The complete classification of six-dimensional iso-edge domains

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Abstract

In this paper, we report on the full classification of generic iso-edge subdivisions of six-dimensional translational lattices. We obtain a complete list of 55 083 357 affine types of iso-edge subdivisions. We report on computational techniques that were used for this computer-assisted enumeration which are of general interest.

1. Introduction

The study of the Voronoi and Delaunay polytopes of lattices was initiated in (Lejeune Dirichlet, 1850; Voronoi, 1908) and the Voronoi polytope of a lattice is an extremely useful object in crystallography under the name of the Wigner–Seitz Cell and Brillouin zone. When the lattice changes the Voronoi and Delaunay polytopes change but in a given dimension there are only a finite number of nonequivalent possibilities, each defining a domain in the space of lattices. Following Voronoi, those domains are named L-type domains. A domain is called generic if it has the maximal possible dimension.

The state of the art of the enumeration of Voronoi polytopes of lattices is reported in Table 3 of (Dutour Sikirić et al., 2016), where the enumeration of all the possible types of Voronoi polytopes in dimension 5 is done. A related enumeration problem is to consider only the edges of the Delaunay polytopes or equivalently the facets of the Voronoi polytopes. This was initiated in (Baranovskii & Ryshkov, 1973; Ryškov & Baranovskii, 1978) and rediscovered in (Engel, 2015). A description of the theory was presented in (Dutour Sikirić & Kummer, 2022) together with applications to algebraic geometry and the Conway-Sloane conjecture. We call those domains iso-edge domains though the name C-type is commonly used¹. Again a domain is called generic if it has the maximal possible dimension.

In this work, we enumerate the generic iso-edge domains in dimension six. The enumeration is relatively difficult and forces us to introduce new computational techniques that are of general interest. It also opens the way for further computations for example of Voronoi polytopes in dimension six. Another related open problem is to prove that the Vallentin lattice (Schürmann & Vallentin, 2006; Vallentin, 2003) gives the best lattice covering in dimension six. See Table 1 for the enumeration results known so far.

Table 1. Number of generic and all combinatorial types, respectively, of iso-edge domain corresponding $GL_d(\mathbb{Z})$ -inequivalent cones.

n	Generic types	All combinatorial types
2	1	2
3	1 (Fedorov, 1885)	5 (Fedorov, 1885)
4	3 (Engel, 2015)	51 (Stogrin, 1975)
5	76 (Ryškov & Baranovskiĭ, 1978)	56 713 (Dutour Sikirić & Kummer, 2022)
	(Engel, 2015)	
6	55 083 357 (This work)	

In Section 2 we start with some notation and background on Delaunay polytopes and on the Gram matrix formalism which is helpful. In Section 3 we give some information

¹ The terminology "C-type" comes from "L-type" introduced by Voronoi. The Cyrillic letter C is pronounced like the Latin letter S and refers to "skeleton", that is the graph determined by the edges of the Delaunay subdivision.

on the methods used to do the effective computer enumeration. In Section 4 we report on the obtained enumeration results.

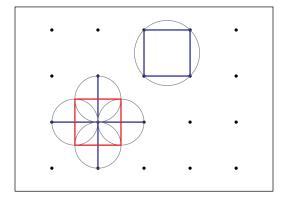
2. Definitions

For a lattice L in the Euclidean space \mathbb{R}^d Voronoi introduced a polytopal decomposition induced by the closest neighbor points:

$$P_V(L) = \left\{ x \in \mathbb{R}^d \text{ s.t. } ||x|| \le ||x - v|| \text{ for } v \in L - \{0\} \right\}.$$

This polytope is now named the *Voronoi polytope* and it shows up in many different applications in crystallography under the names of Wigner–Seitz Cell and Brillouin zone (Okabe *et al.*, 2000). Voronoi polytopes are also important in computational geometry (Aurenhammer *et al.*, 2013) and higher dimensional constructions (Schürmann, 2009).

For a lattice L a sphere S(c,r) of center c and radius r is called an *emphy sphere* if for all lattice vectors $v \in L$ we have $||v - c|| \ge r$. A *Delaunay polytope* of a lattice L is the polytope whose vertex set is $S(c,r) \cap L$ for an empty sphere S(c,r).



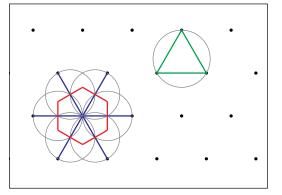


Fig. 1. Example of a Voronoi Cell (red) and Delaunay polytopes (blue and green). The centrally symmetric Delaunay polytopes are indicated in blue. The hexagonal lattice (right) is generic and the integer lattice (left) is not generic.

2.1. Working with Gram matrices

The set of positive definite quadratic forms is denoted by $\mathcal{S}_{>0}^d$. When dealing with lattices up to orthogonal transformations, it is often convenient to work with Gram matrices $Q = B^{\top}B$ instead of using matrices of lattice bases B. Up to orthogonal transformations, the basis B can be uniquely recovered from the Gram matrix. Every positive definite symmetric matrix defines a corresponding positive definite quadratic form $x \mapsto Q[x] := x^{\top}Qx$ on \mathbb{R}^d .

The Gram matrix is an easier and more practical system to work with but the problem is that there are many possible lattice bases of a given lattice. Any two lattice basis B_1 and B_2 of the same lattice are related by an integral matrix U of determinant ± 1 , i.e., an unimodular matrix, such that $B_2 = B_1 U$ and so the corresponding positive definite matrices satisfy $Q_2 = U^{\top} Q_1 U$. We call such positive definite matrices (arithmetically) equivalent.

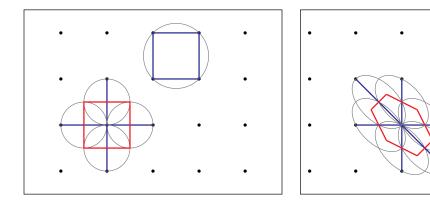


Fig. 2. Same as Figure 1 but in the Gram setting with (up to scaling) $Q = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$ respectively.

2.2. Iso-Delaunay and iso-edge domains

Let $A \in S^d_{>0}$ be a positive definite quadratic form on \mathbb{R}^d . We formulate the notion of Delaunay polytopes in terms of A in the following way: a lattice polytope $P \subset \mathbb{R}^d$ is called a *Delaunay polytope* if there is some $c \in \mathbb{R}^d$ and r > 0 such that $A[x-c] \geq r$ IUCr macros version 2.1.15: 2021/03/05

for all $x \in \mathbb{Z}^d$ with equality if and only if x is a vertex of P. The set $\mathrm{Del}(A)$ of all Delaunay polytopes is the *Delaunay subdivision* associated to A. The *iso-Delaunay domain* $\Delta(\mathcal{D})$ of a Delaunay subdivision \mathcal{D} is

$$\Delta(\mathcal{D}) := \{ Q \in S^d_{>0} : \operatorname{Del}(Q) = \mathcal{D} \},$$

also known as an L-type domain. The iso-Delaunay domain $\Delta(A)$ of $A \in S^d_{>0}$ is defined to be $\Delta(\mathrm{Del}(A))$. Voronoi's second reduction theory (Voronoi, 1908) states that the set of all iso-Delaunay domains is a polyhedral subdivision of the cone $S^d_{>0}$ of positive definite symmetric matrices on which the group $\mathrm{GL}_d(\mathbb{Z})$ of unimodular matrices acts on the right by $A \circ U = U^{\top} A U$. See (Schürmann, 2009) for an overview of such decompositions. For any fixed d this group action on the set of all iso-Delaunay domains has only finitely many orbits.

The *iso-edge domain*, introduced in (Ryškov & Baranovskiĭ, 1978) is a coarser subdivision of $S_{>0}^d$: The iso-edge domain of a Delaunay subdivision \mathcal{D} is defined as

$$C(\mathcal{D}) = \left\{ \begin{array}{c} Q \in S^d_{>0} : E \in \mathrm{Del}(Q) \text{ for all } E \in \mathcal{D} \\ \text{with } E \text{ centrally symmetric} \end{array} \right\}.$$

We call the iso-edge domains of maximal dimension generic. In this generic case, the only centrally symmetric Delaunay polytopes are the edges justifying the name. The iso-edge domain C(A) of $A \in S^d_{>0}$ is defined to be C(Del(A)).

Quadratic forms in an iso-edge domain have exactly $2^n - 1$ translation classes of edges. If one chooses the representatives $[0, v_i]$ for $1 \le i \le 2^n - 1$ for the translation classes then the defining inequalities for the domain are of the form

$$Q\left[\frac{v_i}{2}\right] \le Q\left[\frac{v_i}{2} - v\right] \text{ for } v \in Z^d.$$

Those inequalities are linear in the quadratic form Q. It was proven in (Baranovskii & Ryshkov, 1973) that only a finite number of inequalities suffices and that the generic iso-edge domains are polyhedral.

It was shown in (Ryškov & Baranovskiĭ, 1978) that the set of all iso-edge domains is a polyhedral subdivision of $S_{>0}^d$ and that there are finitely many iso-edge domains up to $GL_d(\mathbb{Z})$ -equivalence.

In (Ryškov & Baranovskiĭ, 1978) the iso-edge domains of dimension 5 were enumerated resulting in 76 different types. Then the iso-Delaunay domains were enumerated (the enumeration was unfortunately wrong in term of missing one case and was corrected later in (Engel, 2000; Engel & Grishukhin, 2002)). Finally, the lattice covering problem was solved in dimension 5 with A_5^* giving the thinnest covering (This conclusion was confirmed in (Schürmann & Vallentin, 2006)). The classification of iso-edge domains in dimension 5 was confirmed in (Engel, 2015).

3. Algorithms

The enumeration of the generic iso-edge domains is done in the following standard way. We start from one iso-edge domain and compute its facets. From each facet, we compute the adjacent iso-edge domain. We check if this new iso-edge domain is isomorphic to an already known one and if not we insert it into the list of iso-edge domains. The enumeration terminates when all domains have been treated.

3.1. Canonical form of iso-edge domains

Determining whether two iso-edge domains are isomorphic may be fast but if we have say $M = 10^7$ cases, then the number of pairwise equivalence tests is M(M-1)/2, which is not computationally feasible. One speed-up is to compute some invariants for the iso-edge domain. But an even better approach is to compute a canonical form of the C-type. The isomorphism test then becomes a simple equality test that has an amortized constant cost since it uses a hash-map.

Such a canonical form for graphs is a common construction in graph computations

(McKay & Piperno, 2014). It allows to obtain a canonical ordering of the vertices that transform isomorphism checks into a string equality check. It is used in combinatorics for enumerating purposes (McKay, 1998).

One key aspect of the enumeration is that we can compute a canonical form of an iso-edge domain. We encode an iso-edge domain by the family of facet-defining vectors of the corresponding Voronoi polytope $\mathcal{V} = (v_i)_{1 \leq i \leq N} \subset \mathbb{Z}^d$, i.e. the set of *Voronoi relevant vectors* of any form in the domain. For a generic iso-edge domain, there are precisely $N = 2 \cdot (2^d - 1)$ such vectors. We follow the approach of (Dutour Sikirić et al., 2020) for the canonical form of quadratic forms which we adapt to our case. We compute the matrix $Q = \sum_{1 \leq i \leq N} v_i v_i^{\mathsf{T}}$ and define the edge weighted graph $G_{\mathcal{V}}$ on the N vectors with edge weights $w_{ij} = v_i^{\mathsf{T}} Q^{-1} v_j$. We then compute the canonical form of this graph (see (McKay & Piperno, 2014)) which allows us to define a canonical ordering of the vectors \mathcal{V} . Once the ordering is canonical we can use a Hermite normal form computation to obtain a unique representation $\mathcal{V}' = (v_i')_{1 \leq i \leq N}$ of the iso-edge domain.

In the case of positive definite quadratic forms, we use a configuration of short vectors which span \mathbb{Z}^d over the integers. In the following lemma, we prove that the Voronoi relevant vectors $(v_i)_{1 \leq i \leq N}$ generate \mathbb{Z}^d , and that they transform well under the action of $GL_d(\mathbb{Z})$. This allows us to apply the whole methodology of (Dutour Sikirić et al., 2020) to our case and prove that the family $\mathcal{V}' = (v_i')_{1 \leq i \leq N}$ is indeed a canonical form for the vectors $\mathcal{V} = (v_i)_{1 \leq i \leq N}$.

Lemma 3.1 Consider the map $A \mapsto \mathcal{V}(A) \subset \mathbb{Z}^d$ that sends a positive definite form $A \in S^d_{>0}$ to its set of Voronoi-relevant vectors. Then for all $A \in S^d_{>0}$

- V(A) spans \mathbb{Z}^d as a \mathbb{Z} -module, and
- for all $U \in \mathrm{GL}_d(\mathbb{Z})$ we have $\mathcal{V}(UAU^\top) = U^{-1}\mathcal{V}(A)$.

Proof. For the form A define the Voronoi polytope as follows

$$V_A = \left\{ x \in \mathbb{R}^d \text{ s.t. } A[x] \le A[x - v] \text{ for } x \in \mathbb{Z}^d \right\}.$$

The family of polytopes $(v + V_A)_{v \in \mathbb{Z}^d}$ realize a tiling of \mathbb{R}^d . As a consequence for each vector $v \in \mathbb{Z}^d$ there exists a path of Voronoi polytopes $\{h_1 + V_A, \dots, h_k + V_A\}$ such that $h_1 = 0$, $h_k = v$ and the polytopes $h_i + V_A$ and $h_{i+1} + V_A$ share a facet. As a consequence $h_{i+1} - h_i$ is a relevant vector and v is an integer sum of Voronoi relevant vectors. This shows that $\mathcal{V}(A)$ spans the lattice. The second part corresponds simply to a basis transformation.

This algorithm can be sped up in several ways. First, we can use the program Traces for computing the canonical form of a graph (See (McKay & Piperno, 2014) for a presentation of the algorithm of traces). Second when reducing an edge-weighted graph to a classical graph that **Traces** can process, we can use an edge reduction technique (see last paragraph of the section "Isomorphism of edge-coloured graphs" of the user manual of (McKay, 2014)). The third optimization is more subtle and uses the fact that the facet vectors of the graph occur in pairs $\{v, -v\}$. Therefore we can write the vectors as $(v_1, v_2, \ldots, v_{2p})$ with p = N/2 and $v_{2i} = -v_{2i-1}$. We consider an edge weighted graph $G_{abs,\mathcal{V}}$ on the p pairs with edge weight $\left|v_{2i}^{\top}Q^{-1}v_{2j}\right|$. This smaller edge weighted graph is easier to work with and as we shall see as powerful an invariant as the full graph. If every automorphism of $G_{abs,\mathcal{V}}$ can be extended to an automorphism of $G_{\mathcal{V}}$ then the canonical form of $G_{abs,\mathcal{V}}$ will give a canonical form of $G_{\mathcal{V}}$. If the graph formed by the non-zero weights is connected then an automorphism of $G_{abs,\mathcal{V}}$ admits at most two extensions to an automorphism of $G_{\mathcal{V}}$. Lemma 3.2 below proves the connectedness. For a more extensive explanation of this trick see Section 9.7.2 of (van Woerden, 2023). With all these reductions the running time for computing the canonical form in dimension 6 is 3 milliseconds per iso-edge domain.

Lemma 3.2 [Connectedness] For a generic iso-edge domain the edge-weighted graphs $G_{\mathcal{V}}$ and $G_{abs,\mathcal{V}}$, when removing all weight 0 edges, are connected.

Proof. It suffices to prove the lemma for $G_{abs,\mathcal{V}}$. Consider a generic iso-edge domain with vectors $S = \{\pm v_1, \ldots, \pm v_N\}$ for $N = 2^d - 1$, and let $Q = \sum_i v_i v_i^{\top}$. Note that due to Lemma 3.1 Q has full rank and is positive definite. Suppose for contradiction that $G_{abs,\mathcal{V}}$ is not connected, then there exists two sets $S_i = \{\pm v_1^i, \ldots, \pm v_{k_i}^i\}$ for i = 1, 2 such that $S = S_1 \cup S_2$, $S_1 \cap S_2 = \emptyset$, $N = |S| = |S_1| + |S_2|$ and such that $x^{\top}Q^{-1}y = 0$ for all $x \in S_1, y \in S_2$. Because Q^{-1} is positive definite the orthogonality implies that $\operatorname{rk}(S_1) + \operatorname{rk}(S_2) \leq d$. Consider the rank $\operatorname{rk}(S_i)$ lattice $L_i = \operatorname{span}_{\mathbb{Z}}(S_i) \subset \mathbb{Z}^d$ w.r.t. some form R in the interior of the iso-edge domain. By definition S_i is contained in the set of Voronoi relevant vectors L_i , and thus $|S_i| \leq 2^{\operatorname{rk}(S_i)} - 1$. This gives however the following contradiction:

$$N = |S| = |S_1| + |S_2| \le (2^{\operatorname{rk}(S_1)} - 1) + (2^{\operatorname{rk}(S_2)} - 1) < 2^d - 1 = N.$$

3.2. Parallelization of the enumeration

We can express the canonical form as a string and thus compute its hash. The hash function that we use does not have to be cryptographically secure and so we use Robin Hood Hash (Celis *et al.*, 1985) which is a fast hashing function adequate for database purposes.

The parallelization strategy chosen is Message Passing Interface (MPI) in which P processes are run simultaneously. No data is shared between the processes but data is exchanged using synchronization primitives. For each iso-edge domain, we compute its canonical form expression. We then compute the hash which we reduce modulo P. This allows us to assign an iso-edge domain to a specific process.

Then on each process, we have an associative container that uses the same hash function but with a different seed in order to store the iso-edge domains. If we were to use the same seed, then the obtained hash on a given node would be in a much smaller set and so the number of collisions would be higher. Using the hash function allows to have very good performance on insertion, essentially O(1). It turns out that the hashes are distinct on all the iso-edge domains that we considered in this work though the algorithms used do not depend on this property.

3.3. Finding adjacent iso-edge domains

From an iso-edge domain having vectors $\{v_1, \ldots, v_N\}$ we compute the triples (i, j, k) with $v_i + v_j + v_k = 0$. From each such triple we get a number of defining inequalities $Q[v_i] \leq Q[v_j] + Q[v_k], \ Q[v_j] \leq Q[v_i] + Q[v_k], \ Q[v_k] \leq Q[v_i] + Q[v_j].$

From all such inequalities, we can determine which ones are facet-defining inequalities. We use Clarkson's method (Clarkson, 1994) implemented in **cdd** (see (Fukuda, 2022; Fukuda *et al.*, 2018)) in order to get the facet-defining inequalities. The problem is that the number of inequalities is large with a minimum of 903. This is fairly high and gives a runtime of 0.2 seconds per form which is too high.

Note that while using the symmetries of the iso-edge domain could in theory lead to a smaller number of cases to consider, in practice 98% of cones have trivial automorphism group so this relatively expensive computation would actually increase the runtime.

Instead, we use an additional criterion to exclude some inequalities from consideration more efficiently. Let $\mathcal{C} \subset \mathbb{Z}^d$ be the set of facet vectors v encoding an iso-edge domain. In other words it defines the edges $\operatorname{conv}(0,v)$ of the Delaunay subdivision $\operatorname{Del}(Q)$ of a positive definite matrix Q.

A 3-homogeneous hypergraph $H_{\mathcal{C}}$ is defined as follows:

$$V(H_{\mathcal{C}}) := \mathbb{Z}^d / 2\mathbb{Z}^d,$$

$$E(H_{\mathcal{C}}) := \{ \{ \bar{x}, \bar{y}, \bar{z} \} : x, y, z \in \mathcal{C}, x + y + z = \mathbf{0} \}.$$

Here for every $t \in \mathbb{Z}^d$ we write \bar{t} to denote the parity class $t + 2\mathbb{Z}^d$ ($\in \mathbb{Z}^d/2\mathbb{Z}^d$).

Let $\{i, j, k\} \in E(H_{\mathcal{C}})$. There are two ways to choose $\{x, y, z\} \subseteq \mathcal{C}$ so that $\bar{x} = i$, $\bar{y} = j$, $\bar{z} = k$ and $x + y + z = \mathbf{0}$. Let us write $\{x, y, z\}$ for one of the two choices, then the other choice would be $\{-x, -y, -z\}$. Define a set $\mathcal{C}' \subset \mathbb{Z}^d$ by requiring that the following properties are fulfilled:

$$C \setminus C' = \{z, -z\}, \qquad C' \setminus C = \{x - y, y - x\}.$$

If \mathcal{C}' is the set of facet vectors of an iso-edge domain, then we say that \mathcal{C}' is obtained from \mathcal{C} by swap (i,j;k). This corresponds precisely with flipping to the neighboring iso-edge domain at the defining inequality $Q[z] \leq Q[x] + Q[y]$, as $Q[x-y] \leq Q[x] + Q[y]$ and $x+y+z=\mathbf{0}$ implies that $Q[z] \geq Q[x] + Q[y]$. Note that in the signature of the swap i and j are interchangeable and k is fixed to be the last argument. Note also that the definition of a swap through parity classes is consistent: we obtain the same swap if $\{x,y,z\}$ and $\{-x,-y,-z\}$ are interchanged.

For the set of facet vectors of an iso-edge domain \mathcal{C} and a triple $\{i, j, k\} \in E(H_{\mathcal{C}})$ we will say that (i, j; k) is a *forbidden swap* for an iso-edge domain \mathcal{C} if there is no iso-edge domain \mathcal{C}' such that \mathcal{C}' is obtained from \mathcal{C} by a swap (i, j; k).

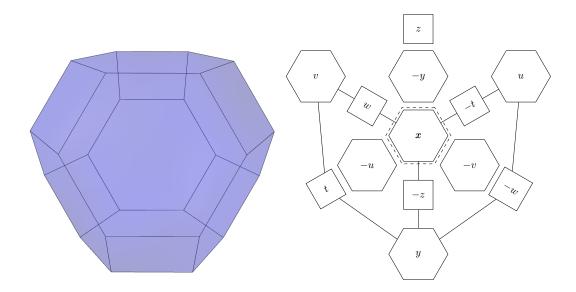


Fig. 3. The unfolded facets of a truncated octahedron. The edges (x, -z, y) between two hexagonal facets with a quadrangular in the middle indicate a triple that satisfies $x + y + z = \mathbf{0}$ as in (the proof of) Theorem 3.3.

Theorem 3.3 Let $\mathcal{C} \subset \mathbb{Z}^d$ be the set of facet vectors of an iso-edge domain. If the inclusion

$$\{\{i, j, k\}, \{i, e, f\}, \{i, g, h\}, \{j, e, g\}, \{j, f, h\}\} \subseteq E(H_{\mathcal{C}})$$

holds for seven pairwise distinct non-zero parity classes

$$e, f, g, h, i, j, k \in \mathbb{Z}^d / 2\mathbb{Z}^d$$

then (i, k; j) and (k, j; i) are forbidden swaps for C.

Proof. Choose seven lattice vectors t, u, v, w, x, y and z from C so that their parity classes are e, f, g, h, i, j and k, respectively. (Thus, there are exactly two choices for each vector; these two choices relate to each other via antipodality.)

We first prove that

$$t, u, v, w, x, y, z \in \text{span}(t, x, y). \tag{1}$$

We note that $t, x, y \in \text{span}(t, x, y)$ for trivial reasons. Since $\{i, j, k\} \in E(H_{\mathcal{C}})$, one concludes that $z \in \text{span}(x, y)$. Similarly, $u \in \text{span}(t, x)$ and $v \in \text{span}(t, y)$ because IUCr macros version 2.1.15: 2021/03/05

 $\{i, e, f\} \in E(H_{\mathcal{C}})$ and $\{j, e, g\} \in E(H_{\mathcal{C}})$, respectively. Therefore, $u, v, z \in \text{span}(t, x, y)$. Finally, $w \in \text{span}(x, v)$ because $\{i, g, h\} \in E(H_{\mathcal{C}})$. Hence $w \in \text{span}(t, x, y)$ and (1) indeed holds.

Further, (1) implies that a Voronoi parallelohedron P, whose set of facet vectors is C, contains 7 pairs of antipodal facet vectors in at most 3-dimensional subspace $\operatorname{span}(t, x, y)$. This is only possible if $\operatorname{dim}\operatorname{span}(t, x, y) = 3$, and if

$$\mathcal{C}^3 := \{\pm t, \pm u, \pm v, \pm w, \pm x, \pm y, \pm z\}$$

is the set of all 14 minimal vectors of the 3-dimensional lattice $\mathbb{Z}^d \cap \operatorname{span}(t, x, y)$. One can view \mathcal{C}^3 as the set of facet vectors of a 3-dimensional iso-edge domain. We remember that a generic 3-dimensional iso-edge domain can have only one combinatorial type — that of a truncated octahedron.

Let F_x^2 , F_y^2 and F_z^2 be facets of P^3 whose facet vectors are x, y and z respectively. F_x^2 , F_y^2 are hexagons because facet vectors of quadrangular faces participate only in 2 triples, while x and y participate in 3 triples. Therefore F_z^2 is quadrangular because each triple contains exactly one facet vector corresponding to a quadrangular face.

For the final step of the proof let x+y+z=0. This can be achieved by interchanging x with -x and y with -y if necessary. Generality is not restricted because the preceding argument does not use any specific choice of signs for facet vectors. We will argue by contradiction, assuming, for instance, that the swap (j, k; i) is admissible. If \mathcal{C}' is the iso-edge domain obtained by the swap, then

$$\tilde{\mathcal{C}}^3 := C' \cap \operatorname{span}(t, x, y) = \{ \pm t, \pm u, \pm v, \pm w, \pm (y - z), \pm y, \pm z \}$$

is also a 3-dimensional iso-edge domain, which can be obtained by a swap from C^3 . A quick computation shows however that a 3-dimensional generic iso-edge domain has only 6 facet defining inequalities and thus 6 possible swaps. For all those swaps both F_y^2 and F_z^2 are hexagonal facets of P^3 , which is not the case as proved earlier. This IUCr macros version 2.1.15: 2021/03/05

contradiction shows that the swap (j, k; i) is forbidden. For similar reasons, the swap (k, i; j) is also forbidden.

The above theorem provides an efficient way to restrict the possible swaps. For each triple $\{i, j, k\}$ we iterate over the vectors e that are in \mathcal{C} . The conditions of the theorem defines the edges f, g and h uniquely if they exist. When they exist, we can forbid some swaps. The cost of this combinatorial check is negligible. This reduces the number of swaps that we have to consider considerably and allow to reduce the runtime of determine the non-redundant facets of the iso-edge domains from an average of 200 milliseconds down to 2 milliseconds per iso-edge domain.

4. Results

The complete runtime of the enumeration was one week on a 20 processors cluster.

The complete results are available at (van Woerden & Dutour Sikiric, 2024).

We report on a few interesting statistics of the 6-dimension iso-edge domains. The total number of triples has a minimum of 1806, a maximum of 2286 and an average of 1887.3. The total number of inequalities generated by those triples has a minimum of 903, a maximum of 1143 and an average of 943.65. After application of Theorem 3.3, we obtain that the minimum number of inequalities is 21, the maximum is 576 and an average of 117.78. The total number of facets has a minimum of 21, a maximum of 216 and an average of 31.87. In Table 2 we give the complete statistics on the number of facets of the iso-edge domains. In Table 3 we give the statistics on the number of automorphisms of the iso-edge domains.

For the set of facet vectors \mathcal{C} of an iso-edge domain a vector v is *free* if for each triple $T = \{x, y, z\} \subset \mathcal{C}$ with $x + y + z = \mathbf{0}$ there exist $w \in T$ such that $v \cdot w = 0$. An iso-edge domain has finitely many free vectors up to scalar multiples and it has at most n(n+1)/2. The notion of free vectors is useful for decomposing Voronoi polytopes as

the Minkowski sum of a polytope and a segment. This notion of geometrical interest has been studied in several papers, see (Grishukhin, 2006a; Dutour Sikirić et al., 2014; Grishukhin, 2004; Grishukhin, 2006b; Engel, 1998) for more details. In Table 4 we give the statistics on the number of free vectors of the iso-edge domains.

The enumeration shows that the iso-edge domain containing the lattice E_6^* is the only one that does not have any free vector. It was discovered in (Engel, 1998) that this polytope has no free vector. In (Grishukhin, 2006a) it was also proved that the lattices D_{2m}^+ for $m \geq 4$ have no free vectors. This implies that all the generic iso-edge domains that contain them have no free vectors. In (Vallentin, 2003) some record coverings in dimension 6 were obtained by doing random walks in the space of iso-Delaunay tessellations. Such random walks can be done as well in the space of iso-edge domains with the goal of minimizing the number of free vectors. By using this technique, we found 225, 455, 135, 55 generic iso-edge domains with no free vectors in dimension 7, 8, 9 and 10, which gives a partial view of the landscape. All such domains were not arithmetically equivalent which indicates that the number of generic iso-edge domains in those dimensions is likely to be extremely large.

Denote by s the number of free vectors of an iso-edge domain. In (Engel, 2020) the number of 6-dimensional cones with s = 0, 1, 2, 3, 18, 19, 20, 21 were determined and the number coincides with the one we found. This provides a rigorous proof of the enumeration results. This enumeration is based on the enumeration of classes with s = 0 and 21 in (Engel, 2019) and computing the adjacent iso-edge domains. The enumeration for s = 0 in (Engel, 2019) in Section 5 is based on the enumeration of iso-Delaunay domains in (Baburin & Engel, 2013). However, since that enumeration is partial we have to consider the proof to be incomplete.

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Table 2. Statistics on the number of facets f of C-types in dimension 6.

f	nb	f	nb	f	nb	f	nb
21	355238	46	313466	71	437	96	9
22	899234	47	242243	72	360	97	7
23	1404333	48	186431	73	257	98	6
24	1974025	49	140903	74	185	99	7
25	2557561	50	107168	75	170	100	1
26	3045565	51	81364	76	140	101	1
27	3443444	52	60849	77	112	102	3
28	3716426	53	45894	78	102	103	4
29	3864881	54	34159	79	79	104	1
30	3865747	55	25589	80	62	105	2
31	3768043	56	19233	81	60	107	1
32	3583995	57	14345	82	59	108	2
33	3333454	58	10928	83	41	109	1
34	3035303	59	8003	84	32	111	1
35	2709025	60	6098	85	22	112	2
36	2373969	61	4609	86	27	113	2
37	2051781	62	3608	87	22	114	1
38	1745716	63	2901	88	18	125	1
39	1467512	64	2053	89	15	129	2
40	1213321	65	1557	90	15	134	1
41	993280	66	1256	91	3	138	1
42	805593	67	987	92	11	166	1
43	644637	68	805	93	7	216	1
44	511780	69	593	94	3		
45	401635	70	515	95	5		

Table 3. Statistics on number h of automorphisms of C-types in dimension 6.

h	nb	h	nb	h	nb	h	nb
2	54319176	20	12	48	52	288	2
4	746925	24	462	72	4	480	4
6	49	28	1 1	96	19	10080	1
8	14200	32	33	120	1	103680	1
12	1999	36	1 1	144	1		
16	402	40	6	240	6		

s	nb	s	nb	s	nb	s	nb
0	1	6	184516	12	3600928	18	15
1	1	7	1351883	13	687446	19	3
$\parallel 2$	6	8	6208175	14	81468	20	1
3	58	9	14706130	15	7622	21	1
$\parallel 4$	1025	10	17467981	16	739		
5	16321	11	10768946	17	91		

Table 4. Statistics on the number s of free vectors of C-types in dimension 6.

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