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Construction of D-Graphs Related to Periodic Tilings

Konstrukcija D-grafova kod periodičkih popločavanja

SAŽETAK

U radu je dan algoritam koji teoretski omogućuje izvođenje metoda za klasifikaciju periodičkih popločavanja u svakoj dimenziju. Pomoću toga se može provjeriti raniji rezulatat dan u radu (e. g. [BM98, BM00]). Primjenom algoritma prikazana je potpuna klasifikacija neizomorfnih trodimenzionalnih $D-$grafova s 5 elemenata.

Ključne riječi: Delaney-Dress simbol, popločavanje u n-dimenzijama

Construction of D-Graphs Related to Periodic Tilings

ABSTRACT

This paper presents an algorithm which allows to derive classification methods concerning periodic tilings in any dimension, theoretically. By the help of this, one can check former results of the topic (e. g. [BM98, BM00]). An implementation of the algorithm yields the complete enumeration of non-isomorphic three-dimensional $D-$graphs with 5 elements, given as illustration.

Key words: Delaney-Dress symbol, tiling in n-dimensions

MSC 2000: 52C22, 57N16, 68R99

1 Introduction

The paper contains the description of an algorithm by which one can solve combinatorial classification problems for tilings in any dimension. The method is based on the well-known concept of Delaney-Dress symbol (or $D-$symbol, shortly, suggested by E. Molnár). This is nothing but a concise representation of the combinatorics and periodicity of a tiling. The symbol consists of a colored graph ($D-$graph) and a matrix function. The theory has been elaborated for the 2-dimensional case in more details (see e. g. [DS84], [DHZ92], [Hus93], [BH96]), however, beside results ([DHM93], [Mol96], [Del95], to name a few) there are a lot of open questions in higher dimensions.

In the following we shall briefly recall the points that are necessary to understand the algorithm. Helping the visual imagination we parallelly work out a spatial example.

Assume that a group Γ acts from the right discretely on a $d-$dimensional, simply connected manifold X^d in such a way that one can find a $\Gamma-$*equivariant cell decomposition*. That is, if we denote the set of cells by $\mathcal{T}$, then $\mathcal{T} = \mathcal{T}^\gamma := \{A^\gamma : A \in \mathcal{T}\}$ holds for all $\gamma \in \Gamma$. The elements of $\mathcal{T}$ are the so-called *cells*. Every point of X^d belongs to at least one tile and no two tiles have an inner point in common. The points of X^d, belonging to exactly two tiles, constitute the $(d-1)$-hyperfaces, or *facets* of $\mathcal{T}$. By intersections we consequently define $(d-2)$-faces, ..., r-faces, ..., 1-faces or *edges*, then 0-faces or *vertices*, as usual for compact (topological) d-politopes. The above pair $(\mathcal{T},\Gamma)$ is called *equivariant tiling*. In our examinations the *symmetry group* Γ contains at least d independent translations, so it is always *periodic*.

Two tilings $(\mathcal{T},\Gamma)$ and $(\mathcal{T}',\Gamma')$, will be considered equivalent if they are topologically equivariant (homeomeric). It means that there exists a homeomorphism ψ that maps $\mathcal{T}$ onto $\mathcal{T}'$ preserving all incidences of tiles, r-faces $(0 \le r \le d-1)$ such that $\psi^{-1}\Gamma\psi = \Gamma'$.

Our Fig. 1 shows a periodic tiling of regular tetrahedra and octahedra filling the Euclidean 3-space. The construction can be derived from a particioned cube by reflecting it in each of its faces, step by step. (See Fig. 2.) "Melting" tiles together we may get octahedra from 8 corner tetrahedra. It is easy to see that the (periodic) space group $Fm\bar{3}m =: \Gamma$ acts on the tiles forming the pair $(\mathcal{T},\Gamma)$ to be equivariant.

We can speak about the vertices, edges and faces of the tetrahedra and octahedra in a usual sense.

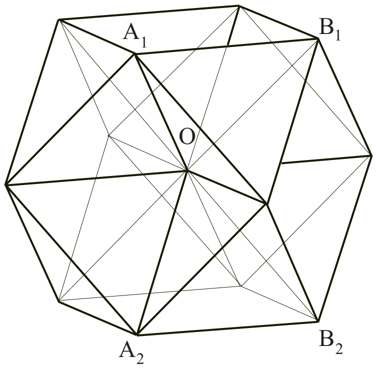

Fig. 1 The tiling can be constructed as follows. Take first 8 regular tetrahedra in the position illustrated above. Then extend the configuration with reflections on the planes A_1A_2O, B_1B_2O, the bisector plane of the segment A_1A_2 and the planes determined by the squares around. Finally we get a tiling with regular tetrahedra and octahedra.

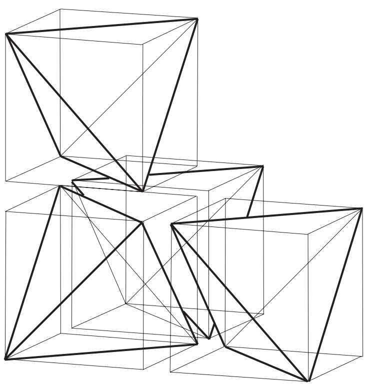

Fig. 2 Take a cube and a tetrahedron in it. In order to get the tiling reflect the bodies in the faces of the cube. The octahedra are divided into 8 smaller simplices.

Now we define the *formal barycentric subdivision* of $\mathcal{T}$ in the usual way: For every $r-$dimensional constituent of $\mathcal{T}$ $(r = 0,\dots,d)$ we choose an interior point, called r-center of $\mathcal{T}$ $(r = 0,\dots,d)$. Consider a fixed tile, one of its $(d-1)$-faces; an incident $(d-2)$-face, ..., finally an incident vertex. These $(d+1)$ centers form the vertices of a $d-$dimensional simplex. Other sequence of $r-$centers leads to other simplex in the tile. Using the method for every tile we finally get the barycentric subdivision made up by simplices called *chambers*. The chamber-system is denoted by $\mathcal{C}$. Every chamber has an *i-face* opposite to its $i-$vertex ($i \in I := \{0,\dots,d\}$). It is obvious that for every chamber $C_1 \in \mathcal{C}$ there exists exactly one chamber C_2 such that their $i-$face is common. In this case we say that C_1 and C_2 are $i-$*adjacent* or $i-$*neighbors*. These adjacencies imply the so-called *adjacency operations* σ_i for $i = 0,\dots,d$:

$$\sigma_i : \mathcal{C} \to \mathcal{C}, \quad C \mapsto \sigma_i C$$

that maps every $C \in \mathcal{C}$ onto its i-neighbor.

The adjacency operations form a free Coxeter group:

$$\Sigma_I := \langle \sigma_i \big| 1 = \sigma_i\sigma_i = \sigma_i^2 : i = 0,\dots,d \rangle$$

that acts transitively from the left on $\mathcal{C}$, if Γ acts from the right, by our convention.

Our Fig. 3 illustrates how the barycentric subdivision can be built up from the given tiling. As an interior point of an $r-$face we have chosen the midpoint for every $r \in \{0,1,2,3\}$.

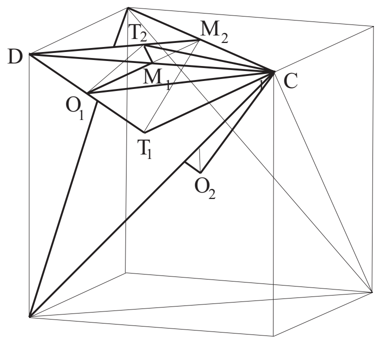

Fig. 3 Take the centers of the two solids (O_1 and O_2), the centers of two faces (T_1 and T_2), the midpoints of edges (M_1 and M_2) and two vertices in common (C,D). The barycentric simplices are $O_2T_1M_2C$, $O_1T_1M_2C$, $O_1T_2M_2C$, $O_1T_2M_1C$, $O_1T_2M_1D$, numbered as 1, 2, 3, 4, 5, respectively, in Fig. 5. O_2M_2CD is the fundamental domain of $Fm\bar{3}m$.

Note that the chamber system $\mathcal{C}$ can always be constructed in a way compatible with the action of Γ on $\mathcal{T}$, and suppose in the following that this is the case. Take a chamber $C \in \mathcal{C}$ and form its *orbit* by Γ:

$$C^\Gamma := \{C^\gamma : \gamma \in \Gamma\}.$$

Our Fig. 4 a–d try to visualize the different simplex orbits by equally coloring the $\Gamma-$equivalent chambers. To avoid any confusion we restrict our attention just to a small part of the tiling.

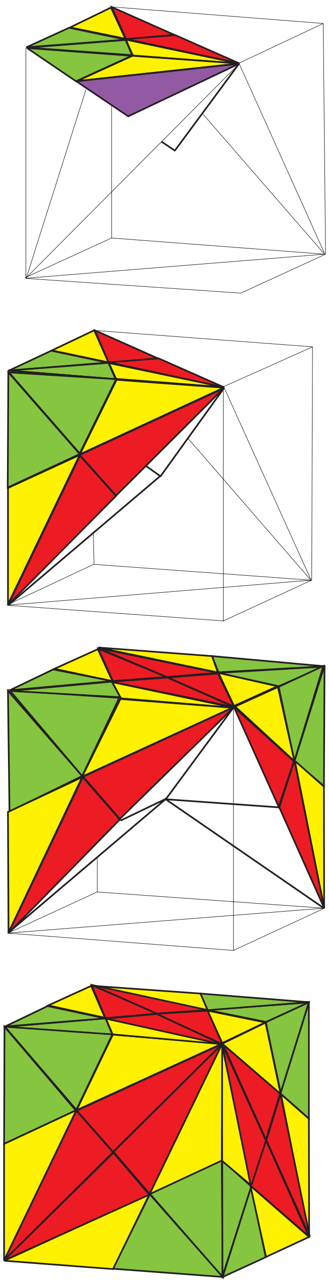

Fig. 4 Take first the 5 simplices above and let act $Fm\bar{3}m$ on them. The polyhedra which can be mapped onto each other are colored in the same way. Step by step we have filled the cube. By reflections we can develop the tiling further.

Fig. 3 shows a polyhedron O_2M_2CD containing barycentric simplices of each kind. This reflection simplex O_2M_2CD can serve as a fundamental domain for Γ. By the so-called Poincare-algorithm one can confirm that the corresponding symmetry group is just $Fm\bar{3}m$ (for more details, see e. g. [Mol83]).

Let $\mathcal{D} := \mathcal{C}/\Gamma$ be the set of different chamber orbits under Γ and let D_k be any orbit ($1 \leq k \leq n$, now $n = 5$). Any $\gamma \in \Gamma$ maps i-neighbors onto i-neighbors, hence the operations σ_i commute with Γ on $\mathcal{C}$, for any i. Thus we can introduce the concept of *i-adjacencies of D_k's*: D_j and D_k are i-adjacent or i-neighbor iff for any $C_j \in D_j$ there exists $C_k \in D_k$ such that $C_k = \sigma_i C_j$ holds.

The set $\mathcal{D}$ and the mappings σ_i define a finite, connected, $(d+1)$-colored graph in which the nodes refer to the orbits and two nodes are linked by an i-colored edge ($i = 0, \ldots, d$) if the corresponding orbits are i-neighbors. Such a graph is called a *Delaney-Dress graph (diagram)* or shortly *D-graph*. Of course, $D = \sigma_i D$ is also possible, in this case we get an $i-$loop.

In Fig. 5, where the loops are not indicated, we can see the $D-$graph of our spatial example from which the Reader may identify the correspondence between colors and numberings.

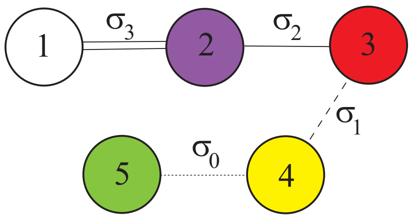

Fig. 5 The D-graph of our example. The loops are not indicated. The colors and numbers are in correspondence with the numbers of matrices and with Fig. 4.

For short D_k will simply be denoted by $k, (k = 1, 2, \ldots, 5)$ in the following.

Let us introduce a matrix function $(m_{ij}) : \mathcal{D} \to \mathbf{N}_{I \times I}$ in the following way. For any $D \in \mathcal{D}$ let

$$m_{ij}(D) := \min \left\{ m \middle| (\sigma_j \sigma_i)^m C = C, \quad C \in D \subset \mathcal{C} \right\}, \qquad (0 \leq i \leq j \leq d).$$

It is easy to see that in a tiling this function has the properties 1-5:

1. $m_{ii}(D) = 1$;
2. $m_{ij}(D) = m_{ji}(D)$;
3. $m_{ij}(D) = m_{ij}(\sigma_i D) = m_{ij}(\sigma_j D)$;
4. $m_{ij}(D) = 2$, if $|i-j| > 1$;
5. $m_{ij}(D) > 2$, if $|i-j| = 1$ in the usual tilings.

Here we give the matrix function m in our example:

$$m(1) = m(2) = m(3) \quad = \quad \begin{bmatrix} 1 & 3 & 2 & 2 \\ 3 & 1 & 3 & 2 \\ 2 & 3 & 1 & 6 \\ 2 & 2 & 6 & 1 \end{bmatrix},$$

$$m(4) = m(5) \quad = \quad \begin{bmatrix} 1 & 3 & 2 & 2 \\ 3 & 1 & 3 & 2 \\ 2 & 3 & 1 & 4 \\ 2 & 2 & 4 & 1 \end{bmatrix}.$$

A pair $(\mathcal{D};m)$, consisting of a finite, connected, colored D-graph and the matrix function fulfilling the properties 1-5, is called a *d-dimensional Delaney-Dress symbol*, or shortly *D-symbol.*

Two D-symbols $(\mathcal{D};m)$, $(\mathcal{D}';m')$ are called *isomorphic* if there exists a bijection $\pi : \mathcal{D} \to \mathcal{D}'$ such that $\sigma_k\left(D^\pi\right) = \left(\sigma_k D\right)^\pi$ moreover, $m'_{ij}\left(D^\pi\right) = m_{ij}(D)$ hold for any $D \in \mathcal{D}$, $0 \le k \le d$, $0 \le i \le j \le d$.

The following basic lemma provides the advantages of D-symbols concerning classification problems :

Lemma 1 *Two tilings $(\mathcal{T},\Gamma)$ and $(\mathcal{T}',\Gamma')$ are equivariantly equivalent (homeomeric, or lying in the same homeomorphism equivariance class), if and only if the corresponding D-symbols $(\mathcal{D};m)$and $(\mathcal{D}';m')$ are isomorphic.* [Dre87] □

Analogously as before, we can introduce other important matrix functions r and v:

$$r : \mathcal{D} \to \mathbf{N}_{I\times I} \qquad r_{ij}(D) := \min\left\{r : \left(\sigma_j\sigma_i\right)^r D = D\right\}$$

for any $D \in \mathcal{D}$, $(0 \le i \le j \le d)$; and

$$v : \mathcal{D} \to \mathbf{N}_{I\times I} \qquad v_{ij}(D) := m_{ij}(D)/r_{ij}(D),$$

where the above division is meant for the elements of matrices.

These functions have the following values in our example (Fig. 5).

$$r(1) = \begin{bmatrix} 1 & 1 & 1 & 2 \\ 1 & 1 & 1 & 2 \\ 1 & 1 & 1 & 3 \\ 2 & 2 & 3 & 1 \end{bmatrix}, \; r(2) = \begin{bmatrix} 1 & 1 & 2 & 2 \\ 1 & 1 & 3 & 2 \\ 2 & 3 & 1 & 3 \\ 2 & 2 & 3 & 1 \end{bmatrix},$$

$$r(3) = \begin{bmatrix} 1 & 3 & 2 & 1 \\ 3 & 1 & 3 & 2 \\ 2 & 3 & 1 & 3 \\ 1 & 2 & 3 & 1 \end{bmatrix}, \; r(4) = \begin{bmatrix} 1 & 3 & 2 & 2 \\ 3 & 1 & 3 & 2 \\ 2 & 3 & 1 & 1 \\ 2 & 2 & 1 & 1 \end{bmatrix},$$

$$r(5) = \begin{bmatrix} 1 & 3 & 2 & 2 \\ 3 & 1 & 1 & 1 \\ 2 & 1 & 1 & 1 \\ 2 & 1 & 1 & 1 \end{bmatrix};$$

$$v(1) = \begin{bmatrix} 1 & 3 & 2 & 1 \\ 3 & 1 & 3 & 1 \\ 2 & 3 & 1 & 2 \\ 1 & 1 & 2 & 1 \end{bmatrix}, \; v(2) = \begin{bmatrix} 1 & 3 & 1 & 1 \\ 3 & 1 & 1 & 1 \\ 1 & 1 & 1 & 2 \\ 1 & 1 & 2 & 1 \end{bmatrix},$$

$$v(3) = \begin{bmatrix} 1 & 1 & 1 & 2 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 2 \\ 2 & 1 & 2 & 1 \end{bmatrix}, \; v(4) = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 4 \\ 1 & 1 & 4 & 1 \end{bmatrix},$$

$$v(5) = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 3 & 2 \\ 1 & 3 & 1 & 4 \\ 1 & 2 & 4 & 1 \end{bmatrix}.$$

It is easy to see that r and v have the properties 1-3 of the matrix function m, as well. We emphasize that 4 and 5 do not necessarily hold but r_{ij} has to be the divisor of m_{ij}. Particularly, $r_{ij}(D) = 1$ or 2, if $|i-j| > 1$. This observation has a basic role in the following algorithm and results in theorems 1 and 2.

2 An algorithm for creating *D*-graphs

The point of this section is to describe an algorithm by that we can derive D-graphs for any number of nodes in any dimension. On the one hand the method provides us checking previously published results ([BM98, BM00] - made by hands, in a different way), on the other hand we get new results given at the end of the paper.

In order to construct D-graphs firstly we describe them algebraically. Let be given a D-graph. Suppose that the nodes have already been numbered. Any adjacency operation (or, the set of i-colored edges of the graph) refers to an involutive permutation. This $i-$permutation will be encoded by a sequence of $n := \left|\mathcal{D}\right|$ numbers as follows: the j-th number for σ_i expresses the number of the node with whom the node number j is $i-$adjacent, i. e. is linked by an $i-$colored edge. Let a_n denote the number of all involutive permutations of n elements.

For calculation of a_n we have the formulas:

$a_0 = 1, a_1 = 1, a_2 = 2$

and for $n \geq 3$:

$a_n = a_{n-1} + (n-1)a_{n-2}$, i. e.

$$a_n = 1 + \sum_{k=1}^{n} \frac{(2n)(2n-1)\dots(2n-[2k-1])}{2^k k!}.$$

The complexity of a_n is at most $O(n^{\frac{n}{2}})$.

Proof Pick out a node. If it is adjacent to itself (loop), then we have a_{n-1} permutations. If it is adjacent to any other node, then we have a_{n-2} permuatations for the $(n-1)$ possibilities each. The second formula comes from combinatorics easily.

Now we give rough estimates for a_n.

$$\begin{aligned} a_n &= a_{n-1} + (n-1)a_{n-2} \\ &= a_{n-2} + (n-2)a_{n-3} + (n-1)a_{n-2} \\ &= na_{n-2} + (n-2)a_{n-3} \end{aligned}$$

$na_{n-2} < a_n < n\,(a_{n-2} + a_{n-3}) < 2na_{n-2}$.

If n is odd ($n = 2t+1$), then

$$a_{2t+1} > (2t+1)a_{2t-1} > \dots$$
$$\dots > (2t+1)(2t-1) \quad \dots \overbrace{a_1}^{1} = \frac{(2t+1)!}{2^t t!},$$

and analogously

$$\frac{2^t(2t+1)!}{2^t t!} > a_{2t+1}.$$

If n is even ($n = 2t$), then

$$a_{2t} > 2ta_{2t-2} > \dots > 2t(2t-2)\dots \overbrace{a_2}^{2} = 2^t t!,$$

and

$$2^{2t-1}t! > a_{2t}, \text{ respectively.}$$

By the Stirling-formula $\left(t! \approx (\frac{t}{e})^t \sqrt{2\pi t}\right)$ we get:

$$\frac{(2t+1)^{2t+1}}{t^t e^{t+1}} \sqrt{\frac{2t+1}{t}} > a_{2t+1} > \frac{(2t+1)^{2t+1}}{(2t)^t e^{t+1}} \sqrt{\frac{2t+1}{t}},$$

and

$$\left(\frac{4t}{e}\right)^t \sqrt{\frac{\pi t}{2}} > a_{2t} > \left(\frac{2t}{e}\right)^t \sqrt{\frac{\pi t}{2}}.$$

From these estimates we see that $a_n = O(n^{\frac{n}{2}})$, indeed. □

Remark The above calculations give us just a rough asymptotics for a_n. There are several conjectures of E. Makai concerning this problem. In his opinion $a_n = \frac{n^{\frac{n}{2}}}{e^{\frac{n}{2}}} e^{\sqrt{n}+o(1)}$ or, even better $a_n \approx c\frac{n^{\frac{n}{2}}}{e^{\frac{n}{2}}} e^{\sqrt{n}}\sqrt{n}$.

Here we sketch the main steps of our algorithm. In this approach the candidates of a D-graph are represented as ordered $(d+1)$-tuples of involutive permutations. The number of entries depends on the dimension d of the tiling. Having all the possible $(d+1)$-tuples we exclude those ones which do not provide connected D-graph, and for which the property $r_{ij}(D) = 1$ or 2 does not hold. Since many different $(d+1)$-tuple can describe the same graph (according to the numberings) at the end we have to choose representants. More precisely the algoritm will be the following.

ALGORITHM

Assume that the D-graph to be constructed has n nodes and dimension d, i. e. $d+1$ colors.

- Construct first the a_n involutive permutations for a given fixed numbering and order them (e. g. lexicographically).

- Subsequently form ordered $(d+1)$-tuples of involutive permutations in such a way that the $(i+1)$-th element of a $(d+1)$-tuple can not be less than the i-th element according to the order above. (We do not need the $(d+1)$-tuples as a set!) Therefore the $(d+1)$-tuples themselves are ordered.

- Consider a $(d+1)$-tuple and decide whether it is connected. If no, then step back and form the next $(d+1)$-tuple. If yes, then step further.

- Take an element of the symmetric group S_n, conjugate all the involutive permutations of the $(d+1)$-tuple and order them. If this latter one is less then the original $(d+1)$-tuple of permutations (according to the ordering of $(d+1)$-tuples), then continue from the previous item. If no then choose another element of S_n, step by step. If no derived $(d+1)$-tuple is less than the original one, then store it and continue from the previous item. At the end we have a set of $(d+1)$-tuples that will be called the set of representants.

- Choose a representant and permute all the $d+1$ involutive permutations in it. In any case check whether the square of the product of two permutations standing on the k-th and $(k+2)$-th places is the identity. If this property holds for all the products, we store the representant, otherwise continue with another representant.

- Work with this subset of representants further and adopt to them a procedure similar to that before two items. However, there is a big difference, namely the $(d+1)$-tuples are not ordered more. In this way one have to compare the conjugate in question to each of the stored $(d+1)$-tuples. Having used up all the elements of S_n finally we get the representants of non-isomorphic d-dimensional D-graphs with n nodes.

Theorem 1 *Using the ALGORITHM one can construct all the non-isomorphic D-graphs with n nodes and of dimension d.*

Proof Using lexicographic ordering for permutation $(d+1)$-tuples (by that of the involutive permutations) we could considerably reduce the number of cases to be treated with. E. g. if all the involutive permutations of a $(d+1)$-tuple are different, then it is enough to check the connectedness of just one $(d+1)$-tuple instead of $(d+1)!$ ones. The involutive permutations are made inductively, as in the proof of Lemma 2 above. The connectedness procedure is the following.

Take the $(d+1)$-tuple in question. Consider the first number in every involutive permutation. Now we have the numbers of those nodes with whom the first node is linked at all. Take these new numbers (if they exist) and collect the numbers from the involutive permutations which stand on the places whose number is as much as these new numbers. Continue this procedure until new numbers appear. If we get all the numbers, then the $(d+1)$-tuple is connected, otherwise not.

However, since the numbers of the nodes were fixed, it is possible that different $(d+1)$-tuples describe the same graph. The fourth item of the algorithm provides us to avoid this phenomenon. It is easy to see that each renumbering can be presented by a permutation from S_n. Conjugating the involutive permutations, we have another involutive ones, according to the change of numbering. Using the fact that each graph has a a minimal $(d+1)$-tuple according to the ordering, it is enough to find this minimal one. At the end of the procedure we get the representants of connected graphs of each kind.

Beside the advantages of the ordering of $(d+1)$-tuples there is a huge disadvantage, too. That is, the adjacency operations of a graph ought to be distinguished. It means that we have to take into consideration any coloring of the edges, any sequence of the $(d+1)$ involutive permutations of any representant.

Since the product of adjacencies refers algebraically to the product of permutations we can apply the previously mentioned restriction ($r_{ij}(D)=1$ or 2, if $|i-j|>1$) by comparing the square of any $(d+1)$-tuple with the identity.

Finally, since we fail the restriction of being ordered we have to search for the representants, again.

In this way the proof of the algorithm is complete. We mention that this relatively complicated structure of the algorithm seems to be the most effective in practice.

The complexity of our algorithm is at most $O(n^{d\frac{n}{2}})$, asymptotically. □

We have implemented our algorithm to computer. We found the earlier results of [BM98] and [BM00] correct. As a new result we get the complete enumeration of the 3-dimensional D-graphs with 5 barycentric simplex orbits.

Theorem 2 *The number of non-isomorphic 3-dimensional D-graphs with 5 simplex orbits is 33. The table below contains the permutation description of them. (The permutations refer to the adjacency operations in the following order: $\sigma_0,\sigma_1,\sigma_2,\sigma_3$.)* □

12345,12345,13254,21435	12345,13254,21435,12345
13254,21435,12345,12345	12345,12354,21435,13245
12345,13245,21435,12354	12354,21435,13245,12345
13245,21435,12354,12345	12345,12354,21435,13254
12345,13254,21435,12354	12354,21435,13254,12345
13254,21435,12354,12345	12345,12354,42513,13254
12345,13254,42513,12354	12354,42513,13254,12345
13254,42513,12354,12345	12345,21435,12354,34125
21435,12354,34125,12345	12345,13254,21435,13254
13254,21435,13254,12345	12345,13254,21354,14523
12345,14523,21354,13254	13254,21354,14523,12345
14523,21354,13254,12345	12345,13254,21435,14523
13254,21435,14523,12345	12354,12435,13245,21345
12354,12435,13254,21345	21345,13254,12435,12354
12354,43215,21354,13245	12354,45312,13245,21354
21354,13245,45312,12354	12354,14523,21354,13254
13254,21354,14523,12354	

We mention that the introductory example of tiling of regular octahedra and tetrahedra is just of the type $12354, 12435, 13245, 21345$ (No. 30 in the table) which has Euclidean realization with the earlier described function m.

We hope that our algorithm can further be developed in a reasonable way for more number of orbits or for higher dimensions.

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