_1\lambda_2\lambda_3$ is bounded from below by $1/27$. In the case $\lambda_1 > 1/3$, this is clear, since in this case $\lambda_1\lambda_2\lambda_3 \geq \lambda_1^3 > 1/27$. We switch to the case $\lambda_1 \leq 1/3$. Applying (2.13) for $i = 1$, we get $\lambda_2 \geq \mu_2 - \mu_1$ and applying (2.13) for $i = 2$ yields $\mu_2 \geq \mu_3 - \lambda_1$. Combined, we obtain $\lambda_2 \geq \mu_3 - \lambda_1 - \mu_1$. Since P is lattice-free, we have $\mu_3 \geq 1$. We further have $\mu_1 \leq 1/3$ because $1/\mu_1 = \operatorname{lw}(P) \geq 3$. Hence, $\lambda_2 \geq 2/3 - \lambda_1$ and thus, $\lambda_1\lambda_2\lambda_3 \geq \lambda_1(2/3 - \lambda_1)^2$. Therefore, in view of (c), we have to determine the minimum of the function $f(\lambda_1) := \lambda_1(2/3 - \lambda_1)^2$ on the interval $\left(\frac{1}{4}, \frac{1}{3}\right]$. It is straightforward to verify that the function $f(\lambda_1) = \lambda_1(2/3 - \lambda_1)^2$ is monotonously decreasing on this interval, which yields $\lambda_1\lambda_2\lambda_3 \geq f(\lambda_1) \geq f(1/3) = 1/27$.

This leaves us to show (d). We observe the following connection between lattice diameter and first successive minimum. By definition of $\operatorname{ld}(P)$, there exist $z, z' \in P$ such that $u := \frac{1}{\operatorname{ld}(P)}(z - z') \in \mathbb{Z}^3 \setminus \{o\}$ and hence, $u \in \frac{1}{\operatorname{ld}(P)}(P - P)$. From the definition of λ_1, we then immediately obtain

$$\lambda_1 \leq \frac{1}{\operatorname{ld}(P)}.$$

Hence, we have $\operatorname{ld}(P) \leq 1/\lambda_1 < 4$ in view of (c) and since $\operatorname{ld}(P) \in \mathbb{N}$, this shows (d). □

Remark 2.9 (Upper bounds on the lattice width). Note that we do not state anything about upper bounds on $\operatorname{lw}(P)$. The reason for this is that such an upper bound is not needed anywhere in the algorithm we will present in the remainder of this section. It turns out when executing the algorithm, however, that all $\mathbb{Z}^3$-maximal lattice-free polytopes in $\mathcal{P}(\mathbb{Z}^3)$ have lattice width at most three. By a result of Dash et al. [DDG+14], one actually has that the lattice width of lattice-free elements of $\mathcal{P}(\mathbb{Z}^d)$ is at most four. Moreover, the following argumentation underlines why one should expect (already prior to executing the algorithm) not to find any polytopes with lattice width four: if one assumes $P \in \mathcal{P}(\mathbb{Z}^3)$ to be lattice-free and have lattice width four, then from (2.15) one has $\lambda_1(P - P) > 1/2$. Consider the dual body $(P - P)^*$ of $P - P$. From [KL88], we know $\lambda_1((P - P)^*) = \operatorname{lw}(P) = 4$. In view of (2.11), we then have

$$\operatorname{vol}(P - P)\operatorname{vol}((P - P)^*) \leq \frac{2^{2\cdot 3}}{\lambda_1(P - P)^3\lambda_1((P - P)^*)^3}. \tag{2.17}$$

For $\operatorname{lw}(P) = 4$ and $\lambda_1(P - P) > 1/2$, the right hand side is strictly less than 8. Recall that by Mahler's conjecture (see [Mah39]) on the minimal volume which the Mahler volume of convex bodies can attain in dimension three, we have $\operatorname{vol}(P - P)\operatorname{vol}((P - P)^*) \geq 64/6 > 10$ if Mahler's conjecture is true. Since this is generally expected to be the case, we did not expect to find any polytopes with lattice width four when running our algorithm. We point out that the proof by Dash et al. of the fact that the lattice width of lattice-free elements of $\mathcal{P}(\mathbb{Z}^3)$ is at most four uses the relation (2.17) in combination with the best known explicit lower bound on the Mahler volume by Kuperberg [Kup08]. ■

Remark 2.10 (Generalization to higher dimensions). Let us briefly discuss how the bounds of this section could potentially be generalized to higher dimensions. Let $d \geq 4$ and let K be a lattice-free convex body. It is known from [KL88, Theorem 2.7] that for every $i \in \mathbb{N}$ there exists a constant $\operatorname{Flt}(i)$ such that $\mu_i(K) \leq \operatorname{Flt}(i)\mu_1(K)$. In the literature, this constant is known as the *flatness constant*. The exact value, in the sense that there exists a polygon for which this value is attained, for $\operatorname{Flt}(2)$ is the one given in (2.14). However, in higher dimensions, no exact value for the flatness constant is known. To the best of our knowledge, the best asymptotical bound available is of order $O(i^{3/2})$; see [BLPS99]. Using the flatness constant, we can generalize (2.15) to $\lambda_1(K - K) \geq 1 - \operatorname{Flt}(d-1)\mu_1(K)$. This yields a positive lower bound on $\lambda_1(K - K)$ whenever $\operatorname{lw}(K) > \operatorname{Flt}(d-1)$. Using the generalization of (2.15) and (2.12), one can obtain a volume bound which has exponential growth in d for $\mathbb{Z}^d$-maximal lattice-free integral polytopes with lattice width larger than $\operatorname{Flt}(d-1)$. Such a bound compares favourably to the best known volume bound, which holds for polytopes of arbitrary lattice width but has doubly exponential growth in d; see

[NZ11, Theorem 2.1]. This supports the intuition that lattice-free polytopes with large lattice width must have 'small' volume. It also suggests that for an attempt at classifying $\mathbb{Z}^d$-maximal lattice-free $\mathbb{Z}^d$-polytopes for given d, polytopes with large lattice width could be viewed separately; and hence suggests that our approach of distinguishing polytopes for $d = 3$ by lattice width could be transferred to higher dimensions. However, it is not known whether for $d \geq 4$ there exist any $\mathbb{Z}^d$-maximal lattice-free $\mathbb{Z}^d$-polytopes with lattice width at least $\operatorname{Flt}(d-1)$ at all. ■

Completing the case of lattice width at least three by a computer search

Based on the bounds on the size of lattice-free polytopes in $\mathcal{P}(\mathbb{Z}^3)$ with lattice width at least three, we can now derive a search algorithm that finds, up to affine unimodular transformations, all polytopes in the set

$$\left\{P \in \mathcal{P}(\mathbb{Z}^3) \, : \, P \text{ is lattice-free and } \mathbb{Z}^3\text{-maximal}, \ \operatorname{lw}(P) \geq 3\right\}. \tag{2.18}$$

We present the algorithm along with mathematical arguments that justify its correctness. We give a rather high-level description omitting algorithmic details that can be resolved in a straightforward manner. We implemented our search algorithm in Python 2.7 – a high-level language with a self-explanatory syntax. The code of this implementation can be found in the appendix. Our implementation contains a straightforward test that checks for each polytope P in (2.18) whether it is also $\mathbb{R}^3$-maximal: we check whether the relative interior of each facet of P contains an integral point. As a result, an execution of our code confirms (within less than half an hour) that every polytope in (2.18) is indeed $\mathbb{R}^3$-maximal.

Since all $\mathbb{R}^3$-maximal lattice-free polytopes in $\mathcal{P}(\mathbb{Z}^3)$ were enumerated in [AWW11], our intention was not to output an irredundant list of all polytopes in (2.18). In fact, our algorithm enumerates many polytopes that are pairwise unimodularly equivalent and excluding such redundancy would require additional code. However, we decided to keep the implementation as simple as possible and hence do not elaborate on this.

Step 1: Fixing a boundary fragment

Let $P \in \mathcal{P}(\mathbb{Z}^3)$ be $\mathbb{Z}^3$-maximal lattice-free and let $\ell := \operatorname{ld}(P)$. In view of Proposition 2.8, the possible values of ℓ are 1, 2, and 3. Because P is lattice-free, there exists a facet F of P with $\operatorname{ld}(F) = \operatorname{ld}(P) = \ell$ and by applying an appropriate unimodular transformation, we can assume $F \subseteq \mathbb{R}^2 \times \{0\}$. Let us first treat the case that $\ell = 1$. By Howe's Theorem in the formulation given in [Sca85, Theorem 1.5], we know the following: if $P \in \mathcal{P}(\mathbb{Z}^3)$ is a polytope with the property $P \cap \mathbb{Z}^3 = \operatorname{vert}(P)$, then its vertices are contained in two adjacent parallel lattice hyperplanes. Since the convex hull of these hyperplanes is a lattice-free integral polytope properly containing P, this contradicts the $\mathbb{Z}^3$-maximality of P. Hence, P has to contain an integral point which is not a vertex of P, and since P is lattice-free, this point has to be in the boundary of P. Clearly, there cannot be an integral point in the relative interior of an edge of P, since otherwise this edge has at least three collinear integral points, contradicting $\ell = 1$. This implies that we can choose F such that $\operatorname{relint}(F) \cap \mathbb{Z}^3 \neq \emptyset$. Suppose $|F \cap \mathbb{Z}^3| > 4$. Then two points in $|F \cap \mathbb{Z}^3|$, say x and y, are congruent modulo two and hence, the line segment $[x, y]$ contains $\frac{1}{2}(x + y) \in \mathbb{Z}^3$, a contradiction to $\ell = 1$. Thus, F is a triangle with precisely one integral point in its relative interior. It follows that F is unimodularly equivalent to $\operatorname{conv}\big((-1,-1,0), (1,0,0), (0,1,0)\big)$; see [Rab89a].

It is easy to check that in the the case $\ell = 2$, up to unimodular transformation, F contains the triangle $\operatorname{conv}\big((0,0,0),\ (2,0,0),\ (0,1,0)\big)$ and likewise, in the case $\ell = 3$, up to unimodular transformation, F contains the triangle $\operatorname{conv}\big((0,0,0),\ (3,0,0),\ (0,1,0)\big)$. Thus, we may assume that P contains one of the following three triangles B in its boundary:

$$B := \begin{cases} \operatorname{conv}\big((-1,-1,0),\ (1,0,0),\ (0,1,0)\big) & \text{if } \ell = 1, \\ \operatorname{conv}\big((0,0,0),\ (2,0,0),\ (0,1,0)\big) & \text{if } \ell = 2, \\ \operatorname{conv}\big((0,0,0),\ (3,0,0),\ (0,1,0)\big) & \text{if } \ell = 3. \end{cases} \tag{2.19}$$

Step 2: Inscribing a pyramid

After fixing ℓ and the corresponding B, we can clearly assume that we have $x_3 \geq 0$ for all points $(x_1, x_2, x_3) \in P$. Let $a = (a_1, a_2, h)$ be any vertex of P with maximal third component. Note that since $h \geq \operatorname{lw}(P)$ we have $h \geq 3$ because otherwise, we have $\operatorname{w}(P, e_3) < 3$. By applying another unimodular transformation that leaves the third component unchanged, we may assume that $0 \leq a_1, a_2 \leq h - 1$ holds. To see that, observe that for every pair of integers k, k' the linear mapping φ given by $\varphi(e_1) = e_1$, $\varphi(e_2) = e_2$ and $\varphi(e_3) = ke_1 + k'e_2 + e_3$ is unimodular, since its matrix representation is an upper triangular matrix with all diagonal entries being one, and maps (a_1, a_2, h) to $(a_1 + kh, a_2 + k'h, h)$. In order to obtain an upper bound on h, let us define the tetrahedron $T := \operatorname{conv}(B \cup \{a\})$ and observe that we have

$$\binom{6}{3} \cdot \operatorname{vol}(T) = \operatorname{vol}(T - T) \leq \operatorname{vol}(P - P) \leq 8 \cdot 27,$$

where the first equality follows from [RS57, Theorem 2] and the last inequality follows from Proposition 2.8. Denoting by $\operatorname{area}(B)$ the area of B and using $\operatorname{vol}(T) = \frac{1}{3} \cdot h \cdot \operatorname{area}(B)$, we thus obtain

$$h \leq \left\lfloor \frac{3 \cdot 8 \cdot 27}{\binom{6}{3} \cdot \operatorname{area}(B)} \right\rfloor.$$

In the cases $\ell = 2$ and $\ell = 3$, this bound evaluates to $h \leq 32$ and $h \leq 21$, respectively. However, in the case $\ell = 1$, the following Lemma provides a tighter upper bound on h.

Lemma 2.11. *Let $P \in \mathcal{P}(\mathbb{Z}^3)$ be a lattice-free polytope such that P contains the points $(a_1, a_2, h) \in \mathbb{Z}^3$ as well as $(-1,-1,0)$, $(1,0,0)$ and $(0,1,0)$. Then, $h \leq 12$.*

Proof. We argue by contradiction by assuming $h > 12$ and showing that this contradicts the lattice-freeness of P. Let D denote the triangle $\operatorname{conv}\big((-1,-1,0),(1,0,0),(0,1,0)\big)$ and consider $D' := D \cap (-D)$. Observe that $o \in D$ and hence, $o \in D'$. Furthermore, D' is symmetric with respect to o by construction. We also introduce the double pyramid $R := \operatorname{conv}(D' \cup \{\pm(a_1, a_2, h)\})$. One can verify directly that the area of D' is one and thus, the volume of R is $\frac{2}{3}h > 8$. Since R is an o-symmetric convex body, we can apply (2.11) to obtain $\frac{2^3}{\lambda_1(R)^3} \geq \operatorname{vol}(R) > 2^3$ or, equivalently, $\lambda_1(R) < 1$. By definition of the successive minima, this implies that $\operatorname{int}(R)$ contains a point z of $\mathbb{Z}^3 \setminus \{o\}$. Because of the symmetry of R, this also implies $-z \in \operatorname{int}(R)$. As $D' \cap \mathbb{Z}^3 \setminus \{o\} = \emptyset$, either z or $-z$ has to be contained in $\operatorname{int}(R) \cap \big(\mathbb{R}^2 \times (0, \infty)\big)$. The latter set, however, is contained in $\operatorname{int}(P)$, a contradiction to the lattice-freeness of P. □

We now summarize the previous observations as follows: we may assume that P is contained in $\mathbb{R}^2 \times [0, \bar{h}]$, where

$$\bar{h} := \begin{cases} 12 & \text{if } \ell = 1, \\ 21 & \text{if } \ell = 2, \\ 32 & \text{if } \ell = 3, \end{cases}$$

and that P contains the tetrahedron $T = \operatorname{conv}(B \cup \{a\})$, where B is defined as in (2.19) and

$$a \in S_{\bar{h}} := \Big\{(x_1, x_2, x_3) \in \mathbb{Z}^3 \;:\; 0 \le x_1, x_2 \le x_3 - 1,\, 0 \le x_3 \le \bar{h}\Big\}. \tag{2.20}$$

We now enumerate all elements of the set in (2.20). Without further qualifications, this enumeration yields several ten thousand points. However, recall that P is lattice-free and satisfies $\lambda_1(P - P) > \frac{1}{4}$ by Proposition 2.8. Since $T \subseteq P$, these two properties also have to be satisfied by T. Furthermore, because P has lattice diameter ℓ and $T \subseteq P$, we have $\operatorname{ld}(T) \le \ell$, while on the other hand $B \subseteq T$ yields $\operatorname{ld}(T) \ge \operatorname{ld}(B) = \ell$. Hence, we obtain that T is lattice-free and satisfies $\operatorname{ld}(T) = \ell$ as well $\lambda_1(T - T) > \frac{1}{4}$. The computer search checks for each of the possible choices for $a = (a_1, a_2, h)$ whether these three properties are fulfilled for the tetrahedron $\operatorname{conv}(B \cup \{(a_1, a_2, h)\})$. As a consequence, we end up with only 69 valid choices for a in total.

Step 3: Collecting all candidate vertices

In the next step, for a given combination of fixed lattice diameter ℓ and pyramid T (i.e., fixed B and $a = (a_1, a_2, h)$ as introduced above), we want to determine all lattice-free polytopes P in $\mathcal{P}(\mathbb{Z}^3)$ which have lattice diameter ℓ and contain T. In order to do so, we compute a set $\operatorname{cand}(T) \subseteq \mathbb{Z}^3$ such that each vertex of P has to be contained in $\operatorname{cand}(T)$. This is done as follows. First, recall that every vertex $v = (v_1, v_2, v_3)$ of P satisfies $0 \le v_3 \le h$ by our choice of h. By Proposition 2.8, we further have that

$$\operatorname{vol}\Big(\operatorname{conv}(T \cup \{v\})\Big) \le \operatorname{vol}(P) \le 27$$

holds. In order to describe a set of points $x \in \mathbb{R}^3$ satisfying $\operatorname{vol}\Big(\operatorname{conv}(T \cup \{x\})\Big) \le 27$, we make use of the following Lemma.

Lemma 2.12. *Let $T \subseteq \mathbb{R}^3$ be a tetrahedron and denote the barycenter of its vertices by c. Then for any $t \ge \operatorname{vol}(T)$, we have*

$$\Big\{x \in \mathbb{R}^3 \;:\; \operatorname{vol}\Big(\operatorname{conv}(T \cup \{x\})\Big) \le t\Big\} \subseteq \lambda \cdot T + (1 - \lambda) \cdot c,$$

where $\lambda := 4 \cdot \Big(\frac{t}{\operatorname{vol}(T)} - 1\Big) + 1$.

Proof. Let $v_1, \dots, v_4$ denote the vertices of S. Then the barycenter c of T is $\frac{1}{4}\sum_{i=1}^{4} v_i$. Thus, for $i \in \{1, \dots, 4\}$, the point

$$w_i = \Big(\lambda + \frac{1-\lambda}{4}\Big)v_i + \sum_{j=1, j\neq i}^{4} \frac{1-\lambda}{4} v_j$$

is a vertex of $\lambda T + (1 - \lambda)c$ given by its barycentric representation with respect to the vertices of T. Now let $x \in \mathbb{R}^3$ not be contained in $\lambda T + (1 - \lambda)c$. We show that then one has $\operatorname{vol}\Big(\operatorname{conv}(T \cup \{x\})\Big) > t$. Let $x = \sum_{i=1}^{4} \gamma_i w_i$ be the barycentric representation of x with respect to $\lambda T + (1 - \lambda)c$. Since $x \notin \lambda T + (1 - \lambda)c$ and $\gamma_1 + \ldots + \gamma_4 = 1$, at least one of $\gamma_1, \dots, \gamma_4$ is negative. By appropriately ordering the vertices of $\lambda T + (1 - \lambda)c$ and T, we can assume $\gamma_1 < 0$. We now determine the barycentric coordinate β_1 of x with respect to the vertex v_1 of T, which is

$$\beta_1 = \gamma_1\Big(\lambda + \frac{1-\lambda}{4}\Big) + (1 - \gamma_1)\frac{1-\lambda}{4} = \gamma_1\lambda + \frac{1-\lambda}{4}.$$

By definition of λ, one has

$$\beta_1 = \gamma_1\left(4\Big(\frac{t}{\mathrm{vol}(T)} - 1\Big) + 1\right) - \frac{t}{\mathrm{vol}(T)} + 1 < -\frac{t}{\mathrm{vol}(T)} + 1,$$

where the inequality follows from $t \geq \mathrm{vol}(T)$ and $\gamma_1 < 0$.

Let $F := \mathrm{conv}(v_2, v_3, v_4)$ and let d_{v_1} denote the distance of v_1 from $H := \mathrm{aff}(v_2, v_3, v_4)$ and let d_x denote the distance of x from H. Then from the geometric interpretation of the barycentric coordinates, one has $d_x = |\beta_1| d_{v_1}$. Observe that since $|\beta_1| > \frac{t}{\mathrm{vol}(T)} - 1$, this yields the following chain of inequalities:

$$\begin{aligned}
\mathrm{vol}\Big(\mathrm{conv}(T \cup \{x\})\Big) &\geq \mathrm{vol}(T) + \mathrm{vol}\Big(\mathrm{conv}(F \cup \{x\})\Big) \\
&= \mathrm{vol}(T) + |\beta_1|\,\mathrm{vol}\Big(\mathrm{conv}(F \cup \{v_1\})\Big) \\
&= (1 + |\beta_1|)\,\mathrm{vol}(T) > \mathrm{vol}(T)\Big(1 + \frac{t}{\mathrm{vol}(T)} - 1\Big) = t,
\end{aligned}$$

which proves the statement. □

Thus, if c denotes the barycenter of the vertices of T, each vertex of P is contained in the search region

$$\mathrm{sreg}(T) := \Big\{(x_1, x_2, x_3) \in \Big(\lambda \cdot T + (1 - \lambda) \cdot c\Big) \cap \mathbb{Z}^3 \;:\; 0 \leq x_3 \leq h\Big\},$$

where $\lambda := 4 \cdot \Big(\frac{27}{\mathrm{vol}(T)} - 1\Big) + 1$. Similar to the previous step, for each vertex v of P we have that $\mathrm{conv}(T \cup \{v\})$ is lattice-free and its lattice diameter is bounded by ℓ. Hence, a valid choice for the set $\mathrm{cand}(T)$ is

$$\begin{aligned}
\mathrm{cand}(T) := \{v \in \mathrm{sreg}(T) :\; &\mathrm{conv}(T \cup \{v\}) \text{ is lattice free}, \\
&\mathrm{ld}(\mathrm{conv}(T \cup \{v\})) = \ell\}.
\end{aligned}$$

It turns out that computing this set is the most time-consuming step. For that reason, we refrain here from additionally computing the first successive minimum of the difference body of $\mathrm{conv}(T \cup \{v\})$.

Step 4: Combining the candidate vertices

In the final step, for each fixed ℓ and T it remains to enumerate all lattice-free polytopes with lattice diameter ℓ and lattice width at least three which can be obtained by taking the convex hull of T and a set of elements of $\mathrm{cand}(T)$, i.e., all polytopes in the set

$$S := \Big\{P \in \mathcal{P}(\mathbb{Z}^3) \;:\; \mathrm{vert}(P) \subseteq \mathrm{cand}(T),\ T \subseteq P,\ P \text{ lattice-free},\ \mathrm{ld}(P) = \ell,\ \mathrm{lw}(P) \geq 3\Big\}.$$

This is done in the following way. Denoting the points in $\mathrm{cand}(T)$ by $v_1, \ldots, v_k$, let us define the sets S_i for $i \in \{0, \ldots, k\}$ as follows. We set $S_0 = \{T\}$ and for every $i \in \{1, \ldots, k\}$, the set S_i is the set of all polytopes in $\mathcal{P}(\mathbb{Z}^3)$ satisfying the following conditions:

$$\mathrm{vert}(P) \subseteq \mathrm{vert}(T) \cup \{v_1, \ldots, v_i\}, \tag{2.21}$$

$$T \subseteq P,\ P \text{ is lattice-free},\ \mathrm{ld}(P) = \ell, \tag{2.22}$$

$$\mathrm{lw}(P \cup \{v_{i+1}, \ldots, v_k\}) \geq 3. \tag{2.23}$$

Observe that we have $S = S_k$ and that each S_i can be iteratively computed as the union of the set of all polytopes of S_{i-1} satisfying (2.23) and the set of all polytopes $P = \mathrm{conv}(P' \cup$

$\{v_i\})$, where $P' \in S_{i-1}$, satisfying conditions (2.22) and (2.23). Only the third condition needs explaining: this is to ensure that for our preliminary polytope 'built' from T and the first i elements of cand(T), which might not have lattice width three, it is still possible to obtain a polytope of lattice width at least three by 'adding' points of cand(T) which have not yet been considered. If this is not possible, there is no need to consider this polytope any further.

For an arbitrary order of the v_j's, the cardinalities of the S_i's grow extremely fast, making a computation practically impossible. However, this can be avoided by sorting the v_j's decreasingly according to the absolute value of their second coordinates. The idea behind this order is that, for most T, the majority of points in cand(T) together with T are contained in a small strip with respect to the second coordinate. Thus, in order to arrive at a polytope with lattice width at least three, at least one of the v_j's appearing early in the sorted list has to belong to P. Due to condition (2.23), any polytope not containing one of the first v_j's is then discarded from the sets S_i for already small i. Furthermore, for any computed polytope containing one of the v_j's from the beginning of the sorted list, the number of further candidates that can be added to arrive at a lattice-free polytope turns out to be very small.

In the described procedure, for all constructed polytopes we need to decide whether their lattice width is at least three. This is done by simply computing the width with respect to a few explicit directions; more specifically, the directions in the set V defined in the following lemma.

Lemma 2.13. *Let $P \subseteq \mathbb{R}^3$ be a polytope containing a tetrahedron $T = \operatorname{conv}(B \cup \{a\})$, where*

$$B \in \Big\{ \operatorname{conv}\Big((-1,-1,0),\ (1,0,0),\ (0,1,0)\Big), \\ \operatorname{conv}\Big((0,0,0),\ (2,0,0),\ (0,1,0)\Big), \\ \operatorname{conv}\Big((0,0,0),\ (3,0,0),\ (0,1,0)\Big)\Big\}$$

and $a = (a_1, a_2, h) \in \mathbb{Z}^3$ with $h \geq 3$. Then $\operatorname{lw}(P) \geq 3$ holds if and only if

$$\max_{p\in P}\langle v\,,\,p\rangle - \min_{q\in P}\langle v\,,\,q\rangle \geq 3 \tag{2.24}$$

holds for all v in the set $V :=$

$$\Big\{ v = (v_1, v_2, v_3) \in \mathbb{Z}^3 : (v_1, v_2) \in \{(0,1),(1,-1),(1,0),(1,1),(1,2),(1,-2),(2,-1),(1,3)\}, \\ \tfrac{1}{h}(-2 - v_1a_1 - v_2a_2) \leq v_3 \leq \tfrac{1}{h}(2 - v_1a_1 - v_2a_2)\Big\}.$$

Proof. If $\operatorname{lw}(P) \geq 3$, then by definition of the lattice width, (2.24) holds for every $v \in \mathbb{Z}^3 \setminus \{o\}$ and hence in particular for all $v \in V$. To show the reverse implication, it suffices to show that if $\operatorname{lw}(P) \leq 2$ holds, then there exists some $v \in V$ violating (2.24). Suppose we have $\operatorname{lw}(P) \leq 2$. Then there exists a primitive vector $v^* = (v_1^*, v_2^*, v_3^*) \in \mathbb{Z}^3 \setminus \{o\}$ with $\max_{p\in P}\langle v^*, p\rangle - \min_{q\in P}\langle v^*, q\rangle \leq 2$. In particular, since $B \subseteq P$, we have $\max_{p\in B}\langle v^*, p\rangle - \min_{q\in B}\langle v^*, q\rangle \leq 2$. Note that B contains four integral points. Thus, denoting the projection of B onto the first two coordinates by B', we must have that (v_1^*, v_2^*) is orthogonal to a line containing at least two of the integral points of B'. Simple enumeration shows that the possible choices of (v_1^*, v_2^*) are

$$(0,1),(1,-1),(1,0),(1,1),(1,2),(1,-2),(2,-1),(1,3)$$

and their negatives. Since we may replace v^* by $-v^*$ in the above argumentation, it remains to show that

$$\tfrac{1}{h}(-2 - v_1^* a_1 - v_2^* a_2) \le v_3^* \le \tfrac{1}{h}(2 - v_1^* a_1 - v_2^* a_2)$$

holds. Since each T contains the origin, we must have

$$|\langle v^*, a\rangle - \langle v^*, o\rangle| \le 2,$$

which is equivalent to

$$-2 \le v_1^* a_1 + v_2^* a_2 + v_3^* h \le 2,$$

as claimed. □

Finally, having computed the set S_k, we check for each polytope $P \in S_k$ heuristically whether it can possibly be $\mathbb{Z}^3$-maximal. This is done by selecting a few points $p \in \mathbb{Z}^3 \setminus P$ and test if $\operatorname{conv}(P \cup \{p\})$ is still lattice-free. If this check fails for all considered choices of p, P is regarded as being potentially $\mathbb{Z}^3$-maximal and we then test whether P is even $\mathbb{R}^3$-maximal. It turns out that P is indeed $\mathbb{R}^3$-maximal in all these cases and hence, we obtain the following result.

Proposition 2.14. *Let $P \in \mathcal{P}(\mathbb{Z}^3)$ be a lattice-free polytope with $\operatorname{lw}(P) \ge 3$. Then, P is $\mathbb{Z}^3$-maximal if and only if P is $\mathbb{R}^3$-maximal.*

As a consequence, we obtain the proof of Theorem 1.3.

Proof of Theorem 1.3. Let $P \in \mathcal{P}(\mathbb{Z}^3)$ be lattice-free. If P is $\mathbb{R}^3$-maximal, then it is also $\mathbb{Z}^3$-maximal by definition of $\mathbb{Z}^3$-maximality. Conversely, if P is $\mathbb{Z}^3$-maximal and bounded, then in view of Propositions 2.7 and 2.14 we have that P is also $\mathbb{R}^3$-maximal. If P is $\mathbb{Z}^3$-maximal and unbounded, then in view of Theorem 1.2(b) it is unimodularly equivalent to $\operatorname{conv}(o, 2e_1, 2e_2) \times \mathbb{R}$ or to $[0,1] \times \mathbb{R}^2$. In both cases, we have that P is also $\mathbb{R}^3$-maximal. □

2.4 Results on $\mathbb{Z}^d$-maximal lattice-free rational polytopes

In this section, we prove Theorem 1.5 by extending results from [NZ11] and [AWW11], and also complete the proof of Theorem 1.6. We need the definition of Λ-*freeness* in this section, which is a natural generalization of lattice-freeness but is not needed throughout the rest of the thesis: for a set Λ, we say that a d-dimensional convex set C is Λ-free if $\operatorname{int}(C) \cap \Lambda$ is empty. Furthermore, we will use the *recession cone* of a non-empty polyhedron P, which is defined as $\operatorname{rec}(P) := \{x \in P : x + P \subseteq P\}$. We also point out that every linear unimodular transformation φ preserves $\frac{1}{s}\mathbb{Z}^d$ (as it preserves $\mathbb{Z}^d$ and hence, by linearity, one has $\varphi(\frac{1}{s}\mathbb{Z}^d) = \frac{1}{s}\varphi(\mathbb{Z}^d) = \frac{1}{s}\mathbb{Z}^d$).

We will make use of the following lemma. We refer to the original source [NZ11] for a proof, remarking that there are the following differences to our formulation: in [NZ11], $s\mathbb{Z}^d$-free polytopes in $\mathcal{P}(\mathbb{Z}^d)$ are considered, which are precisely the lattice-free polytopes in $\mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$ up to scaling with the factor s, and the notion s-hollow is used instead of our notion $s\mathbb{Z}^d$-free.

Lemma 2.15. [NZ11, Theorem 2.1] *Let $d, s \in \mathbb{N}$. Up to unimodular equivalence, there exist only finitely many lattice-free polytopes $P \in \mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$ such that $P + \operatorname{lin}(u)$ is not lattice-free for every $u \in \mathbb{Z}^d \setminus \{o\}$.*

Proof of Theorem 1.5. Assertion (a): Let $P \in \mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$ be lattice-free. Then P has a representation as $\mathrm{conv}(V) + \mathrm{rec}(P)$ (see, e.g., [Sch86, §7, §8.2 (4)]), where V is a finite subset of $\frac{1}{s}\mathbb{Z}^d$ and $\mathrm{rec}(P)$ is generated by elements of $\mathbb{Z}^d$. Note that $P + \mathrm{rec}(P) = P$ and hence, $P - \mathrm{rec}(P) = P + \mathrm{lin}(\mathrm{rec}(P))$. Since P is lattice-free, by [Ave13, Lemma 4] we have that $P + \mathrm{lin}(\mathrm{rec}(P))$ is lattice-free. Let M be a linear space generated by vectors of $\mathbb{Z}^d$ satisfying $M \supseteq \mathrm{lin}(\mathrm{rec}(P))$ and having largest possible dimension such that $P + M$ is lattice-free. Obviously, we can assume the vectors generating M to be primitive. Thus, by applying a suitable linear unimodular transformation to $P + M$, we can assume $M = \{o\} \times \mathbb{R}^k$ for some $k \in \{0, \dots, d-1\}$ (where $k = 0$ means $M = \{o\}$). Let P' be the projection of P onto the first $d-k$ coordinates. Then P' is also the projection of $\mathrm{conv}(V)$ onto the first $d-k$ coordinates and thus, P' is a polytope in $\mathcal{P}(\frac{1}{s}\mathbb{Z}^{d-k})$ with the following properties: first, P' is $\mathbb{Z}^{d-k}$-free since otherwise $\mathrm{int}(P') \times \mathbb{R}^k$, which is contained in $\mathrm{int}(P+M)$, contains integral points. Second, since by our choice of M we have that $P + M + \mathrm{lin}(u)$ is not lattice-free for every $u \in \mathbb{Z}^d \setminus M$, we have that $P' + \mathrm{lin}(u')$ is not lattice-free for every $u' \in \mathbb{Z}^{d-k} \setminus \{o\}$. Let $Z \subseteq \mathbb{Z}^{d-k}$ be such that $\mathrm{conv}(P' \cup Z)$ is lattice-free. Then since $P' \subseteq \mathrm{conv}(P' \cup Z)$, we have that $\mathrm{conv}(P' \cup Z) + \mathrm{lin}(u')$ is not lattice-free for every $u' \in \mathbb{Z}^{d-k} \setminus \{o\}$. By Lemma 2.15, there are only finitely many elements of $\mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$ fulfilling this condition up to unimodular equivalence and it is therefore possible to choose among all such sets Z a set Z' with maximal cardinality. Then $L := \mathrm{conv}(P' \cup Z') \times \mathbb{R}^k$ is a $\mathbb{Z}^d$-maximal lattice-free polyhedron in $\mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$ containing P. This proves (a).

Assertion (b): Let $P \in \mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$ be unbounded and $\mathbb{Z}^d$-maximal lattice-free. Let M, k and Z' be as in the proof of assertion (a). Observe that since P is unbounded, we have $\mathrm{rec}(P) \neq \{o\}$ and hence we also have $M \neq \{o\}$ and $k \in \{1, \dots, d-1\}$. Since P is $\mathbb{Z}^d$-maximal lattice-free, obviously, we must have $Z' = P' \cap \mathbb{Z}^{d-k}$. We will now prove that $P' \cap \mathbb{Z}^{d-k}$ is not empty. Assume the contrary and let $z_1 \in \mathbb{Z}^{d-k}$. Then if $T_1 := \mathrm{conv}(P' \cup \{z_1\})$ is not lattice-free, choose an integral point $z_2 \in \mathrm{int}(T_1) \cap \mathbb{Z}^{d-k}$ and replace T_1 by $T_2 := \mathrm{conv}(P' \cup \{z_2\})$. Since the number of integral points in T_1 is finite, repeating this step finitely many times yields some lattice-free T_j such that $P \subseteq T_j$. Since T_j contains a point $z_j \in \mathbb{Z}^{d-k} \setminus P'$, this is a contradiction to $Z' = P' \cap \mathbb{Z}^{d-k}$. Thus, since M is generated by elements of $\mathbb{Z}^d$, we have that $P + M$ contains integral points. Furthermore, for every proper subspace M' of M, we have $(P + M') \cap \mathbb{Z}^d \subsetneq (P + M) \cap \mathbb{Z}^d$. Hence, the $\mathbb{Z}^d$-maximality of P yields $P = P + M$.

Assertion (c): In view of assertion (b), it suffices to prove (c) for polytopes. Let $P \in \mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$ be bounded and $\mathbb{Z}^d$-maximal lattice-free. We have shown in the proof of (b) that P contains at least one integral point. Hence, for every $u \in \mathbb{Z}^d \setminus \{o\}$, the set $P + \mathrm{lin}(u)$ contains infinitely many points of $\mathbb{Z}^d$. The $\mathbb{Z}^d$-maximality of P therefore implies that $P + \mathrm{lin}(u)$ is not lattice-free for every $u \in \mathbb{Z}^d \setminus \{o\}$. In view of Lemma 2.15, this shows (c). □

We now complete the proof of Theorem 1.6. In the proof, we will make use of the following lemma. The essence of this lemma is the very basic fact that the convex hull of a lattice-free polytope P and a point which lies *beyond*[1] a blocked facet of P is not lattice-free. This fact is also used in the proof that $\mathbb{Z}^d$-maximality and $\mathbb{R}^d$-maximality are not equivalent for integral polytopes of dimension $d \geq 4$ in [NZ11, Theorem 3.2]. Our constructions for the cases of non-equivalence in the proof of Theorem 1.6 are motivated by the family of polytopes given in [NZ11, Theorem 3.2].

Lemma 2.16. *Let L be an $\mathbb{R}^d$-maximal lattice-free d-dimensional polyhedron. Let $P \subseteq L$ be a d-dimensional polyhedron such that $P \cap \mathbb{Z}^d = L \cap \mathbb{Z}^d$ and such that for every facet F of L, there exists a facet F' of P such that $F' \subseteq F$ and* $\mathrm{relint}(F') \cap \mathbb{Z}^d \neq \emptyset$*. Then, P is $\mathbb{Z}^d$-maximal lattice-free.*

[1] For a precise definition of beyond, see, e.g., [Zie95].

Proof. Let $p \in \mathbb{Z}^d \setminus P$. Since $P \cap \mathbb{Z}^d = L \cap \mathbb{Z}^d$, we have $p \notin L$. Thus, there exists a facet F of L such that for the hyperplane H spanned by F and the two open half-spaces H^+, H^- associated with H we have: $P \subseteq L \subseteq H \cup H^+$ and $p \in H^-$. By the assumptions of the lemma, there exists a facet $F' \subseteq F$ such that there exists a $z \in \mathbb{Z}^d$ with $z \in \text{relint}(F)$. Obviously, $P \subseteq P \cup \{p\}$ and thus, $F' = P \cap H \subseteq \text{conv}(P \cup \{p\}) \cap H$. Taking into account that $P \cap H \not\subseteq \text{relbd}(\text{conv}(P \cup \{p\}) \cap H)$, in view of [Roc97, Corollary 6.5.2] we have $\text{relint}(P \cap H) \subseteq \text{relint}(\text{conv}(P \cup \{p\}) \cap H)$. Hence, for F', we have the following relations:

$$\begin{aligned} z \in \text{relint}(F') &= \text{relint}(P \cap H) \\ &\subseteq \text{relint}(\text{conv}(P \cup \{p\}) \cap H) \\ &= \text{relint}(\text{conv}(P \cup \{p\}) \cap H \\ &\subseteq \text{relint}(\text{conv}(P \cup \{p\}) = \text{int}(\text{conv}(P \cup \{p\}), \end{aligned}$$

where the third line follows from [Roc97, Corollary 6.5.1]. This proves that P is $\mathbb{Z}^d$-maximal. □

Proof of Theorem 1.6. Let us first prove the cases in which (1.5) holds. Obviously, every $\mathbb{Z}$-maximal rational one-dimensional polyhedron is unimodularly equivalent to $[0, 1]$ and hence also $\mathbb{R}$-maximal. Thus, (1.5) holds for $d = 1$. For $d = 2$, let P be a $\mathbb{Z}^2$-maximal lattice-free polyhedron in $\mathcal{P}(\frac{1}{2}\mathbb{Z}^2)$. Then by Theorem 2.2 we have that P is unimodularly equivalent to one of the polygons Q_i, $i \in \{1, 2, 3, 4, 5\}$. All of those sets are obviously $\mathbb{R}^2$-maximal lattice-free and hence, (1.5) holds for $d = 2$ and $s = 2$. Furthermore, since $\mathcal{P}(\mathbb{Z}^2) \subseteq \mathcal{P}(\frac{1}{2}\mathbb{Z}^2)$, we have that (1.5) also holds for $d = 2$ and $s = 1$. For $d = 3$, $s = 1$ it follows from Theorem 1.3 that (1.5) holds.

To prove the cases in which (1.5) does not hold, we first observe that if (1.5) does not hold for some pair $(d, s) = (d_1, s_1)$, then it also does not hold for any pair (d_2, s_1) where $d_2 \geq d_1$. To see this, observe that if (1.5) does not hold for (d_1, s_1), this means that there exists a polyhedron $P \in \mathcal{P}(\frac{1}{s_1}\mathbb{Z}^{d_1})$ which is $\mathbb{Z}^{d_1}$-maximal but not $\mathbb{R}^{d_1}$-maximal. Hence, the polyhedron $P \times \mathbb{R}^{d_2 - d_1}$ is a polyhedron in $\mathcal{P}(\frac{1}{s_1}\mathbb{Z}^{d_2})$ which is $\mathbb{Z}^{d_2}$-maximal but not $\mathbb{R}^{d_2}$-maximal. Therefore, it suffices to prove that (1.5) does not hold in the cases $d = 2$, $s \geq 3$, $(d, s) = (3, 2)$ and $(d, s) = (4, 1)$.

For these cases, our construction is the following: we give an example of an $\mathbb{R}^d$-maximal lattice-free polytope $L \notin \mathcal{P}(\frac{1}{s}\mathbb{Z}^d)$ with the property that $P := \text{conv}(L \cap \frac{1}{s}\mathbb{Z}^d)$ fits the setting of Lemma 2.16. Then in view of Lemma 2.16 and the fact that $P \subsetneq L$, we have that P is $\mathbb{Z}^d$-maximal but not $\mathbb{R}^d$-maximal. For the choice of L, we rely on the following known fact: an axis-aligned simplex $\text{conv}(o, a_1e_1, \dots, a_de_d)$, where $a_1, \dots, a_d > 0$, is $\mathbb{R}^d$-maximal lattice-free if and only if

$$\frac{1}{a_1} + \cdots + \frac{1}{a_d} = 1; \tag{2.25}$$

see, e.g., [AWW09, Proof of Theorem 3.1].

Now, let $d = 2$ and $s \geq 3$. Let $L(s) := \text{conv}\left(o, (2 - \frac{1}{s})e_1, (2 + \frac{1}{s-1})e_2\right)$. Since (2.25) is fulfilled by $L(s)$, the polygon $L(s)$ is $\mathbb{R}^2$-maximal lattice-free. Consider $P(s) := \text{conv}(L \cap \frac{1}{s}\mathbb{Z}^d) = \text{conv}\left(o, (2 - \frac{1}{s})e_1, (2 + \frac{1}{s})e_2, 2e_2 + \frac{1}{s}e_1\right)$. This is a $\frac{1}{s}\mathbb{Z}^2$-polygon which is, by construction, properly contained in $L(s)$. Hence, $P(s)$ is lattice-free but obviously not $\mathbb{R}^2$-maximal lattice-free. However, it is straightforward to verify that each facet of $L(s)$ contains a facet of $P(s)$ which is blocked. Hence, in view of Lemma 2.16, we get that $P(s)$ is $\mathbb{Z}^2$-maximal.

We switch to the case $d = 3$, $s = 2$. Consider the polytope $L = \text{conv}\left(o, \frac{7}{2}e_1, \frac{7}{2}e_2, \frac{7}{3}e_3\right)$ and let $P = \text{conv}(L \cap \frac{1}{2}\mathbb{Z}^3)$. In view of (2.25), L is $\mathbb{R}^3$-maximal lattice-free. Obviously, $P \subsetneq L$ and hence, P is not $\mathbb{R}^3$-maximal. Observe that $-e_1, -e_2, -e_3$ are outer normal vectors of facets of L and it is easy to check that P has blocked facets with normal vectors $-e_1, -e_2, -e_3$. In view of Lemma 2.16, to show that P is $\mathbb{Z}^3$-maximal it therefore suffices to check that the facet of L given by $F = \{(x_1, x_2, x_3) \in L : 2x_1 + 2x_2 + 3x_3 = 7\}$ contains a facet of P which is blocked. Note that $(\frac{7}{2}, 0, 0), (0, \frac{7}{2}, 0), (\frac{1}{2}, 0, 2)$ are elements of $\frac{1}{2}\mathbb{Z}^3$ which are contained in F and which are obviously affinely independent. Hence, there exists a facet F' of P which contains those three points and is itself contained in F. Furthermore, one can write $(1, 1, 1)$ as convex combination of those three points using only positive coefficients:

$$(1,1,1) = \frac{3}{14}\left(\frac{7}{2}, 0, 0\right) + \frac{2}{7}\left(0, \frac{7}{2}, 0\right) + \frac{1}{2}\left(\frac{1}{2}, 0, 2\right).$$

This implies that $(1, 1, 1) \in \operatorname{int}\Big(\operatorname{conv}\big((\frac{7}{2}, 0, 0), (0, \frac{7}{2}, 0), (\frac{1}{2}, 0, 2)\big)\Big) \subseteq \operatorname{int}(F')$ and hence, the facet of P contained in F is blocked. Thus, P is $\mathbb{Z}^3$-maximal.

The case $d = 4, s = 1$ was treated in [NZ11, Theorem 3.2]. We give an example of our own here, the construction of which follows the same pattern as the examples for the previous two cases. Consider the axis-aligned rational polytope $L = \operatorname{conv}(o, 7e_1, 7e_2, \frac{7}{2}e_3, \frac{7}{3}e_4)$. Equivalently, we can express L by inequalities:

$$L = \left\{(x_1, x_2, x_3, x_4) \in \mathbb{R}^4 : x_1 \geq 0, x_2 \geq 0, x_3 \geq 0, x_4 \geq 0, x_1 + x_2 + 2x_3 + 3x_4 \leq 7\right\}.$$

Again, by (2.25) we have that L is $\mathbb{R}^4$-maximal lattice-free. We now define the polytope $P := \operatorname{conv}(L \cap \mathbb{Z}^4) \subsetneq L$, which is obviously not $\mathbb{R}^4$-maximal. We show that P is $\mathbb{Z}^4$-maximal. To that end, in view of Lemma 2.16, it suffices to show that for every $u \in U(L)$ we have $F(P, u) \subseteq F(L, u)$, $\dim(F(P, u)) = d - 1$ and $\mathbb{Z}^4 \cap \operatorname{relint}(F(P, u)) \neq \emptyset$.

From the description of L via inequalities, one has $U(L) = \{-e_1, -e_2, -e_3, -e_4, \tilde{u}\}$, where $\tilde{u} = e_1 + e_2 + 2e_3 + 3e_4$. For $i \in \{1, 2, 3, 4\}$, the facet $F(P, -e_i)$ is the convex hull of integral points in $F(L, -e_i)$. It can be verified in a straightforward way that for each i, the resulting facet is a simplex of dimension $d - 1$ which contains $(1, 1, 1, 1) - e_i$ in its relative interior. That leaves the facet

$$F(L, \tilde{u}) = \{(x_1, x_2, x_3, x_4) \in L : x_1 + x_2 + 2x_3 + 3x_4 = 7\}.$$

Consider the set $S := \{(7, 0, 0, 0), (0, 7, 0, 0), (1, 0, 3, 0), (1, 0, 0, 2)\} \subseteq F(L, \tilde{u})$. Note that the elements of S are affinely independent (which can be seen from the fact that the matrix having the elements of S as rows is a lower triangular matrix). Thus, $\operatorname{conv}(S)$ is a simplex of dimension 3 and by construction, $\operatorname{conv}(S)$ is contained in $F(P, \tilde{u})$. In particular, we have $\operatorname{relint}(\operatorname{conv}(S)) \subseteq \operatorname{relint}(F(P, \tilde{u})) \subseteq \operatorname{relint}(F(L, \tilde{u}))$. Consider the point $(1, 1, 1, 1) \in \mathbb{Z}^4$. One can write

$$(1,1,1,1) = \frac{1}{42}(7,0,0,0) + \frac{1}{7}(0,7,0,0) + \frac{1}{3}(1,0,3,0) + \frac{1}{2}(1,0,0,2),$$

which shows that $(1, 1, 1, 1)$ can be written as convex combination of the points of S using only positive coefficients. Thus, $(1, 1, 1, 1)$ is in the relative interior of $\operatorname{conv}(S)$. This completes the proof that P is $\mathbb{Z}^4$-maximal. □

The reason why we gave another example in the case $d = 4, s = 1$ in addition to that already known from [NZ11] is that we can also use the polytope we constructed to show the following remark concerning Theorem 2.6.

Remark 2.17. For given P, P_0, P_1, P_{-1} as in Theorem 2.4, we have $P_1 + P_{-1} \subseteq 2P_0$ by Theorem 2.4 (b1). Under the additional assumption of unimodularity of the integral vertices of P_0 made in Theorem 2.6, we get the stronger statement $P_1 + P_{-1} = 2P_0$. We point out that in general, this improvement cannot be obtained. Consider the polytope $P = L \cap \mathbb{Z}^4$, where $L = \operatorname{conv}(o, 7e_1, 7e_2, \frac{7}{2}e_3, \frac{7}{3}e_4)$. In the proof of Theorem 1.6, we have shown that P is $\mathbb{Z}^4$-maximal lattice-free. It is also straightforward to see that P has lattice width two and is contained in $\mathbb{R}^3 \times [0, 2]$. For $i \in \{-1, 0, 1\}$, let P_i be such that $P_i := \left\{x \in \mathbb{R}^3 : (x, i + 1) \in P\right\}$. Then $P_0 = \operatorname{conv}\left((0, 0, 0), (4, 0, 0), (0, 4, 0), (0, 0, 2)\right)$. Not all vertices of P_0 are unimodular: the vertex $(0, 0, 2)$ has normal vectors $-e_1, -e_2, e_1+e_2+2e_3$ (to be interpreted here as elements of $\mathbb{R}^3$), which do not form a basis of $\mathbb{Z}^3$. Furthermore, we introduce the following polytopes in $\mathbb{R}^3$: let $L_i := \left\{x \in \mathbb{R}^3 : (x, i + 1) \in L\right\}$ for $i \in \{-1, 0, 1\}$. Then we have $L_0 = P_0$ and $L_1 + L_{-1} = 2L_0$. On the other hand, we have $P_i \subsetneq L_i$ for $i \in \{-1, 1\}$, since L_i is not integral for $i \in \{-1, 1\}$. Hence, $P_1 + P_{-1} \neq 2P_0$ and thus, assertion (b) of Theorem 2.6 does not hold. Finally, observe that L_1 and L_{-1} are homothetic copies of L_0. Because $P_i \subsetneq L_i$ for $i \in \{-1, 1\}$ and P_i and L_i have all but one vertex in common, P_i cannot be a homothetic copy of L_i for $i \in \{-1, 1\}$ and thus, also not of P_0. This shows that assertion (a) does also not hold for P. ■

Chapter 3

Integral simplices with one interior integral point

In this chapter, the proofs of the results presented in Section 1.4 are given. All results and proofs in this chapter were obtained jointly by Gennadiy Averkov, Benjamin Nill and the author of this thesis and were published in [AKN15].

Structure of the chapter, main proof ideas and background results

Let $S \in \mathcal{S}^d(1)$ and let $\beta_1 \geq \ldots \geq \beta_{d+1} > 0$ be the barycentric coordinates of the interior integral point of S. Results from [Ave12] show that, on the one hand, the inequalities

$$\beta_1 \cdots \beta_j \leq \beta_{j+1} + \ldots + \beta_{d+1}$$

hold for every $j \in \{1, \ldots, d\}$ and, on the other hand, the volumes of faces of S can be bounded from above in terms of values $\frac{1}{\beta_a \cdots \beta_b}$ with $a, b \in \{1, \ldots, d+1\}$ and $a < b$. Thus, if one views $\beta_1, \ldots, \beta_{d+1}$ as arbitrary non-negative variables satisfying $\beta_1 + \ldots + \beta_{d+1} = 1$ and $\beta_1 \cdots \beta_j \leq \beta_{j+1} + \ldots + \beta_{d+1}$ for every $j \in \{1, \ldots, d\}$, the determination of the minimum of $\beta_a \cdots \beta_b$ (for given $1 \leq a \leq b \leq d$) allows us to find upper bounds on the volumes of faces of S. This purely analytical problem is treated in the first part of Section 3.1. The second part of Section 3.1 is concerned with uniqueness in the special case of minimizing a single barycentric coordinate. We link this problem to the problem of unit partitions from number theory and modify a result on unit partitions to derive uniqueness. In Sections 3.2–3.5, we then make use of the information about barycentric coordinates obtained in Section 3.1 and translate it into the size bounds for integral polytopes given in the results from Section 1.4. Furthermore, we characterize the equality cases where possible. These characterizations are carried out directly using number-theoretical properties of the Sylvester sequence.

First, we state some well-known theorems which we will make use of during this chapter.

Theorem 3.1 (Blichfeldt's theorem; [Bli14], [Cas97, p. 69]). *Let $C \subseteq \mathbb{R}^d$ be a d-dimensional convex set. Then*

$$|C \cap \mathbb{Z}^d| \leq d + d! \operatorname{vol}(C).$$

We will use the following generalization of Minkowski's theorem (see (2.11)) to non-symmetric convex sets, which is due to Mahler.

Theorem 3.2 (Mahler's theorem; [Mah39], [GL87, §7, Theorem 2]). *Let $C \subseteq \mathbb{R}^d$ be a d-dimensional compact convex set and let $\operatorname{int}(C) \cap \mathbb{Z}^d = \{o\}$. Then $\operatorname{vol}(C) \leq (1 + \operatorname{ca}(C, o))^d$.*

We will frequently use the Sylvester sequence, as defined in the introduction. For this sequence the following properties are easy to see.

PROPOSITION 3.3 ([LZ91, Lemma 2.1], [ZPW82, p. 44]). *For the Sylvester sequence $(s_i)_{i\in\mathbb{N}}$ and every $i \in \mathbb{N}$, the following statements hold:*

(a)

$$s_{i+1} = s_i^2 - s_i + 1.$$

(b)

$$\frac{1}{s_1} + \ldots + \frac{1}{s_i} + \frac{1}{s_{i+1} - 1} = 1.$$

(c)

$$2^{2^{i-2}} \leq s_i \leq 2^{2^{i-1}}$$

and, furthermore, for $i \geq 2$,

$$2^{2^{i-2}} + 1 \leq s_i.$$

REMARK 3.4. In view of Proposition 3.3, one can now verify in a straightforward way that the simplices $T^d_{1,j}$ are indeed in $\mathcal{S}^d(1)$ for $j \in \{1, \ldots, d+1\}$. The set $\mathrm{int}(T^d_{1,j}) \cap \mathbb{Z}^d$ is the set of points $(n_1, \ldots, n_d) \in \mathbb{N}^d$ fulfilling

$$\frac{n_1}{s_1} + \ldots + \frac{n_{j-1}}{s_{j-1}} + \frac{n_j + \ldots + n_d}{(d-j+2)(s_j - 1)} < 1. \tag{3.1}$$

If for $(n_1, \ldots, n_d) \in \mathbb{N}^d$ one has $n_1 = \ldots = n_d = 1$, then (3.1) holds in view of Proposition 3.3(b). Otherwise, one of the components $n_1, \ldots, n_d$ is at least 2. Taking into account that $s_1, \ldots, s_{j-1}, (d-j+2)(s_j - 1)$ is an increasing sequence, one sees that for $(n_1, \ldots, n_d) \in \mathbb{N}^d \setminus \{\mathbb{1}\}$ the smallest value of the left hand side of (3.1) is attained for $n_1 = \ldots = n_{d-1} = 1$ and $n_d = 2$. With this choice, the left hand side of (3.1) is

$$\frac{1}{s_1} + \ldots + \frac{1}{s_{j-1}} + \frac{d-j+2}{(d-j+2)(s_j - 1)} = 1.$$

Hence, (3.1) is not fulfilled for $(n_1, \ldots, n_d) \in \mathbb{N}^d \setminus \{\mathbb{1}\}$. ■

The following two theorems from [Ave12] deal with simplices $S \in \mathcal{S}^d(1)$. Let p be the unique interior integral point of S and let $\beta_1, \ldots, \beta_{d+1}$ be the barycentric coordinates of p with respect to S. It is clear that $\beta_i > 0$ for every $i \in \{1, \ldots, d+1\}$ because p is in the interior of S. Our analysis of S relies mainly on two different results from [Ave12]. The first one is a general statement establishing a system of inequalities for $\beta_1, \ldots, \beta_{d+1}$.

THEOREM 3.5 ([Ave12, Theorem 1.1]). *Let $S \in \mathcal{S}^d(1)$. Let $\beta_1 \geq \ldots \geq \beta_{d+1} > 0$ be the barycentric coordinates of the unique interior integral point of S. Then, for every $j \in \{1, \ldots, d\}$,*

$$\beta_1 \cdots \beta_j \leq \beta_{j+1} + \ldots + \beta_{d+1}. \tag{3.2}$$

Theorem 1.1 in [Ave12] has a somewhat different but equivalent formulation; see the discussion in [Ave12, page 7]. The second result from [Ave12] which we use here links the barycentric coordinates to the face volumes of the simplex.

THEOREM 3.6 ([Ave12, Theorem 3.7]). *Let $S \subseteq \mathbb{R}^d$ be a d-dimensional simplex with $\mathrm{vert}(S) \subseteq \mathbb{Q}^d$ containing precisely one interior integral point, which we denote by p. Let $\beta_1 \geq \ldots \geq \beta_{d+1} > 0$ denote the barycentric coordinates of p with respect to S. Let F be an l-dimensional face of S, where*

$l \in \{1, \ldots, d\}$. *Let* $\beta_{i_1}, \ldots, \beta_{i_{l+1}}$ *be the barycentric coordinates of* p *associated with the vertices of* F, *where* $1 \le i_1 < \ldots < i_{l+1} \le d+1$. *Then*

$$\mathrm{vol}_{\mathbb{Z}}(F) \le \frac{1}{l!\beta_{i_1} \cdots \beta_{i_l}}.$$

Direct application of Theorem 3.6 yields

$$\max_{F \in \mathcal{F}_l(S)} \mathrm{vol}_{\mathbb{Z}}(F) \le \frac{1}{l!\beta_{d-l+1} \cdots \beta_d} \tag{3.3}$$

and

$$\min_{F \in \mathcal{F}_l(S)} \mathrm{vol}_{\mathbb{Z}}(F) \le \frac{1}{l!\beta_1 \cdots \beta_l}, \tag{3.4}$$

where $l \in \{1, \ldots, d\}$.

Note that Theorem 3.6 was only formulated in [Ave12] for the case of an integral simplex. One can see, however, that the proof from [Ave12] can be applied to our more general setting without any changes. Also, for $l = d$, this result can be found in [Pik01, Lemma 5]; see also [Hen83, Theorem 3.4] and [LZ91, Lemma 2.3].

3.1 Bounds on barycentric coordinates

Izhboldin-Kurliandchik type problems

Because of (3.3) we are interested in the minimal value the product $\beta_a \cdots \beta_d$ can attain for any given $a \in \{1, \ldots, d\}$. In this section, we will treat a more general problem which we call 'Izhboldin-Kurliandchik' problem. First, we introduce some notation which will be used frequently throughout. For the sake of brevity, let $n := d+1$. Let $\mathcal{X}^n$ denote the set of n-tuples $(x_1, \ldots, x_n) \in \mathbb{R}^n$ which fulfil the conditions

$$x_1 + \ldots + x_n = 1, \tag{3.5}$$

$$1 \ge x_1 \ge \ldots \ge x_n \ge 0, \tag{3.6}$$

$$x_1 \cdots x_j \le x_{j+1} + \ldots + x_n \quad \forall\, j \in \{1, \ldots, n-1\}. \tag{3.7}$$

Theorem 3.5 shows that every decreasingly sorted $(d+1)$-tuple of barycentric coordinates of the interior integral point of a simplex from $\mathcal{S}^d(1)$ belongs to the set $\mathcal{X}^n$. Throughout this section, we shall assume $x_0 := 1$ and $x_{n+1} := 0$. Furthermore, we introduce additional notation to keep the presentation simple: ORD(j) denotes the inequality $x_j \ge x_{j+1}$ for $j \in \{0, \ldots, n\}$ and will be called the j-th *ordering inequality*. Similarly, PS(j) denotes the inequality $x_1 \cdots x_j \le x_{j+1} + \ldots + x_n$ and will be called the j-th *product-sum inequality* for $x \in \mathbb{R}^n$ and $j \in \{1, \ldots, n-1\}$.

Given a continuous function $f : \mathcal{X}^n \to \mathbb{R}$, we denote by $\mathrm{IK}^n(f)$ the optimization problem of minimizing f over the set $\mathcal{X}^n$. This notation is short for 'Izhboldin-Kurliandchik problem', as Izhboldin and Kurliandchik determined the optimal value and the unique optimal solution of $\mathrm{IK}^n(x_1 \cdots x_n)$ as well as $\mathrm{IK}^n(x_n)$; see [IK87] and [IK95]. For $\mathrm{IK}^n(f)$, we shall use the standard optimization terminology such as optimal value, optimal solution and feasible solution.

Furthermore, we introduce the following notation to denote special elements of $\mathcal{X}^n$: for $l \in \{1, \ldots, n\}$, we define the vector $y(l) \in \mathbb{R}^n$ by

$$y(l) := \left(\frac{1}{s_1}, \ldots, \frac{1}{s_{l-1}}, \frac{1}{(n-l+1)(s_l - 1)}, \ldots, \frac{1}{(n-l+1)(s_l - 1)} \right).$$

For $l \in \{1, n\}$, the degenerate cases should be interpreted as $y(1) = \left(\frac{1}{n}, \dots, \frac{1}{n}\right)$ and $y(n) = \left(\frac{1}{s_1}, \dots, \frac{1}{s_{n-1}}, \frac{1}{s_n - 1}\right)$. We can then define the set $\mathcal{Y}^n$ for every $n \geq 2$ as

$$\mathcal{Y}^n := \{y(l) \,:\, l = 1, \dots, n\}\,.$$

One can check that every vector $y(l)$ fulfils conditions (3.5)–(3.7) and thus, $\mathcal{Y}^n \subseteq \mathcal{X}^n$.

Problem $\mathrm{IK}^n(x_a \cdots x_b)$ for general a and b

We modify the arguments of Izhboldin and Kurliandchik given in [IK87] and [IK95] to give a more general result about the relation of $\mathcal{Y}^n$ to the set of optimal solutions of $\mathrm{IK}^n(x_a \cdots x_b)$, which we state in Lemma 3.8. In Theorem 3.9, we then show which elements of $\mathcal{Y}^n$ are optimal solutions of $\mathrm{IK}^n(x_a \cdots x_b)$.

Clearly, $\mathcal{X}^n$ is a compact set. It turns out that for every $x \in \mathcal{X}^n$ one has $x_1 < 1$ and $x_n > 0$ for every n. This and two other basic but important properties, which characterize equality cases for the inequalities describing $\mathcal{X}^n$, are proven in the following lemma. Assertion (c) also establishes the link to the Sylvester sequence.

Lemma 3.7 (Basic properties of $\mathcal{X}^n$). *Let $x \in \mathcal{X}^n$, where $n \geq 3$. Then the following statements hold:*

(a) $0 < x_n$ and $1 > x_1$.

(b) For $l \in \{1, \dots, n-1\}$, the inequalities $\mathrm{ORD}(l)$ and $\mathrm{PS}(l)$ for x cannot simultaneously be fulfilled with equality.

(c) If for some $l \in \{1, \dots, n-1\}$, the inequality $\mathrm{PS}(i)$ for x is fulfilled with equality for every $i \in \{1, \dots, l\}$, then $x_i = \frac{1}{s_i}$ for every $i \in \{1, \dots, l\}$.

Proof. To prove assertion (a), observe that if $x_n = 0$, then by $\mathrm{PS}(n-1)$ also $x_1 \cdots x_{n-1} = 0$ and the ordering inequalities then imply $x_{n-1} = 0$. Iteratively, the above argument leads to $x_i = 0$ for every $i \in \{1, \dots, n\}$, yielding a contradiction to $x_1 + \ldots + x_n = 1$. If $x_1 = 1$, then in view of $x_1 + \ldots + x_n = 1$, we get $x_2 = \ldots = x_n = 0$, a contradiction to $\mathrm{PS}(1)$.

We show assertion (b) by proving that if for some $l \in \{1, \dots, n-1\}$ we have $x_1 \cdots x_l = x_{l+1} + \ldots + x_n$, this implies $x_l > x_{l+1}$. Since $n \geq 3$, the product $x_1 \cdots x_l$ contains more than one factor or the sum $x_{l+1} + \cdots + x_n$ contains more than one summand. Hence, in view of (a),

$$x_l \geq x_1 \cdots x_l = x_{l+1} + \ldots + x_n \geq x_{l+1},$$

where at least one of the two inequalities is strict. Thus, we obtain $x_l > x_{l+1}$.

Assertion (c) follows by induction on i. For $i = 1$, from $x_1 = 1 - x_1$ we get $x_1 = 1/2 = 1/s_1$. Assuming the statement holds up to some $i \in \{1, \dots, l-1\}$, we get from the definition of the Sylvester sequence, Proposition 3.3 and $x_1 \cdots x_i x_{i+1} = 1 - (x_1 + \ldots + x_i + x_{i+1})$:

$$\frac{x_{i+1}}{s_{i+1} - 1} = \frac{1}{s_{i+1} - 1} - x_{i+1}$$

and hence $x_{i+1} = \frac{1}{s_{i+1}}$. □

The aim of this section is to find optimal solutions for $\mathrm{IK}^n(x_a \cdots x_b)$, where $1 \leq a \leq b \leq n$. In the following lemma, we deal with the more general problem $\mathrm{IK}^n(x_1^{\alpha_1} \cdots x_n^{\alpha_n})$ for real numbers $\alpha_1, \dots, \alpha_n$. Using a limit argument, we can then derive assertions about $\mathrm{IK}^n(x_a \cdots x_b)$.

Lemma 3.8 (On optimal solutions of $\mathrm{IK}^n(x_1^{\alpha_1}\cdots x_n^{\alpha_n})$). *Let $n \ge 2$, $b \in \{1,\dots,n\}$ and $\alpha_1,\dots,\alpha_n \in \mathbb{R}$ be such that $0 \le \alpha_i \le \alpha_j$ for all $1 \le i \le j \le b$ and $\alpha_i = \alpha_j \le 0$ for all $i, j > b$. Then the following assertions hold:*

(a) There exists an optimal solution x^* for $\mathrm{IK}^n(x_1^{\alpha_1}\cdots x_n^{\alpha_n})$ with $x^* \in \mathcal{Y}^n$.

(b) If $\alpha_i \neq 0$ for all $i \in \{1,\dots,n\}$, then all optimal solutions of $\mathrm{IK}^n(x_1^{\alpha_1}\cdots x_n^{\alpha_n})$ are in $\mathcal{Y}^n$.

(c) If $b = n-1$, $\alpha_i > 0$ for all $i \neq n$ and $\alpha_n = 0$, then all optimal solutions of $\mathrm{IK}^n(x_1^{\alpha_1}\cdots x_n^{\alpha_n})$ are in $\mathcal{Y}^n$.

(d) If $a = 1$, $b = n$ and $\alpha_i > 0$ for all $i \in \{1,\dots,n\}$, then the unique optimal solution to $\mathrm{IK}^n(x_1^{\alpha_1}\cdots x_n^{\alpha_n})$ is

$$\left(\frac{1}{s_1},\dots,\frac{1}{s_{n-1}},\frac{1}{s_n-1}\right).$$

Proof. The proof is organized as follows. We start by proving an auxiliary claim. Then we prove (b) and subsequently deduce (a) as a consequence of (b). Next, we observe that the proof of (b) can be slightly modified to give a proof of (c). Finally, we prove (d) by showing that under the additional assumptions, the arguments used in the proof of (b) allow an explicit description of the optimal solution.

Claim 3.8.1. If $b < n$ and $\alpha_i < 0$ for all $i \in \{b+1,\dots,n\}$, then every optimal solution x^* of $\mathrm{IK}^n(x_1^{\alpha_1}\cdots x_n^{\alpha_n})$ has the property

$$x_b^* = \ldots = x_n^*. \tag{3.8}$$

Proof of the claim. We assume the contrary, i.e., the existence of an optimal solution $x^* \in \mathcal{X}^n$ which does not satisfy (3.8). Let $j \in \{b,\dots,n-1\}$ be the maximal index such that $\mathrm{ORD}(j)$ is strict for x^*. This allows us to construct an element $x' \in \mathcal{X}^n$ by subtracting a small $\delta > 0$ from the j-th component of x^* and adding δ to the $(j+1)$-th component. To see that x' is indeed an element of $\mathcal{X}^n$, observe that its components still sum to one and all ordering inequalities are still fulfilled. It remains to check that $\mathrm{PS}(i)$ remains valid for every i. For $i < j$, this is obviously the case: neither the product part nor the sum part of the inequalities $\mathrm{PS}(1),\dots,\mathrm{PS}(j-1)$ are affected. $\mathrm{PS}(j)$ also remains valid as its product part becomes smaller while its sum part becomes larger. For $i > j$, by maximality of j, we have that $\mathrm{ORD}(i)$ is fulfilled with equality for x^*. So, by Lemma 3.7(b), the inequality $\mathrm{PS}(i)$ has to be strict for x^* and hence remains valid if δ is chosen small enough. Now we show that x' is a better feasible solution of $\mathrm{IK}^n(x_1^{\alpha_1}\cdots x_n^{\alpha_n})$. First we treat the case $j > b$, for which the values of the objective function at x^* and x' differ by the factor

$$\frac{(x_1')^{\alpha_1}\cdots(x_n')^{\alpha_n}}{(x_1^*)^{\alpha_1}\cdots(x_n^*)^{\alpha_n}} = \left(1-\frac{\delta}{x_j^*}\right)^{\alpha}\left(1+\frac{\delta}{x_{j+1}^*}\right)^{\alpha} = \left(1+\frac{\delta}{x_{j+1}^*}-\frac{\delta}{x_j^*}-\frac{\delta^2}{x_j^*x_{j+1}^*}\right)^{\alpha}, \tag{3.9}$$

where $\alpha := \alpha_j = \alpha_{j+1}$. For a sufficiently small $\delta > 0$, this factor is less than one as $\mathrm{ORD}(j)$ is strict for x^* and $\alpha < 0$. This yields the desired contradiction. If $j = b$, then the contradiction is more easily obtained, as in this case $\alpha_j \ge 0 > \alpha_{j+1}$. Hence the contradiction follows immediately from $(x_j^*-\delta)/x_j^* < 1 < (x_{j+1}^*+\delta)/x_{j+1}^*$. This proves the claim. ■

Assertion (b). Assume that $\alpha_i \neq 0$ for all $i \in \{1,\dots,n\}$. Let x^* be an optimal solution of $\mathrm{IK}^n(x_1^{\alpha_1}\cdots x_n^{\alpha_n})$. We show $x^* \in \mathcal{Y}^n$. By $k \in \{0,\dots,n-1\}$ we denote the index such that $x_k^* > x_{k+1}^* = \ldots = x_n^*$. The degenerate case $k = 0$ is trivial, as then $x^* = (1/n,\dots,1/n) \in \mathcal{Y}^n$.

We therefore assume $k \geq 1$. Observe that by Claim 3.8.1, if $b < n$, then this implies $k \leq b - 1$ and hence $\alpha_i > 0$ for $i \in \{1, \dots, k\}$. We show that, for all $j < k$, the inequality ORD(j) is strict. In view of Lemma 3.7(a), the inequality ORD(0) is strict and hence for $k = 1$, there is nothing to show. It remains to show that for $k \geq 2$, the inequality ORD(j) is strict for every $j < k$. Note that ORD(k) is strict by construction and, as stated above, ORD(0) is strict as well. Thus, if there exists $j \in \{1, \dots, k-1\}$ such that ORD(j) is fulfilled with equality, one can determine a pair of indices i_1, i_2 with $1 \leq i_1 < i_2 \leq k$ such that, for x^*, the inequalities ORD($i_1 - 1$) and ORD(i_2) are strict, while ORD(j) is fulfilled with equality for $j \in \{i_1, \dots, i_2 - 1\}$. We can again perturb x^* to some $x' \in \mathcal{X}^n$ by adding a small $\delta > 0$ to $x^*_{i_1}$ and subtracting δ from $x^*_{i_2}$. For convenience, we write y for the value of $x^*_{i_1}$ and $x^*_{i_2}$, which are equal by construction. Again, to prove $x' \in \mathcal{X}^n$ we only need to look at the product-sum inequalities. For $j < i_1$, both sides of PS(j) remain unchanged. For $j \in \{i_1, \dots, i_2 - 1\}$, Lemma 3.7(b) yields that PS(j) is strict for x^* and hence remains valid for x' if $\delta > 0$ is small enough. For $j \geq i_2$, only the product part of PS(j) is affected. To be more precise, the product part changes by the factor $(y + \delta)(y - \delta)/y^2$, which is less than one. Thus, PS(j) is still valid for x' and we conclude that $x' \in \mathcal{X}^n$. Passing from $x^* \in \mathcal{X}^n$ to $x' \in \mathcal{X}^n$, the value of the objective function changes by the factor

$$\left(\frac{y+\delta}{y}\right)^{\alpha_{i_1}} \left(\frac{y-\delta}{y}\right)^{\alpha_{i_2}} \leq \left(1 - \frac{\delta^2}{y^2}\right)^{\alpha_{i_2}} < 1$$

since $\alpha_{i_1} \leq \alpha_{i_2}$. This is a contradiction to the choice of x^*. We deduce that ORD(j) is strict for every $j < k$. Next, we show that for $x^* \in \mathcal{X}^n$ and every $1 \leq j < k$, the inequality PS(j) is fulfilled with equality. We assume the contrary. Then $k \geq 2$ and there exists some index $i \in \{1, \dots, k-1\}$ such that PS(i) is strict. Since ORD($i - 1$) and ORD($i + 1$) are strict, we can again add a $\delta > 0$ to x^*_i and subtract δ from x^*_{i+1} to obtain a new element x' of $\mathcal{X}^n$ by the same arguments as above. This is a contradiction since the values of the objective function $x_1^{\alpha_1} \cdots x_n^{\alpha_n}$ at x' and at x^* differ by the factor

$$\begin{aligned} \frac{(x^*_i + \delta)^{\alpha_i}(x^*_{i+1} - \delta)^{\alpha_{i+1}}}{x_i^{*\alpha_i} x_{i+1}^{*\alpha_{i+1}}} &= \left(1 + \frac{\delta}{x^*_i}\right)^{\alpha_i} \left(1 - \frac{\delta}{x^*_{i+1}}\right)^{\alpha_{i+1}} \\ &\leq \left(1 + \frac{\delta}{x^*_i} - \frac{\delta}{x^*_{i+1}} - \frac{\delta^2}{x^*_i x^*_{i+1}}\right)^{\alpha_{i+1}}. \end{aligned} \tag{3.10}$$

For a sufficiently small $\delta > 0$, this factor is less than one since $\alpha_{i+1} > 0$. This is a contradiction to the choice of x^*.

We show now that PS(k) is also fulfilled with equality. Suppose that this is not the case, i.e., $x^*_1 \cdots x^*_k < x^*_{k+1} + \ldots + x^*_n$. Note that we have $x^*_{k-1} > x^*_k > x^*_{k+1} = \ldots = x^*_n$. By Lemma 3.7(b), this implies that for $k + 1 \leq j \leq n - 1$, the inequality PS(j) is strict for x^*. Let δ be close to 0, but not necessarily positive. We define $x(\delta) := (x^*_1, \dots, x^*_{k-1}, x^*_k + \delta(n - k), x^*_{k+1} - \delta, \dots, x^*_n - \delta)$. Observe that, if δ is sufficiently close to 0, $x(\delta) \in \mathcal{X}^n$. To see this, note that ORD(j) is unaffected for $1 \leq j < k - 1$, while ORD($k - 1$) and ORD(k) remain valid for x if δ is sufficiently close to 0. For $k + 1 \leq j \leq n - 1$, both sides of ORD(j) change by the same amount. PS(j) obviously remains valid for $1 \leq j \leq k - 1$. Since for $k \leq j \leq n - 1$, the inequality PS(j) is strict for x^* it remains valid for x if δ is sufficiently close to 0.

We consider the function f in δ given by

$$f(\delta) = (x^*_1)^{\alpha_1} \cdots (x^*_{k-1})^{\alpha_{k-1}} (x^*_k + \delta(n-k))^{\alpha_k} (x^*_{k+1} - \delta)^{\alpha_k} \cdots (x^*_n - \delta)^{\alpha_n}.$$

We want to show that f does not have a local minimum in $\delta = 0$ and hence, $x^* = x(0)$ cannot be an optimal solution of $\mathrm{IK}^n(x_1^{\alpha_1} \cdots x_n^{\alpha_n})$. As $f(0)$ is fixed (and not 0), it is more convenient to analyze the scaled function $g(\delta) = f(\delta)/f(0)$. For convenience, we also write $y := x^*_{k+1} = \ldots = x^*_n$ and $\beta = \alpha_{k+1} + \ldots + \alpha_n$. Using this notation, we have

$$g(\delta) = \left(1 + \frac{\delta(n-k)}{x^*_k}\right)^{\alpha_k} \left(1 - \frac{\delta}{y}\right)^{\beta}.$$

The first derivative at $\delta = 0$ is

$$g'(0) = \frac{\alpha_k(n-k)}{x^*_k} - \frac{\beta}{y}.$$

If $g'(0) \neq 0$, 0 is not a local minimum of g. If $g'(0) = 0$, we have $\alpha_k(n-k)y = \beta x^*_k$. Let us assume that this holds, as otherwise, we are done. Note that since α_k, $n-k$, y and x^*_k are all positive, this implies $\beta > 0$. We want to show that if $g'(0) = 0$, then 0 is strict local maximum of g. Hence, we need to show $g''(0) < 0$. We now consider the second derivative at $\delta = 0$, which is

$$g''(0) = \alpha_k(\alpha_k - 1)\frac{(n-k)^2}{(x^*_k)^2} - 2\frac{\alpha_k(n-k)\beta}{x^*_k y} + \frac{\beta(\beta-1)}{y^2}.$$

In view of the assumption $\alpha_k(n-k)y = \beta x^*_k$, we get

$$g''(0) = \frac{\beta^2}{y^2} - \frac{(n-k)\beta}{x^*_k y} - 2\frac{\beta^2}{y^2} + \frac{\beta^2 - \beta}{y^2}.$$

As $\beta > 0$ and $y > 0$, for $g''(0) < 0$ it suffices to have

$$-\frac{(n-k)}{x^*_k} - \frac{1}{y} < 0.$$

Since $n-k$, x^*_k and y are positive, this statement is true. Hence, x^* cannot be an optimal solution of $\mathrm{IK}^n(x_1^{\alpha_1} \cdots x_n^{\alpha_n})$, which is a contradiction to the choice of x^*. Thus, we deduce that PS(k) is fulfilled with equality.

Hence, we have that for every optimal solution x^* under the assumptions that $\alpha_i \neq 0$ for every $i \in \{1, \ldots, n\}$, inequality PS(j) is satisfied with equality for every $1 \leq j \leq k$. By Lemma 3.7(c), we get that $x^*_j = 1/s_j$ for $j \in \{1, \ldots, k\}$. Since x_j has been uniquely determined for $j \in \{1, \ldots, k\}$, the value for $x^*_{k+1} = \ldots = x^*_n$ can be uniquely determined from $x_1 + \ldots + x_n = 1$. In view of Proposition 3.3(b), we get

$$x^*_{k+1} = \ldots = x^*_n = \frac{1}{(n-k)(s_{k+1} - 1)}$$

and hence $x^* \in \mathcal{Y}^n$, thereby proving (b).

Assertion (a). We now drop the assumption $\alpha_i \neq 0$ for all $i \in \{1, \ldots, n\}$. Note that since for each $i \in \{1, \ldots, n\}$ and every $x \in \mathcal{X}^n$ we have $x_i > 0$, the expression $x_i^{\alpha_i}$ is continuous in α_i. As a consequence, for every fixed $x \in \mathcal{X}^n$, the expression $x_1^{\alpha_1} \cdots x_n^{\alpha_n}$ is continuous in $(\alpha_1, \ldots, \alpha_n)$. Hence, an optimal solution can be deduced from (b) by a limit argument. For $t \in \mathbb{N}$, we introduce the function $f_t(x) := x_1^{\alpha_1 + \frac{1}{t}} \cdots x_b^{\alpha_b + \frac{1}{t}} x_{b+1}^{\alpha_{b+1} - \frac{1}{t}} \cdots x_n^{\alpha_n - \frac{1}{t}}$. By (b), the problem $\mathrm{IK}^n(f_t)$ has an optimal solution x^*_t belonging to $\mathcal{Y}^n$, i.e.

$$f_t(x^*_t) \leq f_t(x) \tag{3.11}$$

for every $x \in \mathcal{X}^n$. Since $\mathcal{Y}^n$ is finite, there exists an element $y \in \mathcal{Y}^n$ and an infinite set $T \subseteq \mathbb{N}$ such that for every $t \in T$, we have $x_t^* = y$. Passing to the limit in (3.11) as $t \in T$ tends to ∞, we deduce that y is an optimal solution of $\mathrm{IK}^n(x_1^{\alpha_1} \cdots x_n^{\alpha_n})$. This shows (a).

Assertion (c). Note that because we pass to the limit, we cannot guarantee that in the case of a general choice of $(\alpha_1, \ldots, \alpha_n)$ all optimal solutions of $\mathrm{IK}^n(x_1^{\alpha_1} \cdots x_n^{\alpha_n})$ are in $\mathcal{Y}^n$. In particular, one needs a different argument to prove (c). We show that if $\alpha_n = 0$ but $\alpha_i > 0$ for $i \neq n$, we have that $x_{n-1}^* = x_n^*$ holds for every optimal solution x^*. To see this, assume the contrary, i.e. $x_{n-1}^* > x_n^*$. Then, we can perturb x^* into some x' by setting $x_i' := x_i^*$ for $i \in \{1, \ldots, n-2\}$, $x_{n-1}' := x_{n-1}^* - \delta$ and $x_n' := x_n^* + \delta$ for $\delta > 0$ sufficiently small. Obviously, the product-sum inequalities remain valid and thus $x' \in \mathcal{X}^n$. This leads to

$$(x_1')^{\alpha_1} \cdots (x_{n-1}')^{\alpha_{n-1}} < (x_1^*)^{\alpha_1} \cdots (x_{n-1}^*)^{\alpha_{n-1}},$$

a contradiction to the choice of x^*. Now we can apply the arguments of assertion (b) to obtain (c).

Assertion (d). We show that if x^* is an optimal solution, x^* satisfies $\mathrm{PS}(j)$ with equality for every $j \in \{1, \ldots, n-1\}$. Let $i_1, i_2 \in \{1, \ldots, n-1\}$ with $i_1 < i_2$ be such that for x^*, the inequality $\mathrm{PS}(j)$ is strict for $i_1, \ldots, i_2$, but $\mathrm{PS}(i_1 - 1)$ and $\mathrm{PS}(i_2 + 1)$ are fulfilled with equality. Of course, the requirement on $\mathrm{PS}(i_1 - 1)$ is only considered if $i_1 > 1$ and on $\mathrm{PS}(i_2 + 1)$ only if $i_2 < n - 1$. Then by Lemma 3.7(b), $\mathrm{ORD}(i_1 - 1)$ and $\mathrm{ORD}(i_2 + 1)$ are strict. Note that for the degenerate cases $i_1 = 1$ or $i_2 = n - 1$ this still holds and hence we do not need to consider them separately. We consider x' given by $x_i' := x_i^*$ for $i \in \{1, \ldots, n\} \setminus \{i_1, i_2\}$ and $x_{i_1}' := x_{i_1}^* + \delta$, $x_{i_2+1}' := x_{i_2+1}^* - \delta$ for some $\delta > 0$. Since $\mathrm{ORD}(i_1 - 1)$ and $\mathrm{ORD}(i_2 + 1)$ are strict, they remain valid for x' if δ is sufficiently small. To show $x' \in \mathcal{X}^n$, we check that x' satisfies all product-sum inequalities. This can be done in the same way as in the proof of assertion (b). We then argue that x' is a better solution to $\mathrm{IK}^n(x_1^{\alpha_1} \cdots x_n^{\alpha_n})$ by repeating the argumentation leading to (3.10) with i_1 instead of i and $i_2 + 1$ instead of $i + 1$. This yields a contradiction and proves that x^* satisfies $\mathrm{PS}(j)$ with equality for every $j \in \{1, \ldots, n-1\}$. Applying Lemma 3.7(c) then yields $x_j = 1/s_j$ for every $j \in \{1, \ldots, n-1\}$ and from $x_1^* + \ldots + x_n^* = 1$ we obtain $x_n = 1/(s_n - 1)$. □

We remark that Lemma 3.8(d) is a generalization of the result proved by Izhboldin and Kurliandchik, who assumed $\alpha_i = 1$ instead of $\alpha_i > 0$ for every $i \in \{1, \ldots, n\}$. In the following, we analyze the problem $\mathrm{IK}^n(x_a \cdots x_b)$ for specific choices of a and b. Lemma 3.8 states that for every a, b such that $1 \leq a \leq b \leq n$, we find an optimal solution of $\mathrm{IK}^n(x_a \cdots x_b)$ in $\mathcal{Y}^n$. The following theorem now deals with the question which elements of $\mathcal{Y}^n$ are optimal solutions of $\mathrm{IK}^n(x_a \cdots x_b)$ depending on the choice of a and b.

Theorem 3.9 (Localization of optimal solutions of $\mathrm{IK}^n(x_a \cdots x_b)$ within $\mathcal{Y}^n$). *Let $n, a, b \in \mathbb{N}$ be such that $n \geq 4$ and $1 \leq a \leq b \leq n$. Let $l \in \{1, \ldots, n\}$. Then the following statements hold:*

(a) If $a = b$, then $y(b)$ is an optimal solution of $\mathrm{IK}^n(x_b)$.

(b) If $b < n - 1$, $a < b$ and $y(l)$ is an optimal solution of $\mathrm{IK}^n(x_a \cdots x_b)$, then $a \leq l \leq \min\{b, 2 + \log_2 \log_2(ne)\}$ or $l = b$.

(c) If $b = n$, then $y(l)$ is an optimal solution of $\mathrm{IK}^n(x_a \cdots x_n)$ if and only if $l = n$.

(d) If $b = n - 1$, then $y(l)$ is an optimal solution of $\mathrm{IK}^n(x_a \cdots x_b)$ if and only if $l = n - 1$ or $n = 4$, $1 \leq a \leq 2$, $l = 2$.

(e) If $n \geq 5$, $a = 1$ and $b = n - 1$, then

$$y(n-1) = \Big(\frac{1}{s_1}, \cdots, \frac{1}{s_{n-2}}, \frac{1}{2(s_{n-1}-1)}, \frac{1}{2(s_{n-1}-1)}\Big)$$

is the unique optimal solution of $\mathrm{IK}^n(x_1 \cdots x_{n-1})$. *If $n = 4$ and $a = 1$ and $b = 3$, then* $y(2) = (1/2, 1/6, 1/6, 1/6)$ *and* $y(3) = (1/2, 1/3, 1/12, 1/12)$ *are the only optimal solutions of* $\mathrm{IK}^4(x_1x_2x_3)$.

Proof. By Lemma 3.8(a), for every choice of a, b there exists an optimal solution of $\mathrm{IK}^n(x_a \cdots x_b)$ which is in $\mathcal{Y}^n$ and hence can be expressed as $y(l)$. For the proof, we view l as a variable ranging in $\{1, \ldots, n\}$. Let $y(l) = (y(l)_1, \ldots, y(l)_n)$. We introduce the function $f(l) := 1/(y(l)_a \cdots y(l)_b)$. The structure of the proof is as follows: first, we show that $a \leq l \leq b$ if l maximizes $f(l)$. We then show that $f(l)$ is strictly monotonously increasing in l provided l ranges in $\{a, \ldots, b\}$ and is not too close to a or b.

Claim 3.9.1. If $y(l)$ is an optimal solution of $\mathrm{IK}^n(x_a \cdots x_b)$, then $l \in \{a, \ldots, b\}$.

Proof of the claim. We first show that if $y(l)$ is an optimal solution of $\mathrm{IK}^n(x_a \cdots x_b)$, then $l \geq a$. This is obviously true if $a = 1$. Assume $a > 1$ and $l < a$. We compare $f(l)$ and $f(l+1)$ and want to show the inequality

$$f(l) = \Big((n-l+1)(s_l-1)\Big)^{b-a+1} < \Big((n-l)(s_{l+1}-1)\Big)^{b-a+1} = f(l+1).$$

Using $s_{l+1} - 1 = s_l(s_l - 1)$ we can reformulate the desired inequality as

$$(n-l+1)(s_l-1) < (n-l)(s_l-1)s_l$$

or, equivalently, $1 < (s_l - 1)(n - l)$. The latter is clearly true since for $l = 1$, one has $s_l = 2$ and $n - l \geq 3$ while for $l > 1$, one has $s_l \geq 3$ and $n - l \geq 1$. This shows that if l maximizes $f(l)$, we have $l \geq a$. To conclude the proof of the claim it remains to show that if $f(l)$ is maximized for $l \in \{1, \ldots, n\}$, then $l \leq b$. We assume $b < n$, because otherwise there is nothing to show. Observe that by the definition of the Sylvester sequence

$$f(b) = \frac{(n-b+1)(s_b-1)^2}{s_a - 1},$$

while for $l > b$,

$$f(l) = \frac{(s_b-1)s_b}{s_a-1}.$$

Hence, for $l > b$ we have that $f(b) > f(l)$ holds whenever $(n - b + 1)(s_b - 1) > s_b$ or, equivalently, $(n - b)(s_b - 1) > 1$. If $b \geq 2$, i.e., $s_b - 1 \geq 2$, this holds because $n > b$. If $b = 1$, we have $s_b - 1 = 1$ and since $n \geq 4$, we have $n - b \geq 3$. Thus, if $f(l)$ attains the maximal value, then $l \in \{a, \ldots, b\}$. ■

Assertion (a). Claim 3.9.1 shows that if $a = b$, then $l = a = b$. Together with Lemma 3.8(a), this proves assertion (a).

Claim 3.9.2. Let $a \leq l, l' \leq b$. Then $f(l) < f(l')$ if and only if

$$(n-l+1)^{b-l+1}(s_l-1)^{b-l+2} < (n-l'+1)^{b-l'+1}(s_{l'}-1)^{b-l'+2}.$$

Proof of the claim. By definition of f, the inequality $f(l) < f(l')$ is equivalent to

$$\Big((n-l+1)(s_l-1)\Big)^{b-l+1}\prod_{i=a}^{l-1} s_i < \Big((n-l'+1)(s_{l'}-1)\Big)^{b-l'+1}\prod_{i=a}^{l'-1} s_i.$$

Multiplying both sides with $s_1 \cdots s_{a-1}$ and using the definition of the Sylvester sequence proves the claim. ■

We determine a subrange of $\{a,\dots,b\}$ in which $f(l)$ is monotone.

Claim 3.9.3. If $a \le l < b$, $l \ge 2$ and $s_l - e(n-b+2) \ge 0$, where e is the Euler number, then $f(l) < f(l+1)$.

Proof of the claim. By Claim 3.9.2, $f(l) < f(l+1)$ is equivalent to

$$(n-l+1)^{b-l+1}(s_l-1)^{b-l+2} < (n-l)^{b-l}(s_{l+1}-1)^{b-l+1}. \tag{3.12}$$

Note that $n-l \ge b-l \ge 1$. Using this and $s_{l+1}-1 = s_l(s_l-1)$, one sees that (3.12) is equivalent to

$$\left(1+\frac{1}{n-l}\right)^{b-l}(n-l+1)(s_l-1) < s_l^{b-l+1}.$$

Since $n-l \ge b-l$,

$$\left(1+\frac{1}{n-l}\right)^{b-l} \le \left(1+\frac{1}{n-l}\right)^{n-l} < e,$$

where e is the Euler number. Thus, (3.12) holds if

$$s_l^{b-l} - e(n-l+1) \ge 0.$$

We introduce $x := b-l-1$. Then $n-l = n-b+b-l = n-b+x+1$ and we rewrite the latter inequality as

$$s_l^{x+1} - e(x+n-b+2) \ge 0.$$

Note that $x \ge 0$. For a moment, we view x as a variable ranging in $[0,\infty)$ and develop $s_l^{x+1} - e(n-b+x+2)$ into its Taylor series at the point $x=0$:

$$s_l^{x+1} - e(x+n-b+2) = s_l - e(n-b+2) + (s_l \ln s_l - e)x + \sum_{k=2}^{\infty}\frac{s_l(\ln s_l)^k}{k!}x^k.$$

Obviously,

$$\sum_{k=2}^{\infty}\frac{s_l(\ln s_l)^k}{k!}x^k \ge 0$$

for $x \ge 0$ as each of the coefficients is positive. The inequality $s_l \ln s_l - e > 0$ holds whenever $l \ge 2$. Thus, for $l \ge 2$, the expression $s_l^{x+1} - e(n-b+x+2)$ is monotonously increasing for $x \in [0,\infty)$. Hence its value for $x = b-l-1$ is not smaller than the value for $x=0$. Therefore, for (3.12) to hold it suffices to have

$$s_l - e(n-b+2) \ge 0. \tag{3.13}$$

■

Assertion (b). Here, we have $1 \leq a < b$, i.e. $b \geq 2$ and therefore we also have $n-b+2 \leq n$. Let $a \leq l < b$. In view of Proposition 3.3(c), we have $s_l \geq 2^{2^{l-2}}$. Assume now that

$$l > 2 + \log_2 \log_2(en).$$

Combining this with our previous observations yields

$$s_l \geq 2^{2^{l-2}} \geq en \geq e(n-b+2).$$

By Claim 3.9.3, this implies that $f(l) < f(l+1)$ and thus, for $2 + \log_2 \log_2(en) < l < b$, the value $f(l)$ is not the maximum. This proves (b).

Assertion (c). We assume $b = n$ and $a < b$. Let $a \leq l < b$. If $l \geq 3$, we have $s_l - e(n-b+2) = s_l - 2e > 0$ and hence by Claim 3.9.3, we know that $y(l)$ is not an optimal solution of $\mathrm{IK}^n(x_a \cdots x_b)$. Therefore, only $y(1)$, $y(2)$ and $y(n)$ remain as possible optimal solutions. We show directly that $y(n)$ is a better solution than $y(1)$ and $y(2)$, respectively. By Claim 3.9.2, we need to show

$$(n+1-l)^{n+1-l}(s_l - 1)^{n-l+2} < (s_n - 1)^2$$

for $n \geq 4$ and $l \in \{1, 2\}$. We proceed by induction on n. One verifies directly that the inequality holds for $n = 4$ and $l \in \{1, 2\}$. Let us now show that the inequality remains valid when moving from n to $n+1$. By induction hypothesis,

$$(s_{n+1} - 1)^2 = s_n^2(s_n - 1)^2 > (n+1-l)^{2(n+1-l)}(s_l - 1)^{2(n-l+2)}.$$

To complete the induction, we need to show

$$(n+1-l)^{2(n+1-l)}(s_l - 1)^{2(n-l+2)} \geq (n+2-l)^{n+2-l}(s_l - 1)^{n-l+3}.$$

This is equivalent to

$$(n+1-l)^{n-l}(s_l - 1)^{n-l+1} \geq \left(1 + \frac{1}{n+1-l}\right)^{n+2-l}. \tag{3.14}$$

The right-hand side of (3.14) is at most $e\left(1 + \frac{1}{n+1-l}\right)$. As $l \leq 2$ and $n \geq 4$, this is at most $\frac{4e}{3}$. Again employing $l \leq 2$ and $n \geq 4$, the left-hand side of (3.14), is at least $(n+1-l)^{n-l} \geq 9 \geq \frac{4e}{3}$. This completes the induction. Lemma 3.8(a) now yields assertion (c).

Assertions (d) and (e). We assume $b = n - 1$ and $a < b$. Let $a \leq l < b$. If $l \geq 4$, we have $s_l - e(n-b+2) = s_l - 3e > 0$ and hence by Claim 3.9.3, we have that $y(l)$ is not an optimal solution of $\mathrm{IK}^n(x_a \cdots x_b)$. Thus, it remains to compare $y(l)$ and $y(b) = y(n-1)$ directly for $l \in \{1, 2, 3\}$. Note that if $a > 1$, we can exclude the elements $y(l)$ with $l < a$. By Claim 3.9.2, we need to show

$$(n+1-l)^{n-l+1}(s_l - 1)^{n-l+2} < 2(s_{n-1} - 1)^2 \qquad \text{for } l \in \{1, 2, 3\}.$$

Using an inductive argument analogous to the one used for $b = n$, we obtain that this inequality is valid for every $n \geq 5$ and every $l \in \{1, 2, 3\}$. If $n = 4$ and $l = 1$, one can verify directly that the inequality holds. If $n = 4$ and $l \in \{2, 3\}$, a direct computation shows that $y(2)$ and $y(3) = y(n-1)$ yield the same values for each of the problems $\mathrm{IK}^4(x_1x_2x_3)$ and $\mathrm{IK}^4(x_2x_3)$. This proves assertion (d). Lastly, we prove (e) and consider the problem $\mathrm{IK}^n(x_1 \cdots x_{n-1})$ with $n \geq 4$. By Lemma 3.8(c), all optimal solutions of this problem are in $\mathcal{Y}^n$. Hence by our previous arguments, assertion (e) follows. □

Problem $\mathrm{IK}^n(x_a \cdots x_b)$ for $a = b$

One of the well-known topics in number theory (see, e.g., [Cur22, Erd50]) concerns the so-called unit partitions, i.e., representations of 1 in the form $1 = \frac{1}{u_1} + \ldots + \frac{1}{u_n}$ with $n \in \mathbb{N}$ and $u_1, \ldots, u_n \in \mathbb{N}$. By symmetry reasons, there is no loss of generality in assuming the sequence $u_1, \ldots, u_n$ to satisfy $u_1 \le \ldots \le u_n$. With this assumption the vector $x = (\frac{1}{u_1}, \ldots, \frac{1}{u_n})$ belongs to $\mathcal{X}^n$. To see that all product-sum inequalities are satisfied, observe that for every $j \in \{1, \ldots, n-1\}$ we have

$$\frac{1}{u_{j+1}} + \ldots + \frac{1}{u_n} = 1 - \sum_{i=1}^{j} \frac{1}{u_i}.$$

Writing the expression on the right hand side as a fraction with denominator $u_1 \cdots u_j$, one can see that the numerator is at least 1, hence the fraction is at least $\frac{1}{u_1 \cdots u_j}$. Therefore,

$$\left\{ \left(\frac{1}{u_1}, \ldots, \frac{1}{u_n} \right) : u_1, \ldots, u_n \in \mathbb{N}, \ \frac{1}{u_1} + \ldots + \frac{1}{u_n} = 1, \ u_1 \le \ldots \le u_n \right\} \subseteq \mathcal{X}^n.$$

Previous work on this subject has established a link between unit partitions and the Sylvester sequence; see [Cur22] and [Erd50]. A result of Soundararajan, see [Sou05, (1)], provides an elegant way of establishing a sharp upper bound on u_j for each $j \in \{1, \ldots, n\}$.

Here, we use the ideas from [Sou05] to show a generalized result. From Theorem 3.9(a), we already know that $y(a)$ is an optimal solution of $\mathrm{IK}^n(x_a)$ and the only optimal solution contained in $\mathcal{Y}^n$. However, Theorem 3.9(a) does not state anything about uniqueness of this solution within the whole set $\mathcal{X}^n$. Following Soundararajan's approach closely, we can show that $y(a)$ is indeed the unique optimal solution within $\mathcal{X}^n$. The proof strategy from [Sou05] can be adapted by dropping the assumption of unit fractions and replacing it by the less restrictive assumption of product-sum inequalities. This will lead to optimal solutions of $\mathrm{IK}^n(x_a)$ for $a \in \{1, \ldots, n\}$ over the set $\mathcal{X}^n$. First, we need the following proposition from [Sou05]. It is based on Muirhead's inequality. Muirhead's inequality can be found, for example, in [HLP52, Theorem 45].

PROPOSITION 3.10 ([Sou05, Proposition]). *Let $n \in \mathbb{N}$. Let $g_1 \ge g_2 \ge \ldots \ge g_n > 0$ and $h_1 \ge h_2 \ge \ldots \ge h_n > 0$ be such that $h_1 \cdots h_j \le g_1 \cdots g_j$ for every $j \in \{1, \ldots, n\}$. Then*

$$h_1 + \ldots + h_n \le g_1 + \ldots + g_n,$$

with equality if and only if $g_i = h_i$ for every $i \in \{1, \ldots, n\}$.

LEMMA 3.11. *Let $x_1, \ldots, x_k$ ($k \in \mathbb{N}$) be a sequence of positive real numbers satisfying the following conditions:*

$$x_1 + \ldots + x_k < 1, \tag{3.15}$$

$$x_1 \ge \ldots \ge x_k, \tag{3.16}$$

$$x_1 \cdots x_j \le 1 - \sum_{i=1}^{j} x_i \quad \forall\, j \in \{1, \ldots, k\}. \tag{3.17}$$

Then

$$x_1 + \ldots + x_k \le \frac{1}{s_1} + \ldots + \frac{1}{s_k}, \tag{3.18}$$

with equality being attained if and only if $x_i = 1/s_i$ for every $i \in \{1, \ldots, k\}$.

Proof. The proof of Lemma 3.11 is an adaptation of the proof presented in [Sou05]. Since [Sou05] is not intended for publication, we repeat the details of the proof here.

We argue by induction on k. For $k = 1$, inequality (3.17) yields $x_1 \leq 1/2 = 1/s_1$. Let now $k \geq 2$ and assume that the statement holds for all sequences with at most $k - 1$ elements. First, we show that (3.18) holds in the case that

$$x_1 \cdots x_k > \frac{1}{s_1 \cdots s_k}. \tag{3.19}$$

In view of (3.17), we obtain

$$\frac{1}{s_1} + \ldots + \frac{1}{s_k} = 1 - \frac{1}{s_{k+1} - 1} = 1 - \frac{1}{s_1 \cdots s_k} > 1 - x_1 \cdots x_k \geq \sum_{i=1}^{k} x_i.$$

Hence (3.18) holds and is strict. We switch to the case $x_1 \cdots x_k \leq \frac{1}{s_1 \cdots s_k}$. Thus, the inequality

$$x_l \cdots x_k \leq \frac{1}{s_l} \cdots \frac{1}{s_k} \tag{3.20}$$

holds for $l = 1$. We fix $l \in \{1, \ldots, k\}$ to be the maximal index for which (3.20) holds. Since $l - 1 < k$, the induction hypothesis yields

$$\sum_{i=1}^{l-1} x_i \leq \sum_{i=1}^{l-1} \frac{1}{s_i}. \tag{3.21}$$

The choice of l yields a series of inequalities as follows:

$$\begin{aligned} x_l &\leq \frac{1}{s_l}, \\ x_l x_{l+1} &\leq \frac{1}{s_l s_{l+1}}, \\ &\vdots \\ x_l \cdots x_k &\leq \frac{1}{s_l \cdots s_k}. \end{aligned}$$

Thus, $x_l, \ldots, x_k$ and $1/s_l, \ldots, 1/s_k$ fulfil the settings of Proposition 3.10. Hence, we have

$$\sum_{i=l}^{k} x_i \leq \sum_{i=l}^{k} \frac{1}{s_i}. \tag{3.22}$$

Together with (3.21), this proves (3.18).

Now, we characterize the equality case. Observe that, if $x_i = 1/s_i$ for every $i \in \{1, \ldots, k\}$, the inequality (3.18) is trivially fulfilled with equality. Let us now assume we have equality in (3.18) and show that this implies $x_i = 1/s_i$ for every $i \in \{1, \ldots, k\}$. Above, we have shown that (3.19) implies that (3.18) is strict. So, under our assumptions, (3.19) cannot hold. We can hence again fix the maximal l such that (3.20) holds. Then by the induction hypothesis, we have $x_i = 1/s_i$ for every $i \in \{1, \ldots, l - 1\}$. Therefore, (3.21) holds with equality. This implies that (3.22) also has to be fulfilled with equality. By Proposition 3.10, this is the case if and only if $x_i = 1/s_i$ for every $i \in \{l, \ldots, k\}$. ◻

Theorem 3.12. *Let $n \in \mathbb{N}$, $i \in \{1, \dots, n\}$ and $x \in \mathcal{X}^n$. Then*

$$x_i \geq \frac{1}{(n-i+1)(s_i-1)},$$

with equality if and only if $x = y(i)$.

Proof. We have

$$x_i \geq \frac{1}{n-i+1}\Big(1 - \sum_{j=1}^{i-1} x_j\Big) \geq \frac{1}{n-i+1}\Big(1 - \sum_{j=1}^{i-1} \frac{1}{s_j}\Big) = \frac{1}{(n-i+1)(s_i-1)}. \tag{3.23}$$

The first inequality in (3.23) follows from $x_1 + \ldots + x_n = 1$ and $x_i \geq x_{i+1} \geq \ldots \geq x_n$ and the second one is a consequence of Lemma 3.11. Now, let us prove the characterization of the equality case. Clearly, for $x = y(i)$, one has $x_i = \frac{1}{(n-i+1)(s_i-1)}$. On the other hand, if $x_i = \frac{1}{(n-i+1)(s_i-1)}$, both inequalities in (3.23) are attained with equality. Hence, we have $1 - \sum_{j=1}^{i-1} x_j = 1/(s_i - 1)$, which by Lemma 3.11 holds if and only if $x_j = 1/s_j$ for $j \in \{1, \dots, i-1\}$. Furthermore, $x_1 + \ldots + x_n = 1$ yields $x_i + \ldots + x_n = 1/(s_i - 1)$. Since we have $x_i \geq x_{i+1} \geq \ldots \geq x_n$ and $x_i = \frac{1}{(n-i+1)(s_i-1)}$, this implies that we have in fact $x_i = x_{i+1} = \ldots = x_n$. This yields $x = y(i)$. □

Remark 3.13. One can see that Theorem 3.12 solves $\mathrm{IK}^n(x_i)$ for every $i \in \{1, \dots, n\}$. In [IK87], there is an alternative approach to solve $\mathrm{IK}^n(x_n)$. First, Izhboldin and Kurliandchik determine the unique optimal solution of $\mathrm{IK}^n(x_1 \cdots x_n)$ and then show that this is also the unique optimal solution of $\mathrm{IK}^n(x_n)$ in the following way. Let y be the optimal solution of $\mathrm{IK}^n(x_1 \cdots x_n)$. We know from the proof of Lemma 3.8 that y attains all the product-sum inequalities with equality. Let x be an arbitrary element of $\mathcal{X}^n$. Thus, taking into account $\mathrm{PS}(n-1)$ for x, we have

$$x_n^2 \geq x_1 \cdots x_{n-1} x_n \geq y_1 \cdots y_n = y_n^2. \tag{3.24}$$

Thus, $x_n \geq y_n$, which shows that y is also an optimal solution of $\mathrm{IK}^n(x_n)$. Furthermore, y is the unique optimal solution of $\mathrm{IK}^n(x_n)$, because if $x \in \mathcal{X}^n$ minimizes x_n, then all inequalities in (3.24) are attained with equality. Consequently, x is an optimal solution of $\mathrm{IK}^n(x_1 \ldots x_n)$ and by this coincides with y. ■

3.2 Proofs of results on $\mathcal{S}^d(1)$

In this section, we prove Theorems 1.7 and 1.8 by applying the results from Section 3.1 to the $(d+1)$-tuple of barycentric coordinates associated with the interior integral point of a simplex in $\mathcal{S}^d(1)$. Observe that if we assume the barycentric coordinates $\beta_1, \dots, \beta_{d+1}$ of this point to be ordered decreasingly, the tuple $(\beta_1, \dots, \beta_{d+1})$ fulfils conditions (3.5) and (3.6). Because of Theorem 3.5, it also fulfils (3.7) and hence we have $(\beta_1, \dots, \beta_{d+1}) \in \mathcal{X}^{d+1}$.

The following simple proposition will be used for the characterization of the equality cases in Theorems 1.7 and 1.8. It will also be used in Section 3.5, where we prove Theorems 1.14 and 1.15.

Proposition 3.14. *Let $a_1, \dots, a_k$ ($k \in \mathbb{N}$) be pairwise relatively prime integers. Let $m_1, \dots, m_k$ be integers such that*

$$\frac{m_1}{a_1} + \ldots + \frac{m_k}{a_k} \in \mathbb{Z}.$$

Then a_i divides m_i for every $i \in \{1, \dots, k\}$.

Proof. By symmetry of the statement, it suffices to prove the assertion for $i = 1$. Multiplying $\frac{m_1}{a_1} + \ldots + \frac{m_k}{a_k}$ by $a_2 \cdots a_k$, we deduce $\frac{m_1 a_2 \cdots a_k}{a_1} \in \mathbb{Z}$. By the assumptions, a_1 is relatively prime to $a_2 \cdots a_k$. Hence $\frac{m_1}{a_1} \in \mathbb{Z}$ and the assertion follows. □

It follows directly from the definition that the elements of the Sylvester sequence are pairwise relatively prime. Hence, we can apply Proposition 3.14 to the elements of the Sylvester sequence.

Proof of Theorem 1.7. The bound in (1.8) and assertion (b) follow immediately from Theorem 3.12 by setting $n = d+1$ and $x_1 = \beta_1, \ldots, x_n = \beta_n$. Assertion (a) can be checked directly from the fact that $\operatorname{int}(T^d_{1,i}) \cap \mathbb{Z}^d = \{(1,\ldots,1)\}$ and by noticing that $y(i) \in \mathcal{Y}^{d+1}$ is the $(d+1)$-tuple of barycentric coordinates of $(1,\ldots,1)$ with respect to $T^d_{1,i}$.

We will now prove assertion (c). From assertion (a) we have that for $S \simeq T^d_{1,d+1}$ and $i = d+1$, equality is attained in (1.8). To show the reverse implication, consider an arbitrary $S \in \mathcal{S}^d(1)$ such that its interior integral point p has the barycentric coordinate $\beta_{d+1} = \frac{1}{s_{d+1}-1}$. Assertion (b) implies

$$(\beta_1, \ldots, \beta_{d+1}) = \Big(\frac{1}{s_1}, \ldots, \frac{1}{s_d}, \frac{1}{s_{d+1}-1}\Big).$$

Without loss of generality, we can assume that the vertex of S associated with the smallest barycentric coordinate is o. For the remaining barycentric coordinates, let p_i with $i \in \{1,\ldots,d\}$ be the vertices of S such that p_i corresponds to the coordinate $1/s_i$, $i \in \{1,\ldots,d\}$. Then

$$p := \frac{p_1}{s_1} + \ldots + \frac{p_d}{s_d}$$

is the single interior integral point of S. By Proposition 3.14, we get $p_i/s_i \in \mathbb{Z}^d$ for $i \in \{1,\ldots,d\}$. Let $\Lambda := \frac{p_1}{s_1}\mathbb{Z} + \ldots + \frac{p_d}{s_d}\mathbb{Z}$ be the lattice induced by those points. By construction, Λ is a rank d sublattice of $\mathbb{Z}^d$. Recall that for a rank d lattice with basis $b_1, \ldots, b_d \in \mathbb{Z}^d$, the determinant of this lattice can be expressed as the number of lattice points in $(0,1]b_1 + \ldots + (0,1]b_d$ (see, e.g., [Bar02, VII, 2.6]). Using this and the fact that

$$\begin{aligned}\{p\} &\subseteq \left((0,1]\frac{p_1}{s_1} + \ldots + (0,1]\frac{p_d}{s_d}\right) \cap \Lambda \\ &\subseteq \operatorname{int}(S) \cap \Lambda \\ &\subseteq \operatorname{int}(S) \cap \mathbb{Z}^d = \{p\},\end{aligned}$$

we have that Λ is a sublattice of $\mathbb{Z}^d$ with determinant one. Hence $\Lambda = \mathbb{Z}^d$ and, moreover, the linear mapping given by $\frac{p_i}{s_i} \mapsto e_i$ preserves $\mathbb{Z}^d$. Consequently, this mapping is a unimodular transformation. Thus $S \simeq \operatorname{conv}(o, s_1 e_1, \ldots, s_d e_d) = T^d_{1,d+1}$. □

To prove Theorem 1.8(b), we will show that equality in (1.10) for $l \in \{1, d\}$ is attained if and only if the unique interior integral point of the simplex S has a specific tuple of barycentric coordinates with respect to S. The following lemma gives a characterization of the simplices in $\mathcal{S}^d(1)$ for which this is the case. The same tuple of barycentric coordinates will also be of interest when characterizing the equality case in Theorem 1.11.

LEMMA 3.15. *Let $S \in \mathcal{S}^d(1)$. Let the barycentric coordinates $\beta_1, \ldots, \beta_{d+1}$ of the interior integral point with respect to S be*

$$(\beta_1, \ldots, \beta_{d+1}) = \Big(\frac{1}{s_1}, \ldots, \frac{1}{s_{d-1}}, \frac{1}{2(s_d-1)}, \frac{1}{2(s_d-1)}\Big).$$

Then $S \simeq \operatorname{conv}\left(T^{d-1}_{1,d} \times \{0\} \cup \{\pm(a,h)\}\right)$ *for some* $h \in \mathbb{N}$ *and some* $a \in \{0,\dots,h-1\}^{d-1}$.

Proof. Let p_i be the vertex associated with the barycentric coordinate $1/s_i$ for $i \in \{1,\dots,d-1\}$ and p_d, p_{d+1} be the vertices associated with the remaining two coordinates. Then, the single interior integral point of S is

$$p := \frac{p_1}{s_1} + \ldots + \frac{p_{d-1}}{s_{d-1}} + \frac{p_d + p_{d+1}}{2(s_d-1)}.$$

Since $1/(s_d-1) = 1 - 1/s_1 - \ldots - 1/s_{d-1}$, we get

$$2p = p_d + p_{d+1} + \sum_{i=1}^{d-1} \frac{2p_i - p_d - p_{d+1}}{s_i}.$$

As $2p, p_d, p_{d+1} \in \mathbb{Z}^d$, we obtain

$$\sum_{i=1}^{d-1} \frac{2p_i - p_d - p_{d+1}}{s_i} \in \mathbb{Z}^d.$$

Applying Proposition 3.14, we get $(2p_i - p_d - p_{d+1})/s_i \in \mathbb{Z}^d$ for all $i \in \{1,\dots,d-1\}$. In particular, $(p_d + p_{d+1})/2 \in \mathbb{Z}^d$, because $s_1 = 2$ and $p_1 \in \mathbb{Z}^d$. Without loss of generality, we assume that $(p_d + p_{d+1})/2 = o$. The simplex $T := \operatorname{conv}(o, p_1, \dots, p_{d-1})$ is a hyperplane section of S. Furthermore, $p \in \operatorname{relint}(T)$ and the d-tuple of barycentric coordinates of p with respect to T is

$$\Big(\frac{1}{s_1}, \dots, \frac{1}{s_{d-1}}, \frac{1}{s_d - 1}\Big).$$

Theorem 1.7(c) asserts that (up to unimodular equivalence) there is only one $(d-1)$-dimensional simplex with one interior integral point which has these coordinates and thus $T \simeq T^{d-1}_{1,d} \times \{0\}$. By moving to another basis of $\mathbb{Z}^{d-1} \times \{0\}$ if necessary, we can assume $T = \operatorname{conv}(o, s_1 e_1, \dots, s_{d-1} e_{d-1})$. Then, we can write p_d as (a,h), where $a \in \mathbb{Z}^{d-1}$ and $h \in \mathbb{Z}$. Since $p_d + p_{d+1} = o$, this leads to $p_{d+1} = -(a,h)$. Note that $h \neq 0$ because otherwise S would not be full-dimensional. Furthermore, we can assume $h \in \mathbb{N}$ by interchanging the roles of p_d and p_{d+1} if necessary. It remains to show that up to unimodular equivalence, we can choose $a \in \mathbb{Z}^{d-1}$ such that $a \in \{0,\dots,h-1\}^{d-1}$. Assume $a \notin \{0,\dots,h-1\}^{d-1}$. Let $a' \in \{0,\dots,h-1\}^{d-1}$ such that $a' \equiv a \pmod h$. There exists a linear unimodular transformation preserving $\mathbb{R}^{d-1} \times \{0\}$ which maps the simplex $\left(T^{d-1}_{1,d} \times \{0\} \cup \{\pm(a,h)\}\right)$ to the simplex $\left(T^{d-1}_{1,d} \times \{0\} \cup \{\pm(a',h)\}\right)$; cf. page 42, where this unimodular transformation is given for the three-dimensional case. This observation completes the proof. □

In the proof of Theorem 1.8(b), we will show that the simplices for which equality in (1.10) holds for $l \in \{1, d\}$ fulfil the assumptions of Lemma 3.15. We will then proceed by determining the values of a and h as used in the formulation Lemma 3.15. To determine a, we will make use of the following lemma.

Lemma 3.16. *Let* S *be the simplex in* $\mathbb{R}^d$ *given by* $S = \operatorname{conv}(o, a_1 e_1, \dots, a_d e_d)$, *where* $d \geq 2$ *and* $a_1, \dots, a_d > 1$ *satisfy* $\frac{1}{a_1} + \ldots + \frac{1}{a_d} = 1$. *Let* $v \in \mathbb{R}^d$. *Then,* $S + v$ *is lattice-free if and only if* $v \in \mathbb{Z}^d$.

Proof. By (2.25), S is lattice-free and it is obvious that $S + v$ is also lattice-free for every $v \in \mathbb{Z}^d$. Let us now show the reverse implication. Let $v \in \mathbb{R}^d \setminus \mathbb{Z}^d$. Observe that

$$\operatorname{int}(S) = \left\{ x = (x_1, \dots, x_d) \in \mathbb{R}^d \,:\, x_1, \dots, x_d > 0,\ \frac{x_1}{a_1} + \ldots + \frac{x_d}{a_d} < 1 \right\}.$$

Hence, taking into account $\frac{1}{a_1} + \ldots + \frac{1}{a_d} = 1$, we get $(0,1]^d \setminus \{\mathbb{1}\} \subseteq \operatorname{int}(S)$. Then, $(0,1]^d + v$ contains the point $v' := (\lfloor v_1 + 1 \rfloor, \ldots, \lfloor v_d + 1 \rfloor) \in \mathbb{Z}^d$. It is easy to check that since $v \notin \mathbb{Z}^d$, we have $v' \neq v + \mathbb{1}$. Thus, $v' \in (0,1]^d \setminus \{\mathbb{1}\} + v \subseteq \operatorname{int}(S+v)$ and hence $S+v$ is not lattice-free. □

Proof of Theorem 1.8. The proof is divided into four parts. First, we prove (1.10) and assertion (a). Assertion (b) is then proven separately for the cases $l = 1$ and $l = d$.

Inequality (1.10). Let $\beta_1, \ldots, \beta_{d+1}$ be the barycentric coordinates of the interior integral point of S and assume $\beta_1 \geq \ldots \geq \beta_{d+1}$. By (3.3), we have

$$\max_{F \in \mathcal{F}_l(S)} \operatorname{vol}_{\mathbb{Z}}(F) \leq \frac{1}{l! \beta_{d-l+1} \cdots \beta_d}.$$

Minimizing the product $\beta_{d-l+1} \cdots \beta_d$ corresponds to finding an optimal solution to the problem $\mathrm{IK}^{d+1}(x_{d-l+1} \cdots x_d)$. Inequality (1.10) then follows from Theorem 3.9(d) with $n = d+1$.

Assertion (a). We need to show that for every $l \in \{1, \ldots, d\}$, the simplex S_1^d fulfils (1.10) with equality. This can be seen from the fact that for $l \in \{1, \ldots, d\}$, the simplex S_1^d contains the face

$$\operatorname{conv}(o, s_{d-l+1} e_{d-l+1}, \ldots, s_{d-1} e_{d-1}, 2(s_d - 1) e_d),$$

which has normalized volume

$$\frac{2}{l!}(s_d - 1) \prod_{i=d-l+1}^{d-1} s_i = \frac{2(s_d - 1)^2}{l!(s_{d-l+1} - 1)}.$$

Claim 3.16.1. Let $S := \operatorname{conv}\Big(T_{1,d}^{d-1} \times \{0\} \cup \{\pm(s_d - 1) e_d\}\Big)$. Then, $S \simeq S_1^d$.

Proof of the claim. Note that because $(s_d - 1) e_d \in \mathbb{Z}^d$, it suffices to show $S \simeq S_1^d - (s_d - 1) e_d$. Let $\varphi : \mathbb{R}^d \to \mathbb{R}^d$ be the linear mapping given by $\varphi : e_i \mapsto e_i + \frac{s_d - 1}{s_i} e_d$ for $i \in \{1, \ldots, d-1\}$ and $\varphi : e_d \mapsto e_d$. Obviously, φ maps $S_1^d - (s_d - 1) e_d$ to S. Furthermore, φ preserves integrality as s_i divides $s_d - 1$ for every $i \in \{1, \ldots, d-1\}$. The associated transformation matrix is thus an integral lower triangular matrix and all entries on the diagonal are 1 and hence, φ is a unimodular transformation. ■

Assertion (b) for $l = 1$. Assume $l = 1$. As shown above, the simplex S with $S \simeq S_1^d$ fulfils (1.10) with equality for $l = 1$. Conversely, let $l = 1$ and let $S \in \mathcal{S}^d(1)$ be an arbitrary simplex satisfying (1.10) with equality. Let $\beta_1 \geq \ldots \geq \beta_{d+1} > 0$ be the barycentric coordinates of the interior integral point of S and let $p_1, \ldots, p_{d+1}$ the corresponding vertices of S. By our assumptions and Theorems 3.6 and 3.12, we have

$$2(s_d - 1) = \max_{1 \leq i < j \leq d+1} \operatorname{vol}_{\mathbb{Z}}([p_i, p_j]) \leq \max_{1 \leq i < d+1} \frac{1}{\beta_i} = \frac{1}{\beta_d} \leq 2(s_d - 1). \tag{3.25}$$

This implies $\beta_d = 1/(2(s_d - 1))$. By Theorem 1.7(b),

$$(\beta_1, \ldots, \beta_{d+1}) = \Big(\frac{1}{s_1}, \ldots, \frac{1}{s_{d-1}}, \frac{1}{2(s_d - 1)}, \frac{1}{2(s_d - 1)}\Big). \tag{3.26}$$

Thus, by Theorem 3.6 and (3.26), $[p_d, p_{d+1}]$ is the unique edge having normalized volume $2(s_d - 1)$.

As the barycentric coordinates of the interior integral point of S fulfil (3.26), we can apply Lemma 3.15 and obtain $S \simeq \operatorname{conv}(T_{1,d}^{d-1} \times \{0\} \cup \{\pm(a, h)\})$ for some $h \in \mathbb{N}$ and

$a \in \{0, \dots, h-1\}^{d-1}$. Thus, to prove $S \simeq S_d^1$ it suffices to show that $h = s_d - 1$ and $a = o$. Because the barycentric coordinates associated with $\pm(a, h)$ are β_d and β_{d+1}, we have that $[p_d, p_{d+1}]$ is the edge with endpoints $\pm(a, h)$. Therefore, $2(s_d - 1) = \operatorname{vol}_{\mathbb{Z}}([p_d, p_{d+1}]) = \operatorname{vol}_{\mathbb{Z}}([(a, h), -(a, h)]) = \gcd(2(a, h))$. This yields $h \geq s_d - 1$. On the other hand, $h > s_d - 1$ yields $\operatorname{vol}(S) > \frac{2(s_d-1)}{d} \operatorname{vol}(T_{1,d}^{d-1}) = \frac{2(s_d-1)^2}{d!}$. Since $S \in \mathcal{S}^d(1)$, this is a contradiction to Inequality (1.10). Hence, $2(s_d - 1) = \gcd(2(a, s_d - 1))$. As all components of a are between 0 and $h - 1$, this also implies $a = o$, because otherwise $\gcd(2(a, s_d - 1)) < 2(s_d - 1)$. By Claim 3.16.1, this implies $S \simeq S_1^d$.

Assertion (b) for $l = d$. Assume $l = d$. By Theorem 3.6 and Theorem 3.9(d), we have

$$\operatorname{vol}(S) \leq \frac{1}{d!\beta_1 \cdots \beta_d} \leq \frac{2}{d!}(s_d - 1)^2. \tag{3.27}$$

We assume that S fulfils (1.10) with equality for $l = d$, i.e. $\operatorname{vol}(S) = \frac{2}{d!}(s_d-1)^2$. It follows that both inequalities in (3.27) are fulfilled with equality. Hence by Theorem 3.9(e) and because $d \geq 4$, we have that the barycentric coordinates of the interior integral point of S fulfil (3.26). Therefore, we can again apply Lemma 3.15 to obtain $S \simeq \operatorname{conv}(T \times \{0\} \cup \{\pm(a, h), \})$, where $T := T_{1,d}^{d-1}$, $h \in \mathbb{N}$ and $a \in \{0, \dots, h-1\}^{d-1}$. Thus,

$$\operatorname{vol}(S) = \frac{2h \operatorname{vol}(T)}{d} = \frac{2h}{d!}(s_d - 1).$$

On the other hand, by assumption, we have $\operatorname{vol}(S) = \frac{2}{d!}(s_d - 1)^2$. This yields $h = s_d - 1$. It remains to show that $a = o$. By applying an appropriate unimodular transformation if necessary, we may assume $S = \operatorname{conv}(T \times \{0\} \cup \{\pm(a, s_d - 1)\})$. We consider $S' \subseteq \mathbb{R}^{d-1}$ such that $S' \times \{1\}$ is the hyperplane cross-section $S' \times \{1\} = S \cap (\mathbb{R}^{d-1} \times \{1\})$ of S. Then

$$S' = \frac{h-1}{h} T + \frac{1}{h} a = \operatorname{conv}\left(\{o\} \cup \left\{\frac{s_d - 2}{s_d - 1} s_i e_i \; : \; i \in \{1, \dots, d-1\}\right\}\right) + \frac{1}{h} a.$$

Observe that $\frac{h-1}{h} T$ fulfils the assumptions of Lemma 3.16 because

$$\frac{s_d - 1}{s_d - 2} \sum_{i=1}^{d-1} \frac{1}{s_i} = \frac{s_d - 1}{s_d - 2}\left(1 - \frac{1}{s_d - 1}\right) = 1.$$

Thus, $\frac{h-1}{h} T + \frac{1}{h} a$ is lattice-free if and only if $a/h \in \mathbb{Z}^{d-1}$. Assume the contrary, i.e. $a/h \notin \mathbb{Z}^{d-1}$. Then there exists a point $p \in \operatorname{int}(S') \cap \mathbb{Z}^{d-1}$ and hence also in $\operatorname{relint}(S') \cap \mathbb{Z}^d$. Note that we also have $(1, \dots, 1, 0) \in \operatorname{relint}(T \times \{0\})$ and thus $(1, \dots, 1, 0) \in \operatorname{int}(S) \cap \mathbb{Z}^d$. In other words, S contains more than one integral point in its interior, a contradiction. Hence, $a/h \in \mathbb{Z}^{d-1}$ and since $a \in \{0, \dots, h-1\}^{d-1}$, this implies $a = o$. Thus, by Claim 3.16.1, we have $S \simeq S_1^d$. □

Proof of Corollary 1.9. This follows immediately from Theorem 1.8 and Blichfeldt's Theorem 3.1. □

REMARK 3.17 (On minimal h-faces of simplices in $\mathcal{S}^d(1)$). Using the results from Section 3.1, it is also possible to give upper bounds on the volume of minimal h-faces. More precisely, we introduce the following functions on $\mathcal{S}^d(1)$: Let $d \geq 4$ and $g, h \in \{1, \dots, d-1\}$ with $g < h$. Let

$$v_h(S) := \min_{F \in \mathcal{F}_h(S)} \operatorname{vol}_{\mathbb{Z}}(F) \qquad \forall\, S \in \mathcal{S}^d(1)$$

and let

$$\gamma_{h,g}(S) := \min_{H \in \mathcal{F}_h(S)} \max_{G \in \mathcal{F}_g(H)} \operatorname{vol}_{\mathbb{Z}}(G) \qquad \forall\ S \in \mathcal{S}^d(1).$$

By (3.3), bounding $\nu_h(S)$ from above corresponds to bounding $\beta_1 \cdots \beta_h$ from below, which can be done using Theorem 3.9(b). Furthermore, in view of (3.3) and (3.4), one can show that bounding $\gamma_{h,g}(S)$ corresponds to bounding $\beta_{h-g+1} \cdots \beta_h$ from below. Again, one can apply Theorem 3.9(b) to obtain a bound. ■

Remark 3.18 (On dimensions $d \leq 3$). At this point, we want to give a short overview about the validity of the results proved above in dimensions one, two and three. While all results hold for $d \geq 4$, Theorem 1.7 holds even for arbitrary dimension d. This is not true for the statements of Theorem 1.8. The assumption of $d \geq 3$ in Theorem 1.8 cannot be relaxed: it fails to hold for $d = 2$, since the triangle $T^2_{1,1} = \operatorname{conv}(o, 3e_1, 3e_2)$ is the volume maximizer in $\mathcal{P}^2(1)$ (see [Rab89a]) and has volume 4.5, while the upper bound in the theorem would yield 4. Regarding Theorem 1.8(b), we have to differ between the cases $l = 1$ and $l = d$. The assumption of $d \geq 4$ cannot be relaxed for $l = d$, as we know from the enumeration contained in [Kas10] that both S^3_1 and the tetrahedron $T^3_{1,2} = \operatorname{conv}(o, 2e_1, 6e_2, 6e_3)$ satisfy the inequalities in Theorem 1.8(a) with equality for $l = d$ and $l = d - 1$. For $l = 1$, however, we need to have minimal value for β_d, which is the case if and only if the tuple of barycentric coordinates satisfies (3.26); see Theorem 3.12, regardless of the value of d. Hence, for $l = 1$ and $d \geq 1$, $\max_{F \in \mathcal{F}_1(S)} \operatorname{vol}_{\mathbb{Z}}(F) = 2(s_d - 1)$ holds if $S \simeq S^d_1$. For $l = 1$ and $d \in \{1, 2\}$, the reverse implication is also true, i.e., $\max_{F \in \mathcal{F}_1(S)} \operatorname{vol}_{\mathbb{Z}}(F) = 2(s_d - 1)$ holds if and only if $S \simeq S^d_1$ (as can be seen from the enumeration in [Rab89a]). Corollary 1.9 is also valid for $d \in \{1, 2\}$, where the case $d = 1$ is trivial and the case $d = 2$ can be seen again from [Rab89a]. ■

3.3 Proofs of results on $\mathcal{S}^d(1)$ involving dualization

In this section, we turn our attention to duals of simplices in $\mathcal{S}^d(1)$ and prove Theorems 1.10 and 1.11.

The following is a basic result from standard duality (see also [Nil07, Proposition 3.6]).

Proposition 3.19. *Let S be a d-dimensional simplex such that $o \in \operatorname{int}(S)$ and let $v_1, \ldots, v_{d+1}$ be the vertices of S. Let $\beta_1, \ldots, \beta_{d+1}$ be the barycentric coordinates of o such that $o = \sum_{i=1}^{d+1} \beta_i v_i$. Then, there exists a unique sequence $u_1, \ldots, u_{d+1} \in \mathbb{R}^d$ such that*

$$\langle u_i\,,\, v_j \rangle = 1 \quad \forall\ i, j \in \{1, \ldots, d+1\},\ i \neq j. \tag{3.28}$$

For this sequence, one has:

$$\operatorname{vert}(S^*) = \{u_1, \ldots, u_{d+1}\}, \tag{3.29}$$

$$o = \beta_1 u_1 + \ldots + \beta_{d+1} u_{d+1}, \tag{3.30}$$

$$\langle u_i\,,\, v_i \rangle = 1 - \frac{1}{\beta_i} \quad \forall\ i \in \{1, \ldots, d+1\}. \tag{3.31}$$

Next, we prove Theorem 1.10. For that purpose, we need the following proposition.

Proposition 3.20. *Let $d \geq 1$ and $S \subseteq \mathbb{R}^d$ be a d-dimensional simplex such that $o \in \operatorname{int}(S)$. Let $\beta_1, \ldots, \beta_{d+1}$ be the barycentric coordinates of o with respect to S. Then*

$$\operatorname{vol}(S) \operatorname{vol}(S^*) = \frac{1}{(d!)^2 \beta_1 \cdots \beta_{d+1}}.$$

Proof sketch. This result can be deduced from [Nil07, Proposition 3.6]. Since the language used in that paper differs from the one used in this thesis, we give a proof sketch for Proposition 3.20 as a service to the reader.

Let $v_1, \ldots, v_{d+1}$ be the vertices of S such that $o = \sum_{i=1}^{d+1} \beta_i v_i$ and let $u_1, \ldots, u_{d+1}$ as in (3.28). We introduce the matrices

$$V = \begin{pmatrix} v_1 & \cdots & v_{d+1} \\ 1 & \cdots & 1 \end{pmatrix} \quad \text{and} \quad U = \begin{pmatrix} u_1 & \cdots & u_{d+1} \\ -1 & \cdots & -1 \end{pmatrix}.$$

Then, one has $\mathrm{vol}(S) = \frac{1}{d!}|\det V|$ and $\mathrm{vol}(S^*) = \frac{1}{d!}|\det U|$. Furthermore, in view of (3.28) and (3.31), we have that $V^\top U$ is a diagonal matrix with diagonal elements $-1/\beta_1, \ldots, -1/\beta_{d+1}$. We conclude that $(d!)^2 \mathrm{vol}(S)\,\mathrm{vol}(S^*) = |\det V^\top U| = \frac{1}{\beta_1 \cdots \beta_{d+1}}$. □

Proof of Theorem 1.10. By Proposition 3.20 and by applying Lemma 3.8(d) with $n = d + 1$ and $\alpha_i = 1$ for every $i \in \{1, \ldots, n\}$, we get the desired upper bound. Since, by Lemma 3.8(d) and Theorem 1.7(b), the product $\beta_1 \cdots \beta_{d+1}$ is minimal if and only if β_{d+1} is minimal, Theorem 1.7(c) yields that the upper bound is attained if and only if $S = T^d_{1,d+1}$. The lower bound, meanwhile, follows from the fact that $\sum_{i=1}^{d+1} \beta_i = 1$ and hence by the inequality for the geometric and arithmetic means, we have

$$\beta_1 \cdots \beta_{d+1} \leq \frac{1}{(d+1)^{d+1}},$$

with equality if and only if $\beta_1 = \ldots = \beta_{d+1} = 1/(d + 1)$. The latter is the case if and only if the unique interior integral point of S is its centroid. □

Proposition 3.21. *Let P be an integral d-dimensional polytope such that $o \in \mathrm{int}(P)$. Then* $\mathrm{int}(P^*) \cap \mathbb{Z}^d = \{o\}$.

Based on the previous propositions, we can now show the following lemma regarding the dual of S^d_1. This will then be used to characterize the cases in which the dual of a simplex $S \in \mathcal{S}^d(1)$ has maximal volume or an edge of maximal length, respectively. We show that in this case, S^* is equivalent to S^d_1 and hence, we can use the following lemma to describe S.

Lemma 3.22. *Let* $S = \mathrm{conv}\left((T^{d-1}_{1,d} \times \{0\}) \cup \{\pm e_d\}\right) - (1, \ldots, 1, 0)$. *Then* $S^* \simeq S^d_1$.

Proof. For convenience, let $\tilde{e} := e_1 + \ldots + e_{d-1}$. Let us first observe that the barycentric coordinates $\beta_1 \geq \ldots \geq \beta_{d+1}$ of o with respect to S satisfy

$$(\beta_1, \ldots, \beta_{d+1}) := \Big(\frac{1}{s_1}, \ldots, \frac{1}{s_{d-1}}, \frac{1}{2(s_d - 1)}, \frac{1}{2(s_d - 1)}\Big).$$

Furthermore, Proposition 3.21 and (3.30) yield that o is the unique interior integral point of S^* and o has barycentric coordinates $\beta_1, \ldots, \beta_{d+1}$ with respect to S^*. Now define the facets F_i of S as $F_i := \mathrm{conv}(\mathrm{vert}(S) \setminus \{s_i e_i - \tilde{e}\})$ for $i \in \{1, \ldots, d-1\}$. We set $u_i = -e_i$ for $i \in \{1, \ldots, d - 1\}$ and

$$u_d = (s_d - 1)e_d + \sum_{j=1}^{d-1} \frac{s_d - 1}{s_j} e_j, \qquad u_{d+1} = -(s_d - 1)e_d + \sum_{j=1}^{d-1} \frac{s_d - 1}{s_j} e_j$$

and claim that $\operatorname{vert}(S^*) = \{u_1, \dots, u_{d+1}\}$. Observe that for $i, j \in \{1, \dots, d-1\}$ with $j \neq i$ we have $\langle s_j e_j - \tilde{e}\,,\, -e_i\rangle = \langle -\tilde{e}\,,\, -e_i\rangle = 1$ as well as $\langle \pm e_d - \tilde{e}\,,\, -e_i\rangle = 1$. Furthermore, for $i \in \{1, \dots, d-1\}$, we have

$$\langle s_i e_i - \tilde{e}\,,\, u_d\rangle = -\sum_{k=1}^{d-1} \frac{s_d - 1}{s_k} + s_i \frac{s_d - 1}{s_i} = \left(-1 + \frac{1}{s_d - 1} + 1\right)(s_d - 1) = 1$$

and analogously, $\langle e_d - \tilde{e}\,,\, u_d\rangle = 1$. By an analogous computation, one can also verify $\langle s_i e_i - \tilde{e}\,,\, u_{d+1}\rangle = \langle -e_d - \tilde{e}\,,\, u_{d+1}\rangle = 1$. In view of (3.28) and (3.29), this suffices to show that $\operatorname{vert}(S^*) = \{u_1, \dots, u_{d+1}\}$. To complete the proof, we have to show that the simplex

$$S^* = \operatorname{conv}\left(e_1, \dots, e_{d-1}, \pm(s_d - 1)e_d - \sum_{j=1}^{d-1} \frac{s_d - 1}{s_j} e_j\right)$$

is unimodularly equivalent to S_1^d. To this effect, we first use an integral translation that moves $-\sum_{j=1}^{d-1} \frac{s_d-1}{s_j} e_j$ into the origin. The resulting simplex is

$$Q_1 := \operatorname{conv}\left(e_1 + \sum_{j=1}^{d-1} \frac{s_d - 1}{s_j} e_j, \dots, e_{d-1} + \sum_{j=1}^{d-1} \frac{s_d - 1}{s_j} e_j, \pm(s_d - 1)e_d\right)$$

and we want to show that Q_1 is unimodularly equivalent to the simplex

$$Q_2 := \operatorname{conv}(s_1 e_1, \dots, s_{d-1} e_{d-1}, \pm(s_d - 1)e_d).$$

Both of these simplices have $\pm(s_d - 1)e_d$ as vertices. Hence, we can turn our attention to the linear mapping $\varphi : \mathbb{R}^{d-1} \times \{0\} \to \mathbb{R}^{d-1} \times \{0\}$ given by

$$\varphi :\ e_i \mapsto \frac{1}{s_i}\left(e_i + \sum_{j=1}^{d-1} \frac{s_d - 1}{s_j} e_j\right) \qquad \forall\ i \in \{1, \dots, d-1\},$$

which maps the remaining vertices of Q_2 onto those of Q_1. Once we have shown $\varphi(\mathbb{Z}^{d-1} \times \{0\}) = \mathbb{Z}^{d-1} \times \{0\}$, we are done. For $i \in \{1, \dots, d-1\}$, the integrality of the coefficients can be seen quickly from the fact that s_i divides $s_d - 1$ for $i \in \{1, \dots, d-1\}$, hence $\frac{s_d-1}{s_j s_i}$ is obviously an integer for every $j \in \{1, \dots, j\}$ with $j \neq i$. For the coefficient of e_i, we have

$$\frac{1}{s_i} + \frac{s_d - 1}{(s_i)^2} = \frac{1 + s_1 \cdots s_{i-1} s_{i+1} \cdots s_{d-1}}{s_i} = \frac{1 + (s_i - 1)s_{i+1} \cdots s_{d-1}}{s_i}$$

is also an integer, as s_i divides $s_k - 1$ for $k \in \{i+1, \dots, d-1\}$ and hence the numerator of this fraction is $0 \pmod{s_i}$. We claim that $\varphi^{-1} : \mathbb{R}^{d-1} \times \{0\} \to \mathbb{R}^{d-1} \times \{0\}$ is the linear mapping ψ given by $\psi :\ e_i \mapsto s_i e_i - \tilde{e}$ for all $i \in \{1, \dots, d-1\}$. Indeed,

$$\begin{aligned}
\psi(\varphi(e_i)) &= \frac{1}{s_i}\left(s_i e_i - \tilde{e} + \sum_{j=1}^{d-1} \frac{s_d - 1}{s_j}(s_j e_j - \tilde{e})\right) \\
&= e_i + \frac{1}{s_i}\left(-\tilde{e} + (s_d - 1)\tilde{e} - \tilde{e}(s_d - 1)\left(1 - \frac{1}{s_d - 1}\right)\right) \\
&= e_i
\end{aligned}$$

in view of Proposition 3.3(b). Obviously, ψ preserves integrality. Thus, we get the desired statement. □

Proof of Theorem 1.11. The proof is again divided into four parts: the proofs of (1.11) and assertion (a) are followed by proofs of assertion (b) for $l = d$ and $l = 1$, respectively.

Inequality (1.11). Let $l \in \{1, \dots, d\}$. Let $\beta_1 \geq \dots \geq \beta_{d+1}$ denote the barycentric coordinates of o with respect to S. Then (3.30) yields that o has the same barycentric coordinates with respect to S^*. Proposition 3.21 guarantees that S^* is a d-dimensional simplex with precisely one interior integral point. Hence, by (3.3), we have that for every l-dimensional face F,

$$\mathrm{vol}_{\mathbb{Z}}(F) \leq \frac{1}{l!} \prod_{i=d-l+1}^{d} \frac{1}{\beta_i} \leq \frac{2(s_d - 1)^2}{l!(s_{d-l+1} - 1)}, \tag{3.32}$$

where the second inequality follows from Theorem 3.9(d). This proves (1.11).

Assertion (a). Let $S \simeq \mathrm{conv}\,(T \times \{0\} \cup \{\pm e_d\})$ and thus by Lemma 3.22 we have $S^* \simeq S_1^d$. By Theorem 1.8(a), for every $l \in \{1, \dots, d\}$, there is a face $F \in \mathcal{F}_l(S^*)$ such that

$$\mathrm{vol}_{\mathbb{Z}}(F) = \frac{2(s_d - 1)^2}{l!(s_{d-l+1} - 1)}.$$

Thus, S fulfils (1.11) with equality for $l \in \{1, \dots, d\}$.

Assertion (b) for $l = d$. Let $S \in \mathcal{S}^d(1)$ be such that equality holds in (1.11) for $l = d$. Then, by Theorem 3.9(e),

$$(\beta_1, \dots, \beta_{d+1}) = \Big(\frac{1}{s_1}, \dots, \frac{1}{s_{d-1}}, \frac{1}{2(s_d - 1)}, \frac{1}{2(s_d - 1)}\Big). \tag{3.33}$$

By Proposition 3.20, we have

$$\mathrm{vol}(S^*) = \frac{1}{(d!)^2 \beta_1 \cdots \beta_{d+1} \,\mathrm{vol}(S)}.$$

From Lemma 3.15, we know that $S \simeq \mathrm{conv}\Big((T \times \{0\}\Big) \cup \{\pm(a, h)\})$, where $h \in \mathbb{N}$ and $a \in \{0, \dots, h-1\}^{d-1}$. We obtain

$$\mathrm{vol}(S^*) = \frac{1}{(d!)^2 \beta_1 \cdots \beta_{d+1} \frac{2h}{d} \,\mathrm{vol}(T)} = \frac{1}{d! 2h \beta_1 \dots \beta_{d+1} (s_d - 1)}.$$

From $\beta_1 \cdots \beta_{d+1} = \frac{1}{4}(s_d - 1)^{-3}$, we get

$$\mathrm{vol}(S^*) = \frac{2(s_d - 1)^2}{d! h}.$$

Since $\mathrm{vol}(S^*) = \frac{2}{d!}(s_d - 1)^2$, we have $h = 1$.

Assertion (b) for $l = 1$. Let $l = 1$ and let $S \in \mathcal{S}^d(1)$ be such that equality holds in (1.11). Applying Theorem 3.6 for the case of one-dimensional faces and Theorem 3.12, we deduce that (3.33) are again the barycentric coordinates of o with respect to both S and S^*. Applying Lemma 3.15, we get $S \simeq \mathrm{conv}\,(T \times \{o\} \cup \{\pm(a, h)\})$, where $h \in \mathbb{N}$ and $a \in \{0, \dots, h-1\}^{d-1}$. Note that (a, h) and $-(a, h)$ correspond to the barycentric coordinates β_d and β_{d+1}, respectively. We want to show that $h = 1$. We write $\tilde{e} := e_1 + \dots + e_{d-1} \in \mathbb{R}^d$. By applying a unimodular transformation if necessary, we may assume $S = \mathrm{conv}(T \times \{0\} \cup \{\pm(a, h)\}) - \tilde{e}$. By (3.30), we can write

$$o = \sum_{i=1}^{d+1} \beta_i u_i, \tag{3.34}$$

where $u_1, \dots, u_{d+1}$ denote the vertices of S^*. By Theorem 3.6 we have that for every edge $E := [u_i, u_j]$ of S^*,

$$\mathrm{vol}_{\mathbb{Z}}(E) \leq \frac{1}{\min\{\beta_i, \beta_j\}}.$$

As all barycentric coordinates are known, this implies that the unique edge of S^* with largest normalized volume is $[u_d, u_{d+1}]$ and since we assumed equality in Theorem 1.11, we have $\mathrm{vol}_{\mathbb{Z}}([u_d, u_{d+1}]) = 2(s_d - 1)$. Hence, $u_d - u_{d+1} = 2(s_d - 1)b$ for some integral unit vector b. We want to show $S^* \cap \mathrm{lin}(u_d - u_{d+1}) = [b, -b]$. To see this, observe that

$$S^* \cap \mathrm{lin}(u_d - u_{d+1}) = \left[\sum_{i=1}^{d-1} \beta_i u_i + (\beta_d + \beta_{d+1}) u_d, \sum_{i=1}^{d-1} \beta_i u_i + (\beta_d + \beta_{d+1}) u_{d+1}\right].$$

In view of (3.34), we have

$$\sum_{i=1}^{d-1} \beta_i u_i + (\beta_d + \beta_{d+1}) u_d = \beta_{d+1}(u_d - u_{d+1}) = \frac{2(s_d - 1)}{2(s_d - 1)} b = b.$$

An analogous computation for $-b$ shows that $S^* \cap \mathrm{lin}(u_d - u_{d+1}) = [b, -b]$. This implies the equalities $\rho(S^*, b) = 1$ and $\rho(S^*, -b) = 1$ for the radius function of S^*. Now we have the following relation between the radius function and the support function:

$$\rho(S^*, b) h(S, b) = 1, \qquad \rho(S^*, -b) h(S, -b) = 1;$$

see, e.g., [Sch93, Remark 1.7.7]. This yields $h(S, b) = h(S, -b) = 1$. We now show that $b \in \mathrm{lin}(e_d)$. In view of (3.28), for every $i \in \{1, \dots, d-1\}$ and the vertex $s_i e_i - \tilde{e}$ of S we have the equalities $\langle u_d\, , s_i e_i - \tilde{e} \rangle = 1$ and $\langle u_{d+1}\, , s_i e_i - \tilde{e} \rangle = 1$. As a consequence, we have $\langle u_{d+1} - u_d\, , s_i e_i - \tilde{e} \rangle = 0$ for every $i \in \{1, \dots, d-1\}$. Since $\mathrm{lin}(\{s_i e_i - \tilde{e} \,:\, i \in \{1, \dots, d-1\}\}) = \mathbb{R}^{d-1} \times \{0\}$, we obtain $u_{d+1} - u_d \in \mathrm{lin}(e_d)$ and hence $b \in \mathrm{lin}(e_d)$. Together with $h(S, b) = h(S, -b) = 1$, this yields $S \subseteq \mathbb{R}^{d-1} \times [-1, 1]$. This shows $h = 1$ and $S \simeq \mathrm{conv}(T \times \{0\} \cup \{\pm e_d\})$. □

In the remainder of this section we use dualization to show that a uniqueness results as in Theorem 1.7(c) cannot be obtained for $i < d + 1$.

Proposition 3.23. *Let $i \in \{1, \dots, d+1\}$ and $e := e_1 + \dots + e_d$. Then the simplex $(T^d_{1,i} - e)^*$ is integral.*

Proof. Let $i \in \{1, \dots, d+1\}$ and write $Q^d_{1,i} := T^d_{1,i} - e$. For $j \in \{1, \dots, d\}$, let F_j denote the facet of $T^d_{1,i}$ not containing $c_j e_j$, where $c_j e_j$ is a vertex of $T^d_{1,i}$. In other words, $c_j = s_j$ for $j \in \{1, \dots, i-1\}$ and $c_j = (d - i + 2)(s_i - 1)$ for $j \in \{i, \dots, d\}$. Then the facet F_j yields $-e_j$ as a vertex of $(Q^d_{1,i})^*$. To see this, observe that for any $c \in \mathbb{R}$, $\langle c e_i - e\, , -e_j \rangle = 1$ for $i \neq j$, $i, j \in \{1, \dots, d\}$. Hence, $(Q^d_{1,i})^* = \mathrm{conv}(-e_1, \dots, -e_d, v)$, where v is the vertex corresponding to the facet of $T^d_{1,i}$ which does not contain o. Since the barycentric coordinates of o with respect to $(Q^d_{1,i})^*$ are known, we can write

$$o = -\sum_{j=1}^{i-1} \frac{e_j}{s_j} - \sum_{j=i}^{d} \frac{e_j}{(d - i + 2)(s_i - 1)} + \frac{v}{(d - i + 2)(s_i - 1)}.$$

Hence

$$v = \sum_{j=1}^{i-1} \frac{(d - i + 2)(s_i - 1)}{s_j} e_j + \sum_{j=i}^{d} e_j.$$

Since s_j divides $s_i - 1$ for $j \in \{1, \dots, i-1\}$, all vertices of $(Q^d_{1,i})^*$ are integral. □

Remark 3.24 (Non-uniqueness of the minimizers of β_i). The previous proposition implies that for $i \in \{1, \dots, d+1\}$, the lattice simplices $T^d_{1,i} - e$ are reflexive in the sense of [Nil07]. As the following volume computation shows, $T^d_{1,i} - e$ and $(T^d_{1,i} - e)^*$ are not unimodularly equivalent unless $i = d+1$, despite the fact that the origin has the same barycentric coordinates with respect to their vertices. In particular, this shows that the minimizers of the i-th barycentric coordinate are not unique unless $i = d+1$. Let $i \in \{1, \dots, d\}$ and let $\beta_1, \dots, \beta_{d+1}$ denote the barycentric coordinates of o. Observe that by Proposition 3.20, we have

$$\operatorname{vol}(T^d_{1,i} - e)\operatorname{vol}\left((T^d_{1,i} - e)^*\right) = \frac{1}{(d!)^2 \beta_1 \cdots \beta_{d+1}}.$$

As

$$\operatorname{vol}(T^d_{1,i} - e) = \frac{1}{d!}(d-i+2)^{d-i+1}(s_i - 1)^{d-i+1} \prod_{j=1}^{i-1} s_j = \frac{1}{d!}(s_i - 1)^{d-i+2}(d-i+2)^{d-i+1}$$

and

$$\frac{1}{\beta_1 \cdots \beta_{d+1}} = (s_i - 1)^{d-i+3}(d-i+2)^{d-i+2},$$

we have

$$\operatorname{vol}\left((T^d_{1,i} - e)^*\right) = \frac{1}{d!}(s_i - 1)(d-i+2).$$

Hence, $\operatorname{vol}(T^d_{1,i} - e) \neq \operatorname{vol}\left((T^d_{1,i} - e)^*\right)$ for $i \in \{1, \dots, d\}$. ■

3.4 Proofs of results about the coefficient of asymmetry

this section contains the proofs of Theorems 1.12 and 1.13. We first reformulate the definition of the coefficient of asymmetry. This alternative definition then simplifies the proof of Theorem 1.12.

Proposition 3.25 (Alternative definition of $\operatorname{ca}(P, o)$). *Let $P \subseteq \mathbb{R}^d$ be a polytope such that $o \in \operatorname{int}(P)$. Then*

$$\begin{aligned} \operatorname{ca}(P, o) &= \min\{\alpha \geq 0 \,:\, P \subseteq -\alpha P\} \\ &= \min\{\alpha \geq 0 \,:\, \operatorname{vert}(P) \subseteq -\alpha P\}. \end{aligned}$$

Thus, $\operatorname{ca}(P, o)$ is the unique $\alpha > 0$ such that $P \subseteq -\alpha P$ and $\operatorname{vert}(P) \cap -\alpha \operatorname{bd}(P) \neq \emptyset$.

Proof. It is easy to see that we can rewrite $\operatorname{ca}(P, o)$ as

$$\begin{aligned} \operatorname{ca}(P, o) &= \max\left\{\frac{\rho(P, u)}{\rho(P, -u)} \,:\, u \in \mathbb{R}^d \setminus \{o\}\right\} \\ &= \min\left\{\alpha \geq 0 \,:\, \frac{\rho(P, u)}{\rho(P, -u)} \leq \alpha \;\forall\, u \in \mathbb{R}^d \setminus \{o\}\right\} \\ &= \min\left\{\alpha \geq 0 \,:\, \rho(P, u) \leq \alpha\rho(P, -u) \;\forall\, u \in \mathbb{R}^d \setminus \{o\}\right\}. \end{aligned}$$

Because $\alpha\rho(P, -u) = \rho(\alpha P, -u) = \rho(-\alpha P, u)$ and the fact that two polytopes Q, Q' satisfy $\rho(Q, u) \leq \rho(Q', u)$ for every $u \in \mathbb{R}^d \setminus \{o\}$ if and only if $Q \subseteq Q'$, we get

$$\operatorname{ca}(P, o) = \min\{\alpha \geq 0 \,:\, P \subseteq -\alpha P\} = \min\{\alpha \geq 0 \,:\, \operatorname{vert}(P) \subseteq -\alpha P\}, \tag{3.35}$$

where the second equality in (3.35) is obvious from the convexity of P. This implies $\operatorname{vert}(P) \cap -\operatorname{ca}(P, o)\operatorname{bd}(P) \neq \emptyset$, because otherwise $\operatorname{bd}(-\operatorname{ca}(P, o)P) \cap P = \emptyset$ and one could choose $\alpha' < \operatorname{ca}(P, o)$ such that $P \subseteq -\alpha' P \subsetneq -\operatorname{ca}(P, o)P$, a contradiction. □

Proof of Theorem 1.12. By Proposition 3.25, there is a vertex of P such that $\mathrm{ca}(P, o)$ is attained along the line going through this vertex and o. Hence, we can choose $v \in \mathrm{vert}(P)$ and $u \in \mathrm{bd}(P)$ such that $o \in [v, u]$ and $\mathrm{ca}(P, o) = \frac{\|v\|}{\|u\|}$. Considering any proper face of P that contains u and using Caratheodory's theorem (see, e.g., [Bar02, I. 2.3]), we can find an integral simplex T of dimension at most $d-1$ in $\mathrm{bd}(P)$ such that $u \in \mathrm{relint}(T)$. Since we have $o \in \mathrm{int}(P)$, $o \in \mathrm{relint}(S)$ and $S \subseteq P$, we have $\mathrm{relint}(S) \subseteq \mathrm{int}(P)$. Hence, o is the only relative interior integral point of the simplex $S := \mathrm{conv}(T \cup \{v\})$. We denote the barycentric coordinate of o (with respect to this simplex) associated with v by β. Clearly, $\|v\|/\|u\| = (1-\beta)/\beta$. Let h be the dimension of S. Then, in view of (1.8), we have

$$\mathrm{ca}(P, o) = \frac{1-\beta}{\beta} \leq s_{h+1} - 2 \leq s_{d+1} - 2. \tag{3.36}$$

It remains to characterize the equality case. First, observe that if $P \simeq T^d_{1,d+1}$, we have $\mathrm{ca}(P, o) = s_{d+1} - 2$ due to (1.9). Now, let $P \in \mathcal{P}^d(1)$ be such that $\mathrm{int}(P) \cap \mathbb{Z}^d = \{o\}$ and $\mathrm{ca}(P, o) = s_{d+1} - 2$. The assumption $\mathrm{ca}(P, o) = s_{d+1} - 2$ implies that for the simplex S, we have equality in both inequalities in (3.36). Hence, S has dimension d and furthermore, o has the barycentric coordinate $1/(s_{d+1} - 1)$ with respect to the vertex v of S. Theorem 1.7(c) yields that S is unimodularly equivalent to $T^d_{1,d+1}$ and, in particular, the unimodular transformation mapping S onto $T^d_{1,d+1}$ has to map v onto o. Thus, u is in the relative interior of the facet of S which is opposite to v. As u is also in $\mathrm{bd}(P)$, we have that this facet is in the boundary of P. We finish the proof by showing $P = S$. Assume that there exists some $y \in P \setminus S$. Then for some facet F of S, one has $\mathrm{relint}(F) \subseteq \mathrm{int}(P)$. By our previous arguments, this facet cannot be the one opposite to v. As the unimodular transformation mapping S onto $T^d_{1,d+1}$ maps v onto o, F therefore has to be unimodularly equivalent to a facet of $T^d_{1,d+1}$ which contains o. It is easy to check that each such facet of $T^d_{1,d+1}$ contains at least one integral point in its relative interior[1] and hence $\mathrm{relint}(F)$ contains a point of $\mathbb{Z}^d \setminus \{o\}$. Since $\mathrm{relint}(F) \subseteq \mathrm{int}(P)$, this is a contradiction to $\mathrm{int}(P) \cap \mathbb{Z}^d = \{o\}$. □

Remark 3.26. Using the argument of Izhboldin and Kurliandchik as outlined in Remark 3.13, it is possible to determine the maximizer of the asymmetry coefficient within $\mathcal{S}^d(1)$ without any use of Soundararajan's arguments. ■

Proof of Theorem 1.13. As $\mathrm{int}(P) \cap \mathbb{Z}^d = \{o\}$, Theorem 3.2 asserts that $\mathrm{vol}(P) \leq (1 + \mathrm{ca}(P, o))^d$. Applying Theorem 1.12 completes the proof. □

In the previous proof, we made use of Theorem 3.2 as it was proved by Mahler. It should be noted that Sawyer proved a slightly sharper inequality than Mahler's in [Saw54] which does, however, not lead to asymptotically better results.

Remark 3.27 (Asymmetry of the volume-maximizers in $\mathcal{P}^d(1)$). We ask whether the simplex S^d_1 has maximal volume among all elements of $\mathcal{P}^d(1)$. The main reason for this question is the apparent link between asymmetry and large volume. Assume that P has maximal volume among all elements of $\mathcal{P}^d(1)$. Then $\mathrm{vol}(P) \geq \mathrm{vol}(S^d_1) = \frac{2}{d!}(s_d - 1)^2$. Let, without loss of generality, $o \in \mathrm{int}(P)$. Then by Theorem 3.2, we have $\mathrm{vol}(P) \leq (1 + \mathrm{ca}(P, o))^d$. This yields the lower bound

$$\mathrm{ca}(P, o) \geq \left(\frac{2}{d!}(s_d - 1)^2\right)^{1/d} - 1 \geq 2^{2^{d+o(d)}}.$$

[1] Every simplex of the form $\mathrm{conv}(o, a_1 e_1, \ldots, a_d e_d)$ with $a_1, \ldots, a_d > 0$ and $1/a_1 + \ldots + 1/a_d < 1$ contains the point $\mathbb{1} - e_i$ in the relative interior of the facet opposite to $a_i e_i$ for each $i \in \{1, \ldots, d\}$. In view of Proposition 3.3 (b), the simplex $T^d_{1,d+1}$ is of that form.

Thus, every volume maximizer in $\mathcal{P}^d(1)$ has asymmetry coefficient with respect to its interior integral point of double exponential order in d. As simplices are typical examples of highly 'non-centrally-symmetric' polytopes, this leads to the question whether every volume maximizer must be a simplex or at least must be close to a simplex with respect to some metric. A similar argumentation can be applied to $\mathcal{P}^d(k)$ with $k \geq 2$ using a generalization of Theorem 3.2 by Lagarias and Ziegler [LZ91, Theorem 2.5] and Pikhurko's bound on the coefficient of asymmetry of elements in $\mathcal{P}^d(k)$ [Pik01, Theorem 4]. Whether for $d \geq 3$ and $k \geq 1$, the simplex S_k^d has maximal volume among all elements of $\mathcal{P}^d(k)$ is an open question. However, for $k \geq 2$, it is not even known whether S_k^d has maximal volume among all elements of $\mathcal{S}^d(k)$. ■

3.5 Proofs of results on the lattice diameter

In this section, we proof Theorems 1.14 and 1.15. To that end, we review a part of [AWW11] which used the bounds on barycentric coordinates of the interior integral point of a simplex $S \in \mathcal{S}^d(1)$ as they were given by Pikhurko in [Pik01]. In [AWW11], as a byproduct on the way to proving finiteness of the family of $\mathbb{Z}^d$-maximal lattice-free polyhedra in $\mathcal{P}(\mathbb{Z}^d)$ (up to unimodular transformation) for fixed dimension d, a bound on $\operatorname{ld}(P)$ was established for $\mathbb{Z}^d$-maximal polyhedra in $\mathcal{P}(\mathbb{Z}^d)$ which depended on Pikhurko's bounds. Since we now have the exact lower bound on the barycentric coordinates, it is worth to revisit the corresponding arguments of [AWW11]. This will allow us to determine the sharp upper bound on the lattice diameter of ℓ-maximal polytopes in $\mathcal{P}(\mathbb{Z}^d)$, which obviously then also holds for all $\mathbb{Z}^d$-maximal polytopes in $\mathcal{P}(\mathbb{Z}^d)$ for $d \geq 3$. We will repeat here only those details from [AWW11] necessary for our purpose but on the other hand aim to give a self-contained proof of Theorem 1.15. We make use of the following lemma:

LEMMA 3.28 ([AWW11, p.6]). *Let $P \subseteq \mathbb{R}^d$ be an integral polytope for which* $\operatorname{relint}(P) \cap \mathbb{Z}^d$ *is not empty and let $a \in$* $\operatorname{relbd}(P) \cap \mathbb{Z}^d$. *Then P contains an integral simplex S of dimension h, for some $h \in \{1, \dots, d\}$, such that $a \in$* $\operatorname{vert}(S)$ *and* $|\operatorname{relint}(S) \cap \mathbb{Z}^d| = 1$.

Proof of Theorems 1.14 and 1.15. We first prove the bounds on the lattice diameter given in the two theorems. Then, we characterize the equality cases.

The inequalities in Theorems 1.14 and 1.15. We can assume $d \geq 2$. Let $P \subseteq \mathbb{R}^d$ be an integral polytope and let $m := \operatorname{ld}(P')$, where P' denotes the convex hull of $\operatorname{int}(P) \cap \mathbb{Z}^d$. There are two cases: $P' \neq \emptyset$, i.e. $m \geq 0$, or $P' = \emptyset$ and hence $m = -1$. For most of the proof, our argumentation is the same for both cases, with the only difference being that, if $P' = \emptyset$, we make the additional assumption of ℓ-maximality on P as in the formulation of Theorem 1.15. Choose a line g such that $|P \cap \mathbb{Z}^d \cap g|$ is maximal, i.e., such that $\operatorname{ld}(P)$ is attained along g. If $\operatorname{ld}(P) \leq m + 2$, then the statements hold trivially since $s_d \geq 2$. Hence, we can assume $\operatorname{ld}(P) > m + 2$. By applying some unimodular transformation, we can assume $g = \operatorname{lin}(e_d)$. By $\pi : \mathbb{R}^d \to \mathbb{R}^{d-1}$ we denote the projection to the first $d - 1$ components. Then, the polytope $Q := \pi(P)$ is the projection of P along g. Clearly, for every point $p \in P \cap \mathbb{Z}^d \cap g$, we have $\pi(p) = o$. Since $\operatorname{ld}(P) > m + 2$, it follows that $o \in \operatorname{bd}(Q)$. To see this, observe that otherwise $\operatorname{relint}(g \cap P) \subseteq \operatorname{int}(P)$. Now $\pi^{-1}(o) \cap P$ contains $\operatorname{ld}(P) + 1 \geq m + 4$ integral points. This implies that $\operatorname{int}(P)$ contains at least $m + 2$ collinear integral points, a contradiction to the choice of m. Note that $\operatorname{int}(Q) \cap \mathbb{Z}^{d-1}$ is not empty. In the case $\operatorname{int}(P) \cap \mathbb{Z}^d \neq \emptyset$ (i.e. $m \geq 0$), this is obvious as every interior point of P has to be projected to a point in $\operatorname{int}(Q)$. In the case $P' = \emptyset$, we made the additional assumption of ℓ-maximality. It is easy to see that under this assumption, $\operatorname{int}(\pi(P)) \cap \mathbb{Z}^{d-1}$ is not empty (see also [AWW11, Lemma 3.7]).

Hence, from Lemma 3.28, we know that for some $h \in \{1, \dots, d-1\}$ there exists an h-dimensional simplex $S \subseteq Q$ which satisfies $o \in \operatorname{vert}(S)$ and contains exactly one point of $\pi(\mathbb{Z}^d)$ in its relative interior. Denote this point by q and let $q := \sum_{i=0}^{h} \gamma_i v_i$ be a barycentric representation of q, where $v_i \in \operatorname{vert}(S)$ for $i \in \{1, \dots, h\}$ and $v_0 = o$. For $x \in Q$, define $f(x)$ as the length of the intersection between $x + \operatorname{lin}(e_d)$ and P, or more formally, $f(x) := \operatorname{len}(\pi^{-1}(x) \cap P)$. Observe that $f(q) \leq m+2$ as otherwise, there would be at least $m+2$ collinear points in the interior of P. Furthermore, by convexity of P, the function f is concave on Q and we can use Jensen's inequality (see, e.g., [Roc97, Theorem 4.3]) to obtain

$$\begin{aligned} \operatorname{ld}(P') + 2 = m + 2 \geq f(q) = f\left(\sum_{i=0}^{h} \gamma_i v_i\right) &\geq \sum_{i=0}^{h} \gamma_i f(v_i) \\ &\geq \gamma_0 f(v_0) \geq \gamma_0 \operatorname{ld}(P) \\ &\geq \frac{1}{s_{h+1}-1} \operatorname{ld}(P) \geq \frac{1}{s_d - 1} \operatorname{ld}(P)\,. \end{aligned} \tag{3.37}$$

The last line in (3.37) comes from the fact that γ_0 is a barycentric coordinate of the unique interior integral point of an integral simplex of dimension at most $d-1$ and we can apply Theorem 1.7. This proves the inequalities in Theorems 1.14 and 1.15.

Characterization of the equality cases. First, we show that in the case $P' = \emptyset$, P is ℓ-maximal lattice-free as well as in the case $P' \neq \emptyset$, there exist polytopes for which the respective bounds are attained with equality. If $P' \neq \emptyset$ and hence $m \geq 0$, note that the simplex S^d_{m+1} has $m+1$ interior integral points which are collinear (see [LZ91, Proposition 2.6]) and hence $\operatorname{ld}\left(\operatorname{conv}\left(\operatorname{int}\left(S^d_{m+1}\right) \cap \mathbb{Z}^d\right)\right) = m$. Furthermore, this simplex has $[o, (m+2)(s_d-1)e_d]$ as an edge. This edge contains $(m+2)(s_d-1)+1$ integral points and therefore, $\operatorname{ld}\left(S^d_{m+1}\right) \geq (s_d-1)(m+2)$. Together with the bound in (3.37), this yields $\operatorname{ld}\left(S^d_{m+1}\right) = (s_d-1)(m+2)$. In the case $P' = \emptyset$, P is ℓ-maximal lattice-free, i.e. $m = -1$, observe that the simplex S^d_0 does not contain an integral point in its interior but each facet of S^d_0 has an integral point in its relative interior. Thus, S^d_0 is $\mathbb{R}^d$-maximal and therefore also ℓ-maximal. It is easy to check that $\operatorname{ld}\left(S^d_0\right) \geq s_d - 1$ and by our previous arguments, this implies $\operatorname{ld}\left(S^d_0\right) = s_d - 1$.

Now, we assume that P fulfils the inequality in Theorem 1.14 or 1.15, respectively, with equality. More precisely, let $P \subseteq \mathbb{R}^d$ be a polytope with $\operatorname{vert}(P) \subseteq \mathbb{Z}^d$ and $\operatorname{ld}(P') = m$ for some $m \in \mathbb{N} \cup \{0, -1\}$ such that $\operatorname{ld}(P) = (m+2)(s_d-1)$, where $P' := \operatorname{conv}(\operatorname{int}(P) \cap \mathbb{Z}^d)$. We proceed as above, i.e, we project along the direction in which the lattice diameter is attained (we can again assume that this direction is e_d) and write $Q := \pi(P)$. Again, we can then construct the simplex S as we did before. Thus, S is an integral simplex of dimension $h \leq d-1$ with precisely one interior integral point and $v_0 := o$ as one of its vertices. By our assumption on the lattice diameter of P, all inequalities in (3.37) are fulfilled with equality for P. The equality $s_{h+1} - 1 = s_d - 1$ then immediately implies $h = d-1$. Moreover, equality in (3.37) also yields $\gamma_0 = 1/(s_d-1)$. This implies that the interior integral point of S has a barycentric coordinate with minimal value. By Theorem 1.7(b), we know that $S \simeq \operatorname{conv}(o, s_1 e_1, \dots, e_{d-1} s_{d-1})$.

Next, we want to show $Q = S$ by showing that all facets of S are also facets of Q. As P fulfils all inequalities in (3.37) with equality, we have $f(v) = 0$ for all vertices $v \in \operatorname{vert}(S) \setminus \{v_0\}$. This suffices to show $Q = S$ in the case $d = 2$ (and hence $\dim(Q) = \dim(S) = 1$), as the vertex of S which is not v_0 has to be in $\operatorname{bd}(Q)$. Hence, we can assume $d \geq 3$. Denote by F the facet of S such that $v_0 \notin F$. Note that for all facets G of S with $G \neq F$, one has $\operatorname{relint}(G) \cap \mathbb{Z}^{d-1} \neq \emptyset$. If $G \not\subseteq \operatorname{bd}(Q)$, we have $\operatorname{relint}(G) \subseteq \operatorname{int}(Q)$ and one can apply Lemma 3.28 and find a simplex $S' \subseteq G$ of dimension $h' \leq d-2$ which has v_0 as a vertex and contains an interior integral point q'. Let v_i' be the vertices of S' and let $q' = \sum_{i=0}^{h'} \gamma_i' v_i'$ with $\sum_{i=0}^{h'} \gamma_i' = 1$ and $\gamma_i' > 0$ for all $i \in \{0, \dots, h'\}$. By the same construction as before, we get

$$m + 2 \geq f(q') = f\left(\sum_{i=0}^{h'} \gamma_i' v_i'\right) \geq \gamma_0' f(v_0') \geq \gamma_0' \operatorname{ld}(P).$$

This yields $\gamma_0' \leq \frac{1}{s_d - 1}$ by our assumption on $\operatorname{ld}(P)$, a contradiction to (1.8) as S' is of dimension at most $d-2$. This shows that $G \subseteq \operatorname{bd}(Q)$ for all facets $G \neq F$ and therefore, $Q \subseteq \mathbb{R}_{\geq 0}^{d-1}$. It remains to show $F \subseteq \operatorname{bd}(Q)$. Assume the contrary, then $\operatorname{relint}(F) \subseteq \operatorname{int}(Q)$ and therefore, $f(y) > 0$ for every $y \in \operatorname{relint}(F)$. Let y' be the point of $\operatorname{relint}(F)$ such that q is in the relative interior of the line segment $[v_0, y']$. Again employing concavity of f, we have

$$m + 2 \geq f(q) \geq \gamma_0 f(v_0) + (1 - \gamma_0) f(y') \geq m + 2 + (1 - \gamma_0) f(y').$$

As both $1 - \gamma_0$ and $f(y')$ are positive, this is a contradiction.

We have proven $Q = S$. In other words, we have shown that the projection of P along e_d is equivalent to $\operatorname{conv}(o, s_1 e_1, \dots, e_{d-1} s_{d-1})$. We conclude the proof by constructing P from this projection. First, we show that P is a simplex in dimension d. For each vertex v_i of Q, with $i \in \{1, \dots, d-1\}$, the point $p_i := \pi^{-1}(v_i) \cap P$ is a vertex of P (since $f(v_i) = 0$ as we have shown before). Furthermore, the endpoints of $\pi^{-1}(v_0) \cap P$ are two more vertices of P, denoted by p_0 and p_0'. Let $T := \operatorname{conv}(\{p_i : i \in \{0, \dots, d-1\}\} \cup \{p_0'\})$. By construction, all facets of T which contain both p_0 and p_0' are in the boundary of P (as their respective projections lie in the boundary of Q). We can write

$$q_0 := \gamma_0 p_0 + \sum_{i=1}^{d-1} \gamma_i p_i, \qquad q_0' := \gamma_0 p_0' + \sum_{i=1}^{d-1} \gamma_i p_i,$$

which yields a point in the respective relative interior of each of the remaining two facets of T. By construction, the segment $[q_0, q_0']$ has length

$$\operatorname{len}([q_0, q_0']) = \gamma_0 \operatorname{len}([p_0, p_0']) = \gamma_0 (m+2)(s_d - 1) = m + 2.$$

Consequently, one has $q_0, q_0' \in \operatorname{bd}(P)$ since otherwise, the segment $[q_0, q_0']$ has $m+2$ integral points contained in the interior of P, which contradicts $m = \operatorname{ld}(P')$. Thus, all facets of T are contained in the boundary of P and hence $P = T$.

Finally, we show that the simplex P is unimodularly equivalent to S_{m+1}^d. Without loss of generality, we set $p_0 = o$ and $p_0' = \operatorname{ld}(P) e_d = (m+2)(s_d - 1) e_d$. The points p_i, $i \in \{1, \dots, d-1\}$, are of the form $p_i = s_i e_i + c_i e_d$ for some integers c_i. Note that there exists some $c_0 \in \mathbb{R}$ such that $q_0 = (1, \dots, 1, c_0)$ and $q_0' = (1, \dots, 1, c_0 + m + 2)$. Moreover, $c_0 \in \mathbb{Z}$. To see this, assume the contrary, i.e. $c_0 \in \mathbb{R} \setminus \mathbb{Z}$. Then $[c_0, c_0 + m + 2]$ contains $m+2$ integral points which lie in the interior of P, a contradiction to the definition of m. From the definition of q_0, q_0' we get

$$c_0 = \sum_{i=1}^{d-1} \gamma_i c_i.$$

By Proposition 3.14 and because $\gamma_i = 1/s_i$ for $i \in \{1, \dots, d-1\}$, we know that $c_0 \in \mathbb{Z}$ implies that s_i divides c_i for every $i \in \{1, \dots, d-1\}$. Consider the linear mapping φ defined by $e_i \mapsto e_i - \frac{c_i}{s_i} e_d$ for every $i \in \{1, \dots, d-1\}$ and $e_d \mapsto e_d$. Because s_i divides c_i for $i \in \{1, \dots, d-1\}$,

$\varphi(\mathbb{Z}^d) \subseteq \mathbb{Z}^d$. The inverse mapping to φ is given by $e_i \mapsto e_i + \frac{c_i}{s_i} e_d$ for $i \in \{1, \ldots, d-1\}$ and $e_d \mapsto e_d$, which shows that $\varphi(\mathbb{Z}^d) = \mathbb{Z}^d$. Thus, φ is a unimodular transformation. Clearly, $\varphi(P) = S^d_{m+1}$. This proves that, up to unimodular equivalence, P is a uniquely determined simplex, namely $P \simeq S^d_{m+1}$. □

Proof of Corollary 1.16. The upper bound on the lattice point enumerator $G(P)$ follows immediately from (1.6) and the upper bound on the lattice diameter $\operatorname{ld}(P)$ from Theorem 1.15: one has

$$G(P) \leq (\operatorname{ld}(P) + 1)^d \leq (s_d)^d \leq 2^{d2^{d-1}},$$

where the last inequality follows from Proposition 3.3(c).

The volume bound in Corollary 1.16 can be obtained by replacing the bound on the lattice diameter used in the proof of the volume bound in [AWW11] by the sharp bound given in Theorem 1.15. We follow the lines of the proof in [AWW11]. It can be shown that P is a subset of an integral polytope Q whose number of interior integral points is between 1 and $G(P)$. Since a d-dimensional integral polytope with $k \in \mathbb{N}$ interior integral points is known to have volume of order $k2^{2^{2d+o(d)}}$ (see [Pik01]), we conclude $\operatorname{vol}(P) \leq \operatorname{vol}(Q) \leq G(P)2^{2^{2d+o(d)}}$. Thus, in view of the bound on $G(P)$ shown above, we arrive at the bound in Corollary 1.16. □

Appendix A

Implementation of search algorithm

This appendix contains an implementation of the algorithm presented in Section 2.3 in Python 2.7 courtesy of Gennadiy Averkov and Stefan Weltge. Executing this code yields Proposition 2.14. It is divided into three files, the first of which contains the main part of the algorithm, while the other two provide basic functions for computations on three-dimensional polytopes and basic functions and objects needed for geometric computations.

search.py

```
"""
This is the main part of the code. The procedure is executed by calling the
    function "main".
"""

from basics import Vector3d
from fractions import Fraction
from polytopes import Polytope3d

import basics
import math

UPPER_BOUND_VOLUME = 27
STRICT_LOWER_BOUND_SUCC_MIN = Fraction(1, 4)

def main():
    """Executes the search algorithm."""
    # Step 1: enumerate boundary fragments (and run search)
    print "case: lattice diameter = 1"
    run_search(base = [Vector3d(x, y, 0) for (x, y) in [(1, 1), (-1, 0), (0,
        -1)]],
               upper_bound_height = 12,
               lattice_diameter = 1)

    print "case: lattice diameter = 2"
    run_search(base = [Vector3d(x, y, 0) for (x, y) in [(0, 0), (2, 0), (0,
        1)]],
```

```python
               upper_bound_height = 32,
               lattice_diameter = 2)

    print "case: lattice diameter = 3"
    run_search(base = [Vector3d(x, y, 0) for (x, y) in [(0, 0), (3, 0), (0, 1)]],
               upper_bound_height = 21,
               lattice_diameter = 3)

# ------------------------------------------------------------------------

def run_search(base, upper_bound_height, lattice_diameter):
    # Step 2: enumerate apices
    print "  - computing apices ..."
    apices = list(enumerate_apices(base, upper_bound_height, lattice_diameter))
    print "  - apices:", len(apices)

    # Step 3: collect further candidate vertices
    for apex in apices:
        print "  - investigating pyramid with base", base, "and apex", apex
        print "    - computing candidates ..."

        pyramid = Polytope3d(base + [apex])
        candidates = get_sorted_candidates(pyramid, lattice_diameter)
        print "    - candidates:", len(candidates)

        # Step 4: enumerate combinations
        # - searches for a 'critical' polytope (see docstring of 'search_critical_polytope' for a definition) with base
        #   'base', apex 'apex', and lattice diameter 'lattice_diameter'
        # - as a result, no such critical polytope exists, which verifies the claim
        Q = search_critical_polytope(pyramid, apex, lattice_diameter, candidates)
        if Q:
            print "! error, found critical polytope", Q.vertices()
            exit(1)

def enumerate_apices(base, upper_bound_height, lattice_diameter):
    """
    Returns a list of all possible apices for the given boundary fragment 'base', see explanation of Step 2.
    """
    for z in range(3, upper_bound_height + 1):
        for x in range(z):
            for y in range(z):
                apex = Vector3d(x, y, z)
                pyramid = Polytope3d(base + [apex])

```

```python
                if is_valid_pyramid(pyramid, lattice_diameter):
                    yield apex

def is_valid_pyramid(pyramid, lattice_diameter):
    """
    Returns true iff 'pyramid' is lattice-free, has lattice diameter of at most 'lattice_diameter' and has first
    successive minimum less than 1/4.
    """
    if not pyramid.is_lattice_free():
        return False

    if pyramid.has_ld_greater_than(lattice_diameter):
        return False

    if pyramid.successive_minimum_at_most(STRICT_LOWER_BOUND_SUCC_MIN):
        return False

    return True

def get_sorted_candidates(pyramid, lattice_diameter):
    """
    Computes a sorted list of candidates for given pyramid 'pyramid' and lattice diameter 'lattice_diameter' (see the
    explanations of Steps 3 and 4 as well as the remarks on the order of the list).
    """
    candidates = []

    for c in integer_points_in_safe_region(pyramid):
        if not pyramid.contains(c):
            Q = Polytope3d(pyramid.vertices() + [c])
            if Q.is_lattice_free() and not Q.has_ld_greater_than(lattice_diameter):
                candidates.append(c)

    is_in_strip = lambda c: pyramid.ymin() <= c.y and c.y <= pyramid.ymax()

    return [c for c in candidates if is_in_strip(c)] + [c for c in candidates if not is_in_strip(c)]

def integer_points_in_safe_region(pyramid):
    """
    Computes a search region for integer points that can be added to 'pyramid' without exceeding the volume bound
    'volume_bound' (see explanation of Step 3).
    """
    vol = basics.volume_of_simplex(pyramid.vertices())
    assert vol <= UPPER_BOUND_VOLUME
```

```

    vertices = pyramid.vertices()
    center = (vertices[0] + vertices[1] + vertices[2] + vertices[3]) * Fraction(1,4)
    scaling = 1 + 4 * (Fraction(UPPER_BOUND_VOLUME) / Fraction(vol) - 1)
    safe_region = pyramid.homo_copy(scaling, center)

    return safe_region.integer_points(zmin = 0, zmax = pyramid.zmax())

def search_critical_polytope(pyramid, apex, lattice_diameter, candidates):
    """
    This function computes all lattice-free polytopes with lattice diameter <= 'lattice_diameter' and lattice width >= 3
    that can be constructed from 'pyramid' by adding points of 'candidates'. For each such polytope, we check whether it
    is 'critical', i.e., potentially Z^3-maximal lattice-free but not R^3-maximal lattice-free. The method of generating
    such a list is described in the explanation of Step 4.
    """
    if is_critical(pyramid, apex):
        return pyramid

    polytopes_built = set([pyramid])
    num_candidates = len(candidates)

    while candidates:
        c = candidates.pop()
        polytopes_new = set(polytopes_built)

        # For each polytope P, keep P and add P' := P \cup \{ c \} if P' is lattice free and ld(P') <= lattice_diameter
        for P in polytopes_built:
            if not P.contains(c):

                Q = Polytope3d(P.vertices() + [c])
                if Q.is_lattice_free() and not Q.has_ld_greater_than(lattice_diameter):
                    if is_critical(Q, apex):
                        return Q
                    polytopes_new.add(Q)

        # Only keep polytopes that, by adding the remaining candidates, can be extended to ones with lattice width >= 3
        polytopes_built = set([P for P in polytopes_new if
                               not has_lattice_width_at_most_two(P.vertices() + candidates, apex)])
        print "    - completed %d / %d (polytopes stored: %d)" % \
            (num_candidates - len(candidates), num_candidates, len(polytopes_built))
```

```python

        if not polytopes_built:
            return

def is_critical(P, apex):
    """
    Returns true iff P
    - has lattice width at least three,
    - is not R^3-maximal lattice-free, but
    - seems to be Z^3-maximal lattice-free.
    """
    if has_lattice_width_at_most_two(P.vertices(), apex):
        return False
    if P.all_facets_blocked():
        return False

    # Heuristically try to add some integer points outside of P
    (min_x, min_y, min_z, max_x, max_y, max_z) = P.bounding_box()
    return not P.is_lattice_free_extendable([Vector3d(x, y, z) for x in range(min_x - 1, max_x + 2) \
                                                                for y in range(min_y - 1, max_y + 2) \
                                                                for z in range(min_z - 1, max_z + 2)])

def has_lattice_width_at_most_two(points, apex):
    """
    Returns true iff 'points' has lattice width of at most two, see the lemma in explanation of Step 4.
    """
    for (vx, vy) in [(0,1), (1,-1), (1,0), (1,1), (1,2), (1,-2), (2,-1), (1,3)]:
        min_z = basics.custom_ceil(Fraction(- 2 - vx * apex.x - vy * apex.y, apex.z))
        max_z = basics.custom_floor(Fraction(2 - vx * apex.x - vy * apex.y, apex.z))

        for vz in range(min_z, max_z + 1):
            v = Vector3d(vx, vy, vz)

            if max([p * v for p in points]) - min([p * v for p in points]) <= 2:
                return True

# ------------------------------------------------------------------------------
```

```

main()
```

polytopes.py

```
"""Straight-forward implementation of basic functions on three-dimensional
    (rational) polytopes."""

import basics
import itertools

from basics import Vector3d
from fractions import Fraction

class Inequality3d(object):
    """Represents a linear inequality of the form a * x <= b."""

    def __init__(self, lhs, rhs):
        """Creates a linear inequality of the form a * x <= b, where a = 'lhs'
            and b = 'rhs'."""
        self.lhs = lhs
        self.rhs = rhs
        if self.lhs.is_zero():
            raise Exception("trivial inequality: %s" % str(self))

    def __str__(self):
        return str(self.lhs) + " <= " + str(self.rhs)

    def __repr__(self):
        return str(self)

    def __eq__(self, other):
        """Returns true iff all coefficients including the right-hand side of
            'self' and 'other' coincide."""
        return self.lhs == other.lhs and self.rhs == other.rhs

    def __ne__(self, other):
        return self.lhs != other.lhs or self.rhs != other.rhs

    def __hash__(self):
        return hash(str(self))

    def is_satisfied(self, p):
        """Returns true iff 'p' satisfies the inequality."""
        return self.lhs * p <= self.rhs

    def is_strictly_satisfied(self, p):
        """Returns true iff the inequality is strict for 'p'."""
        return self.lhs * p < self.rhs

```

```
    def holds_with_equality(self, p):
        """Returns true iff 'p' satisfies the inequality with equality."""
        return self.lhs * p == self.rhs

# ----------------------------------------------------------------------

class Polytope3d(object):
    """Represents a three-dimensional (rational) polytope."""

    def __init__(self, points):
        """Constructs the convex hull of 'points'."""
        assert(len(points) >= 3)

        # store bounding box
        self._xmin = min([p.x for p in points])
        self._ymin = min([p.y for p in points])
        self._zmin = min([p.z for p in points])
        self._xmax = max([p.x for p in points])
        self._ymax = max([p.y for p in points])
        self._zmax = max([p.z for p in points])

        # Compute facet-defining inequalities
        # - this is done by iterating over all triples of points that span
            some plane H
        # - if all points in 'points' lie on one side of H (including H
            itself), this defines a facet
        self._facets = set()
        for triple in itertools.combinations(points, 3):
            normal = basics.normal_vector_of_triangle(triple)

            if not normal.is_zero():
                max_scal_prod = max([normal * p for p in points])
                min_scal_prod = min([normal * p for p in points])

                if max_scal_prod - min_scal_prod == 0:
                    raise Exception("polytope low-dimensional")

                scal_prod = normal * triple[0]

                if max_scal_prod == scal_prod:
                    self._facets.add(Inequality3d(normal, scal_prod))
                elif min_scal_prod == scal_prod:
                    self._facets.add(Inequality3d(-normal, -scal_prod))

        # determine which points are vertices
        is_vertex = lambda p: len([f for f in self._facets if
            f.holds_with_equality(p)]) >= 3
        self._vertices = frozenset([p for p in points if is_vertex(p)]) #
            frozenset important for hashing
```

```python

    def bounding_box(self):
        """Returns a tuple (xmin, ymin, zmin, xmax, ymax, zmax) containing the minimum and maximum coordinates of 'self'
        with respect to all coordinate directions."""
        return (self._xmin, self._ymin, self._zmin, self._xmax, self._ymax, self._zmax)

    def integer_points_in_bounding_rect_of_slice(self, height):
        """Yields a set S of integer points such that every integer point in 'self' with z-coordinate being equal to
        'height' is contained in S."""
        # First, we compute the intersection of 'self' with the set of points having z-coordinate being equal to
        # 'height'; note that every vertex of this set is
        # - a vertex of 'self' with z-coordinate being equal to 'height', or
        # - the intersection of z = 'height' with a line segment between some vertex above and some vertex below z =
        #   'height'
        above = [v for v in self._vertices if v.z > height]
        inside = [v for v in self._vertices if v.z == height]
        below = [v for v in self._vertices if v.z < height]

        points = inside
        if len(above) > 0 and len(below) > 0:
            for a in above:
                for b in below:
                    mu = Fraction(a.z - height, a.z - b.z)
                    points.append(a * (1 - mu) + b * mu)

        # By construction, 'self' intersected with z = 'height' is the convex hull of 'points'; now we compute a
        # bounding rectangle (xmin, ymin, xmax, ymax) of 'points'
        if len(points) > 0:
            xmin = basics.custom_ceil(min([p.x for p in points]))
            ymin = basics.custom_ceil(min([p.y for p in points]))
            xmax = basics.custom_floor(max([p.x for p in points]))
            ymax = basics.custom_floor(max([p.y for p in points]))

            # Finally, we return all integer points inside the bounding rectangle
            for x in range(xmin, xmax + 1):
                for y in range(ymin, ymax + 1):
                    yield Vector3d(x, y, height)

    def is_lattice_free(self):
        """Returns true iff 'self' does not contain any integer point in its interior."""
```

```
        for height in range(basics.custom_ceil(self._zmin), basics.custom_floor(self._zmax) + 1):
            for p in self.integer_points_in_bounding_rect_of_slice(height):
                if self.contains_in_interior(p):
                    return False

        return True

    def contains_in_interior(self, p):
        """Returns true iff 'p' is contained in the interior of 'self'."""
        for f in self._facets:
            if not f.is_strictly_satisfied(p):
                return False
        return True

    def contains(self, p):
        """Returns true iff 'p' is contained in 'self'."""
        for f in self._facets:
            if not f.is_satisfied(p):
                return False
        return True

    def ymin(self):
        """Returns the minimum y-coordinate of points in the polytope 'self'."""
        return self._ymin

    def ymax(self):
        """Returns the maximum y-coordinate of points in the polytope 'self'."""
        return self._ymax

    def zmax(self):
        """Returns the maximum z-coordinate of points in the polytope 'self'."""
        return self._zmax

    def integer_points(self, zmin = None, zmax = None):
        """
        Returns all integer points of 'self' with z-coordinate between 'zmin' (default: -inf) and 'zmax' (default: inf).
        """
        if zmin is None:
            zmin = basics.custom_ceil(self._zmin)
        if zmax is None:
            zmax = basics.custom_floor(self._zmax)

        for height in range(zmin, zmax + 1):
            for p in self.integer_points_in_bounding_rect_of_slice(height):
```

```
                if self.contains(p):
                    yield p

    def has_ld_greater_than(self, g):
        """Returns true iff 'self' has lattice diameter greater than 'g'."""
        for [p, q] in itertools.combinations(self.integer_points(), 2):
            if (p - q).gcd() > g:
                return True
        return False

    def _eq_(self, other):
        """Returns true iff 'self' and 'other' represent the same polytope."""
        return self.vertices == other.vertices

    def _hash_(self):
        return hash(self._vertices)

    def successive_minimum_at_most(self, value):
        """Returns true iff the first successive minimum of 'self' is at most 'value'."""
        # Note that the first successive minimum of P := 'self' is at most 'value' if and only if P - P contains a
        # non-zero point of 1/'value' * Z^3; setting 'value' =: a/b, this is equivalent to the fact that a * (P-P)
        # contains a non-zero integer point in b * Z^d
        value = Fraction(value)
        difference_body = Polytope3d([(v - w) * value.numerator for v in self._vertices for w in self._vertices
                                      if v != w])

        for p in difference_body.integer_points():
            if p.gcd() >= value.denominator:
                return True
        return False

    def vertices(self):
        """Returns a list of all vertices of 'self'."""
        return list(self._vertices)

    def __mul__(self, multiple):
        """For a scalar 'multiple', this returns 'multiple' * 'self'."""
        V=[v * multiple for v in self._vertices]
        return Polytope3d(V)

    def homo_copy(self, scaling, center):
        """Returns 'scaling' * 'self' + (1 - 'scaling') * 'center'."""
        V = [v * scaling + center * (1 - scaling) for v in self._vertices]
        return Polytope3d(V)

```

```
    def all_facets_blocked(self):
        """Returns true iff every facet of 'self' contains an integer point in its relative interior."""
        intpoints = list(self.integer_points())
        for f in self._facets:
            if not self.is_facet_blocked(f, intpoints):
                return False
        return True

    def is_facet_blocked(self, facet, points):
        """Returns true iff 'facet' containts one point of 'points' in its relative interior."""
        for p in points:
            if facet.holds_with_equality(p):
                if len([g for g in self._facets if g.holds_with_equality(p)]) == 1:
                    return True
        return False

    def is_lattice_free_extendable(self, points):
        """
        Returns true iff there exists a point p in 'points' \ 'self' such that conv('self' union {p}) is lattice-free.
        """
        for p in points:
            if not self.contains(p) and Polytope3d(self.vertices() + [p]).is_lattice_free():
                return True
        return False
```

scripts.py

```
"""Contains very basic functions and objects needed for geometric computations."""

import fractions

def gcd_three(a, b, c):
    """Returns the absolute value of the greatest common divisor of 'a', 'b', and 'c'."""
    return abs(fractions.gcd(a, fractions.gcd(b, c)))

def custom_floor(x):
    """Floor function that does not use floating point arithmetics when applied to fractions."""
    return x // 1

def custom_ceil(x):
    """Ceiling function that does not use floating point arithmetics when applied to fractions."""
```

```
    return -custom_floor(-x)

def normal_vector_of_triangle(points):
    """Returns a primitive nonzero vector 'v' in Z^3 that is perpendicular to the plane containing the
    (three-dimensional) points 'points[0]','poins[1]','points[2]'."""
    a = points[1] - points[0]
    b = points[2] - points[0]
    normal = a.cross(b)
    if normal.is_zero():
        return Vector3d(0,0,0)
    return normal.primitive_vector()

def volume_of_simplex(vertices):
    """Computes the volume of the 3-dimensional simplex whose vertices are 'vertices'."""
    assert len(vertices) == 4
    a = vertices[1] - vertices[0]
    b = vertices[2] - vertices[0]
    c = vertices[3] - vertices[0]
    return abs(fractions.Fraction(a.cross(b) * c, 6))

# ----------------------------------------------------------------------------

class Vector3d(object):
    """Straight-forward implementation of basic functions on vectors with three components."""
    def __init__(self, x, y, z):
        """Creates a vector with coordinates ('x', 'y', 'z')."""
        self.x = x
        self.y = y
        self.z = z

    def __str__(self):
        return "[" + str(self.x) + ", " + str(self.y) + ", " + str(self.z) + "]"

    def __repr__(self):
        return str(self)

    def __eq__(self, other):
        return self.x == other.x and self.y == other.y and self.z == other.z

    def __ne__(self, other):
        return self.x != other.x or self.y != other.y or self.z != other.z

    def __hash__(self):
        return hash(str(self))

```

```
    def __add__(self, other):
        return Vector3d(self.x + other.x, self.y + other.y, self.z + other.z)

    def __sub__(self, other):
        return Vector3d(self.x - other.x, self.y - other.y, self.z - other.z)

    def __neg__(self):
        return Vector3d(-self.x, -self.y, -self.z)

    def __mul__(self, other):
        """If 'other' is a scalar, this returns the vector that arises from 'self' by multiplying each component with
        'other'. If 'other' is a vector, this returns the scalar product of 'self' and 'other'."""
        if type(other) is Vector3d:
            return self.x * other.x + self.y * other.y + self.z * other.z
        return Vector3d(self.x * other, self.y * other, self.z * other)

    def __div__(self, other):
        """Returns the vector that arises from 'self' by dividing each component by 'other'."""
        return Vector3d(self.x / other, self.y / other, self.z / other)

    def gcd(self):
        """Returns the greatest common divisor of the entries of 'self'."""
        return gcd_three(self.x, self.y, self.z)

    def is_zero(self):
        """Returns true iff all entries of 'self' are zero."""
        return self.x == 0 and self.y == 0 and self.z == 0

    def is_integral(self):
        """Returns true iff all entries of 'self' are integer numbers."""
        return all([type(t) is int for t in [self.x, self.y, self.z]])

    def primitive_vector(self):
        """Returns an integral vector that is parallel to 'self' and whose entries have gcd one."""
        x = fractions.Fraction(self.x)
        y = fractions.Fraction(self.y)
        z = fractions.Fraction(self.z)

        v = Vector3d(x.numerator * y.denominator * z.denominator, \
                     y.numerator * x.denominator * z.denominator, \
                     z.numerator * x.denominator * y.denominator)

        return v / v.gcd()

    def cross(self, other):
```

```
        """Returns the 3-dimensional cross product of 'self' and 'other'."""
        return Vector3d(self.y * other.z - self.z * other.y,
                        self.z * other.x - self.x * other.z,
                        self.x * other.y - self.y * other.x)
```

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