Vsep – New Heuristic and Exact Algorithms for Graph Automorphism Group Computation

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Abstract. Three new algorithms Vsep, exact (Vsep-e) and heuristic (Vsep-h1, Vsep-h2) for determining the generators, orbits and order of an undirected graph automorphism group (GAG) are presented. A basic tool of these algorithms is the adjacency refinement procedure that gives finer output partition on a given input partition of graph vertices. The refinement procedure is a simple iterative algorithm based on the criterion of relative degree of a vertex toward a basic cell in the partition. A search tree (denoted ST) is used in the algorithms - each node of the tree is a partition. A non-singleton cell with maximum partitioning ability is selected in this partition. The partition of a given node of the tree is obtained from the parent-node partition by setting in a separate cell a vertex in the selected cell (called individualization). For this vertex is determined that it is not similar to a previous vertex in the cell till the moment of the selection. Then, a refinement follows. This process of individualization and refinement (denoted as IR procedure) continues until a discrete partition is obtained. Then, a move back to the parent-partition follows. A move back takes place also after the whole selected cell of a given selection level has been traversed. That way a tower of finer partitions on every path of the search tree is obtained. The initial partition that is a result of a refinement of the input partition is at the top of the tower (root of the tree). The algorithm stops when the whole selected cell of the root of the tree has been traversed. All nonequivalent discreet partitions derivative of the selected vertices called a “bouquet” are stored in a coded form in a hash table in order to reduce the necessary storage – this is a main difference of Vsep with the known GAG algorithms. The proposed algorithms have polynomial time and space complexity for a class of undirected connected graphs called Class6. Graphs from this class satisfy certain requirements. Large set of graphs including the graphs of the projective planes hold these requirements. A new strategy (novelty in Vsep) is used in the exact algorithm: if during its execution some of the searched or intermediate variables obtain a wrong value then the algorithm continues from a new start point losing some of the results determined so far. The new start point is such that the correct results can be obtained. The proposed algorithms has been tested on the nauy&Traces benchmark graphs and compared with Traces, and the results show that “Vsep-e” has graph families that are best cases for it and worst cases for Traces and vice versa. The heuristic versions of Vsep are based on determining some number of discreet partitions derivative of each vertex in the selected cell of the initial partition and comparing them for an automorphism, i.e. their search trees are reduced. The heuristic algorithms are almost exact and are many times faster than the exact one. The experimental tests exhibit that the worst-cases running time of the exact algorithm is exponential but it is polynomial for the heuristic algorithms. Several cell selectors are used in Vsep, some of them are known and some are new. We also use a chooser of cell selector (another novelty of Vsep) for choosing the optimal cell selector for the manipulated graph! The proposed heuristic Vsep algorithms use two main heuristic procedures (Fork, FRST – novelty of Vsep) that generate two different forests of search trees.

Key words: graphs, isomorphism, automorphism, group, stabilizer, exact algorithm, heuristic algorithm, partition, numbering, generators, orbits and order of the graph automorphism group.

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1. Introduction

We assume some familiarity with the basics in the design and analysis of algorithms [1,2,3], combinatorial algorithms [4,5], graph theory and group theory [6,7,8,9,10]. We consider simple finite undirected graphs (without loops and multiple edges). The graph is denoted by G(V,E), where : V={1,2,3, . . . ,n} is the set of vertices and E - the set of edges (v, w), where v, w ∈ V. If G is not the only graph under consideration, then V and E are denoted by V(G) and E(G), respectively. The number |E| of the edges of G we denote by k, k=O(n^2). Our algorithms are applicable to any undirected graph but for the class of graphs, denoted by CLASS6, the exact algorithm has polynomial time and space complexity. This class contains any undirected connected graph that: a) requires maximum 6 selections from the starting partition to obtain the final discrete partition and b) its number of edges are less or equal to half number of edges of the complete graph with the same number of vertices. Our algorithms are applicable also for disconnected graphs but for them there is more efficient algorithm we do not describe here. The set of all vertices adjacent to a vertex x are denoted by Adj(x). We use a static list representation of a graph (by two static arrays) because of its least required storage and fastest operation of finding all adjacent vertices of a given vertex compared with the adjacency matrix and the dynamic list representation.

An isomorphism f [4,5,6,7,8,9,10,11,12] between two graphs G_1(V_1, E_1) and G_2(V_2,E_2) is called one-to-one correspondence (mapping) y_i= f(x_i) between the vertices of the graphs (x_i∈V_1, y_i∈V_2, i=1,2,...,n, n=|V_1|=|V_2|) such that two adjacent (nonadjacent) vertices from one of the graphs correspond to two
An automorphism \[4,5,6,7,8,9,10,11,12\] of a graph is an isomorphism of the graph onto itself. Or, an automorphism \( h \) of graph \( G(V,E) \) is called one-to-one correspondence \( y_i=h(x_i) \) between the vertices of the graph \( (x_i,y_i) \in V, i=1,2,...,n \) that preserves the adjacency of the vertices, i. e. there is unique corresponding edge (non-edge) \( (h(p),h(q)) \in E \) to each edge (non-edge) \( (p,q) \in E \). A fixed point \( x \) of an automorphism \( h \) is called a vertex \( x \) for which \( x=h(x) \). Trivial automorphism is an automorphism \( h_0 \) if each its vertex is a fixed point, \( x=h_0(x_i) \), \( i=1,2,...,n \) and a non–trivial automorphism is an automorphism for which there is at least one pair of vertices \( x,y \) such that \( y=h(x)\neq x \).

Two vertices \( x_i \) and \( y_i \) in the a graph \( G(V,E) \) are called similar (or symmetric) \[7,8\], \( x_i \sim y_i \), when they are corresponding, \( y_i=h(x_i) \), in some automorphism \( h \) or under some set of automorphisms of the graph. Otherwise, if \( x_i \) and \( y_i \) are not similar we use the notation \( x_i !\sim y_i \). An automorphism \( h \) can be presented by two sequences \( \Pi_a \) and \( \Pi_b \) of graph vertex labels:
\[
a_1, a_2, ..., a_n = \Pi_a
b_1, b_2, ..., b_n = \Pi_b
\]
where the corresponding vertices are \( a_i \) and \( b_i=h(a_i), i=1,2,...,n \). The automorphism \( h \) may be shortly written in the form \( \Pi_b=\Pi_a(h) \). The automorphism can be presented by \( n! \) pairs of rows each row being derived from the other by transposing the positions of the pairs of corresponding vertices. The corresponding pairs of vertices can be set on to any place of the rows, but it is possible the place to depend on the sorting criterion which does not depend on the vertex labeling. Each automorphism can be written uniquely only with the permutation \( \Pi_b \) if we assume that \( \Pi_a=1,2,3,...,n \). Even a simpler notation called cycle notation \[10\] is often used. In a cycle \( (x_1,x_2, ... ,x_i, x_{i+1}, ... ,x_p) \), \( x_i \) maps to \( x_{i+1} \), \( I \leq i \leq p-I \) and \( x_p \) maps to \( x_1 \). For example,
\[
h=(1,8)(2,6,3,7)(4,5) = 1 \ 2 \ 3 \ 4 \ 5 \ 6 \ 7 \ 8 \n\]
\[
8 \ 6 \ 7 \ 5 \ 4 \ 3 \ 2 \ 1
\]
Any automorphism can be written as the product of disjoint cycles and the product is unique up to the order of the cycles \[10\]. The cycles of length 1 are omitted.

The operation function composition (or superposition) \[4,5,6,7,8,9,10,11,12\] of two automorphisms \( \alpha=\left(\begin{array}{c}x \\
... \\
z \end{array}\right) \) and \( \beta=\left(\begin{array}{c}y \\
... \\
z \end{array}\right) \) is a consecutive execution of \( \alpha \) and \( \beta \), i. e. \( \gamma=\alpha.\beta=\left(\begin{array}{c}x \\
... \\
z \end{array}\right) \). This operation is usually called multiplication and is denoted by juxtaposition \( \gamma=\alpha.\beta \).

The set of all automorphisms of a given graph \( G(V,E) \) form a graph automorphism group (under the operation function composition of automorphisms) denoted \( Aut(G) \), shortly \( A(G) \) or \( A \) \[4,5,6,7,8,10,12\]. The trivial automorphism is the identity of the group – we denote it by \( I \). The number of the automorphisms in \( A(G) \), \(|Aut(G)| \), is called an order of the automorphism group. An order of an automorphism is the order of the cyclic group generated by this automorphism. If the automorphism is written in cycle form then its order is the least common multiple of the cycle lengths \[10\].

The subset \( gen(A) \subseteq A \), denoted \( gen(A) \) or \( \langle g_1, g_2, ..., g_d \rangle \), is called a generating set \[4,5,6,10,12\] of the automorphism group if every automorphism \( h \in A \) can be written as a finite product of elements \( g_i, g_i^{-1} \in gen(A) \). The generating sets are not unique.

The subset of the graph vertices \( y \) similar to vertex \( x \) in any automorphism \( h \in Aut(G) \), \( y=h(x) \), is called an orbit of \( x \), denoted \( Orb(x,A) \): \( Orb(x,A)=[h(x)| h \in Aut(G)] \) and \( Orb(x,A) \) is read as ‘orbit of a vertex \( x \) under a group \( A \)’. By \( Orb(A) \) we denote the set of all orbits of the group \( A \).

A graph with only one orbit of \( Aut(G) \) is called transitive, and a graph is called rigid or asymmetric if each of its vertices is in a separate orbit - \(|Aut(G)|=1 \). A stabilizer \( A(x_1, x_2, ..., x_i) \) or point-wise stabilizer \[4,10,12\] is the subgroup of the automorphism group \( A \) that contains only the automorphisms with fixed points \( x_1, x_2, ..., x_i \).

There is a theorem called orbit-stabilizer theorem \[4,7,8,9\] for computing the order \(|A|\) of the automorphism group of graph \( G(V,E) \). We denote it theorem ‘O-S’. The theorem claims that
\[ \|A\| = |A(x_j)|**d \text{ where } Orb(x_j,A) = \{ x_1, x_2, ..., x_d \} \text{ is the orbit of vertex } x_j \text{ under the group } A \text{ and } A(x_j) \text{ is a stabilizer of a representative } x_j \text{ of this orbit. In other words, the order of the graph automorphism group is equal to the product of the order of a stabilizer of one of its vertices and the length of the orbit of this vertex.}

The algorithms Vsepk and some other known graph isomorphism and automorphism algorithms use the orbit-stabilizer theorem.

The stabilizer \( A_j = A(x_1, ..., x_j) \) is called an ancestor stabilizer to the stabilizer \( A_i = A(x_1, ..., x_j) \) if \( j > i \) and \( A_j \) is called a successor (or descendant) stabilizer to \( A_i \). Obviously, the orbits of the successor stabilizer are subsets of the orbits of the ancestor stabilizer and the order of the successor stabilizer is a divisor of the order of the ancestor stabilizer.

Given a set \( S \subseteq V \) a set-wise stabilizer \([10, 12]\), denoted \( Aut(G,S) \), is a subgroup of \( Aut(G) \) defined by:

\[
Aut(G,S) = \{ \alpha \in Aut(G) \mid x, \alpha(x) \in S \}.
\]

The graph isomorphism problem consists in deciding whether two given graphs are isomorphic, i.e., whether there is an isomorphism between them. The graph isomorphism problem belongs to the class \( NP \) problems \([3-14]\), and has been conjectured intractable, although probably not \( NP \)-complete.

It is neither known that this problem has polynomial time complexity nor to belong to the class of \( NP-complete \) problems. Its unknown complexity status is a theoretical and practical challenge. Two problems are called polynomial-time equivalent if there is a polynomial time algorithm that transforms one of the problems to another \([5, 6, 8, 10] \). The problems \([3, 6, 10] \) that are polynomial-time equivalent to graph isomorphism are called graph isomorphism complete.

The following problems are graph isomorphism complete \([15, 16]\): given two graphs \( G1 \) and \( G2 \): existence of isomorphism of the graphs; determine the isomorphism of the graphs if it exists; determine the numbers of isomorphisms from \( G1 \) to \( G2 \); given a graph \( G \): determine the generating set \( gen(Aut(G)) \), determine the orbits \( Orb(Aut(G)) \), determine the order \( |Orb(Aut(G))| \). The problems of determining the orbits and order of the graph automorphism group \( A \) are also called automorphism partitioning and automorphisms counting, respectively. The generators, the orbits and the order of the automorphism group \( A \) of a graph \( G \) we denote by \( GOO(A) \) or \( GOO(Aut(G)) \).

A class of graphs is called graph isomorphism complete if recognition of isomorphism for graphs from this class is a graph isomorphism complete problem. The following classes are graph isomorphism complete \([14, 16]\): connected graphs, graphs of diameter 2 and radius 1, directed acyclic graphs, regular graphs, bipartite graphs without non-trivial strongly regular subgraphs, bipartite Eulerian graphs, bipartite regular graphs, line graphs, chordal graphs, regular self-complementary graphs, etc. However, there are special cases of the graph isomorphism problem with polynomial-time complexity: planar graphs (linear time), trees have a particularly simple algorithm, graphs of bounded degree, interval graphs, permutation graphs and convex graphs. At present it is not known a polynomial time algorithm for solving the graph isomorphism complete problems in the worst-case \([13, 14]\) – all known algorithms have exponential or moderately exponential worst-case time complexity. Graph isomorphism problems are of great practical and theoretical interest \([3, 4, 5, 12, 13, 14]\). There are several practical algorithms (their names are shown below in parentheses) for graph isomorphism and graph automorphism group, due to Brendan McKay (nauty), Adolfo Piperno (Traces), William Kocay (Groups&Graphs), Schmidt and Druffel, Jeffrey Ullman; L.P. Cordella, P. Foggia C. Sansone and M.Vento (VF2), Tommi Junttila and Petteri Kaski (bliss), Hadi Katebi, Karem A. Sakallah, and Igor L. Markov (saucy), Jose Luis Lopez-Presa, Luis Nunez Chiroque, and Antonio Fernandez Anta (conauto), G. Tener and N. Deo (nishe), etc. Their running time on random graphs is quite well but a major disadvantage of these algorithms is their exponential time performance in the worst-case. There are two main generalizations of the graph isomorphism: subgraph problem (given two graphs determine if one of them is a subgraph to another) and largest common subgraph problem (given two graphs determine the common subgraph to both that has the maximum number of vertices or edges). These two problems are \( NP \)-complete and have many applications and the algorithms for them use the graph isomorphism and automorphism algorithms as basic tools. Other important problems related to graph isomorphism are \([4, 12]\): i) Compute a complete invariant (certificate, signature) \( f \) for \( G \), i.e. for all graphs \( G \) and \( H \), \( G \cong H \Leftrightarrow f(G) = f(H) \) (graph certificate identifies a graph uniquely up to isomorphism); ii) Compute a canonical labeling \( g \) for \( G \), i.e., for all graphs \( G \) and \( H \), \( G \cong g(G) \land \{G \cong H \Rightarrow g(G) = g(H)\} \).

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The graph isomorphism related problems (graph isomorphism itself, GOO(Aut(G)), subgraph isomorphism, largest common subgraph, graph certificate and canonization of a graph) arise in such fields as mathematics, chemistry, information retrieval, linguistics, logistics, switching theory, bioinformatics, and network theory [5,17].

Our goal is to develop exact and heuristic algorithms for determining GOO(Aut(G)), i.e. to solve the three problems by one algorithm with time complexity as lower as possible, possibly polynomial. In addition, our requirements to the heuristic algorithms are to give results equal to the results of the exact algorithm with the probability close to 1. As the following text and all experiments show we achieved the goal. The proposed exact algorithm is with the polynomial time complexity for any connected graph which number of edges is less or equal to the half number of edges of the complete graph, i.e. if the graph belongs to the family Class6. There are many heuristic algorithms for the graph isomorphism problem [18-21]. We propose two new heuristic algorithms (Vsep-H1, Vsep-h2) for GOO(Aut(G)) with much lower polynomial time complexity than the exact one and the experiments show that they are many times faster than the exact algorithm even for difficult graphs with different sizes and gave correct results for all graphs we run. The heuristic algorithms are very fast and even for large graphs takes at most several minutes. The algorithm Vsep-H1 can be used independently but we use it as one of the first steps in the exact algorithm to determine a representative of one of the smallest orbits of Aut(G) as a starting selected vertex – this way we speed up the exact algorithm and reduce the required storage.

One of the main differences between this article and the previous one [45] is the absence of the conjecture – firstly B. McKay pointed me counter examples in a private communication. There are many counter examples also in [41] – all graphs with LMAX > 6 when applying the algorithm on them.

2. Partitions and the refinement procedure

A ordered partition (or simply partition) \( \Pi \) or \( \Pi(G) \)

\[ \Pi = C_1C_2\ldots C_p = C_1 \cup C_2 \cup \ldots \cup C_p \]

of the vertices of graph \( G(V,E) \) [4,12,15] is a sequence of disjoint non-empty subsets of \( V \) whose union is \( V \). \( \Pi = \{ x_{1,1}, x_{1,2}, \ldots, x_{1,k_1} \ldots, x_{i,1}, x_{i,2}, \ldots, x_{i,k_i} \ldots, x_{p,1}, x_{p,2}, \ldots, x_{p,k_p} \} \) is a detailed presentation of \( \Pi \), where \( C_i = \{ x_{i,1}, x_{i,2}, \ldots, x_{i,k_i} \} \) and \( x_{i,k_i} \in V \). The subsets \( C_1, C_2, \ldots, C_p \) are called cells (classes, blocks).

We denote the number of the cells in a partition \( \Pi \) by \( |\Pi| \). Two cells are called adjacent if there is at least one edge between their vertices, i.e. cells \( C_i, C_j \in \Pi \) are adjacent if there is at least one edge \( (x,y) \), \( x \in C_i, y \in C_j \). A cell with cardinality one is called trivial (or singleton). The vertex of such a cell is said to be fixed by \( \Pi \) or it is called a fixed point of \( \Pi \). By \( NC(x, \Pi) \) we denote the index of the cell \( C \in \Pi \) that contains vertex \( x \), i.e. \( x \in C \). The position (index) of a vertex \( x \) in the partition (or in the cell) we denote by \( pos(x) \). The relative degree \( \rho(x,C_i) \) of a vertex \( x \in C_i \) toward a cell \( C_i \) is equal to the number of vertices of cell \( C_i \) adjacent to vertex \( x \). We denote by \( v(x, \Pi) \) a cell-degree vector defined as \( v(x, \Pi) = (\rho(x,C_i), i=1,\ldots,p) \) – it is a vector whose components are the relative degrees of \( x \) to each cell in \( \Pi \). We say that the partition \( \Pi_2 \) is finer than \( \Pi_1 \), written \( \Pi_2 \leq \Pi_1 \), if for every cell \( C_i \in \Pi_2 \) there exists a cell \( C_i \in \Pi_1 \) such that \( C_i \subseteq C_j \). In order to get a finer partition \( \Pi_2 = D_1D_2\ldots D_q \) when given \( \Pi_1 = C_1C_2\ldots C_p \), a refinement procedure (RP, \( \Pi_2 = RP(\Pi_1) \)) is used, that assign to each vertex \( x \in V \) a sorting criterion according to which the vertices of each class \( C_i \in \Pi_1 \) are sorted out in increasing or decreasing order of their criteria [4,5,12]. Often a sorting criterion is the relative degree \( \rho(x,W) \) of any vertex \( x \in \Pi \) toward some cell \( W \in \Pi. \) The refinement procedure that uses this criterion is called adjacency refinement procedure. We use only this version of the procedure. Example of another criterion for sorting is the number of the subgraphs of a given type (for example a triangle) that contain vertex \( x \).

Two partitions \( \Pi_1 \) and \( \Pi_2 \) of the vertices of graph \( G(V,E) \) are called compatible [40] if: (1) \( |\Pi_1| = |\Pi_2| = m \); (2) if \( \Pi_1 = W_1W_2\ldots W_m \) and \( \Pi_2 = U_1U_2\ldots U_m \), then for all \( i \in [1:m] \), \( |W_i| = |U_i| \); (3) for all \( x,y \in V \), \( NC(x,\Pi_1) = NC(y,\Pi_2) \) implies \( v(x,\Pi_1) = v(y,\Pi_2) \).

Two partitions \( \Pi_1 = C_1C_2\ldots C_p \) and \( \Pi_2 = D_1D_2\ldots D_q \) are called equivalent if there is an automorphism \( \alpha \in Aut(G) \) such that \( NC(x,\Pi_1) = NC(y,\Pi_2) \) for each pair of vertices \( x,y = \alpha(x) \). In other words, the similar vertices are in cells with the same label of \( \Pi_1 \) and \( \Pi_2 \).
Obviously for the equivalent partitions $\Pi_1$ and $\Pi_2$ we have: $p = q$ and $|C_i| = |D_i|$, $i = 1, 2, \ldots, p$. We denote the equivalent partitions by $\Pi_2 = \alpha(\Pi_1)$. Evidently the equivalence relation is transitive. Two discrete partitions $\Pi_1 = a_1a_2\ldots a_k\ldots a_n$, $\Pi_2 = b_1b_2\ldots b_k\ldots b_n$ of a graph $G(V,E)$ vertices are called equivalent if they form an automorphism $h \in \text{Aut}(G)$, $b_k = h(a_k)$, $k = 1, 2, \ldots, n$. The testing if two discrete partitions $\Pi_1$ and $\Pi_2$ form an automorphism is a basic operation in our algorithms.

Given sequence of equivalent discrete partitions $\Pi_i, \ldots, \Pi_m$, we store one of them, for example $\Pi_i$ and the orbits derived by the automorphisms $\Pi_i = \alpha_i(\Pi_j)$, $i = 2, \ldots, m$.

Now we can define a partition-wise stabilizer $A(G, \Pi) : A(G, \Pi) = \{\alpha \in \text{Aut}(G) \mid x, \alpha(x) \in C_i, \text{where } C_i \text{ is any cell of } \Pi\}$ [12]. This is a subgroup of $\text{Aut}(G)$ such that each automorphism $\alpha \in \text{Aut}(G)$ belongs to $\text{Aut}(G, \Pi)$ if to any vertex $x$ of any cell of $\Pi$ corresponds a vertex $y = \alpha(x)$ from the same cell. The orbits of $A(G, \Pi)$ are subsets of the cells of $\Pi$ as we’ll see below. If $\Pi = \Pi_n$ then $A(G, \Pi_n) = \text{Aut}(G)$.

Algorithms for determining the graph automorphisms and isomorphisms use very often the refinement procedure - each cell of its output partition contains at least one orbit of a graph automorphism group or its stabilizer. It is still not known a refinement algorithm that gives output partition each cell of which coincides with an orbit (orbital partition or automorphism partition) [17] on unit input partition.

There are two versions of the refinement algorithm when the sorting criterion is the relative vertex degree $rdg(x, C_i)$ - with vectors or with a base cell. In the vector refinement algorithm to each vertex $x$ is assigned a characteristic vector $V(x)$ whose length is equal to the number of the partition cells and its $i$-th component $V_i(x)$ is equal to $rdg(x, C_i)$. The sorting is being made for each cell until it reaches a partition in which no cell can be divided into subcells.

The RP with a base cell sorts (counting sort [1,2]) the vertices of any cell $C_i$ according to their relative degree $rdg(x, C_i)$ toward a selected base cell $C_j$. Again, the sorting continues until it reaches a partition $\Pi_2$ in which there is no cell that can be divided into subcells toward any base cell - such partition is called stable (equitable) [4,12]: it holds the property $\Pi_1 = \text{RP}(\Pi_1)$. Vertices in every cell of the stable partition have the same sorting criterion - in our case, the same relative degree toward each cell. The base cell refinement algorithm (developed by the author) has time complexity $O(n \log n)$, where $k$ and $n$ are respectively the number of edges and the number of vertices of the graph [22,23] and its tests show many times faster performance than the vector refinement algorithm. The vector refinement algorithm has a considerably worse time complexity because it uses general sorting algorithms with the complex comparison operation of vectors. The base cell refinement algorithm RPB (fig.1) uses the counting sort that has a linear time complexity and does not use a comparison operation - it sorts integers (the relative degree of the vertices) within the range 0 to some integer. In our algorithms for $\text{GOO}(\text{Aut}(G))$ we use only the adjacency refinement procedure with a base cell (fig.1)[23]. It differs from the known refinement algorithms [4, 12, 17] in the way the base cell is selected – after the current base cell ends sorting the adjacent cells as a new base cell is selected the first new smallest subcell and if there is no such subcell the label of the new base cell is taken from the queue - the first cell label in the queue. There is another version RPB1 of the refinement algorithm with base cell –it always takes the new base cell from the queue.

The individualization-refinement procedure (denoted IR), used in the known GA algorithms, has two steps: individualization and refinement. Given an equitable partition $\pi$ and a vertex $x$ at the individualization step a new partition $\pi_1$ is obtained: the cell $C(x)$ of $\pi$ with index $i$ is divided into 2 subcells: $\{x\}$ - the first subcell, with index $i$ and the second subcell $\{C(x)\setminus\{x\}\}$ with index $i+1$, other cells of $\pi$ are not changed. At the refinement step the partition $\pi_1$ is refined with the refinement procedure RP obtaining a new equitable partition $\pi_2 = \text{RP}(\pi_1)$ finer than $\pi_1$. Given a partition $\pi$ and a vertex $x$ we denote by $\text{IR}(\pi, x)$ the resulting partition from the application of IR on $\pi$ and $x$.

Cells in a partition $\Pi$ are not consecutively labeled by 1, 2, . . . . The label $NC(C_i, \Pi)$ of a cell $C_i$ in a partition $\Pi$ is determined by $NC(C_i, \Pi) = \sum_{j=1}^{i-1} |C_j| + 1$, i.e. the label of the cell $C_i$ (respectively of each of its vertices ) is the first vertex index in the cell, or it is greater by 1 than the number of the vertices in all cells preceding $C_i$ in the partition. $NC(x, \Pi)$ denotes the label of the cell that contains vertex $x$. This way of labeling is time saving because changing the labels of a given cell does not cause change of the labels.
of other cells.
Two cells of a partition are called *non-trivially joined* (have non-trivial join) if the number of edges between them is greater than 0 and less than maximum possible.

A channel of a cell C (new notion), denoted as Ch(C), is the number of the edges adjacent to all vertices of the cell. A channel of two cells C₁, C₂, denoted as Ch(C₁, C₂), is the number of all edges between all vertices of the two cells. Example: Let Π=|1,8|4,5|2,3,6,7|=C₁ C₂ C₃ be a partition on the vertices of the graph on fig.1. The channels of the cells are: Ch(C₁, C₁)=0, Ch(C₁, C₂)=4, Ch(C₁, C₃)=4, Ch(C₂, C₂)=2, Ch(C₂, C₃)=4, Ch(C₃, C₃)=10, Ch(C₃, C₂)=1, Ch(C₃, C₁)=5. The edges of a trivial cell adjacent to the cell C whose channel is determined are excluded from its channel, i.e. from Ch(C). For example, the cells D₅ and D₆ of the partition Π=|1|8|5|4, 6, 7|2, 3|=D₁ D₂ D₃ D₄ D₅ D₆ of the vertices of the above graph have channels Ch(C(D₅))=1, Ch(C(D₆))=1 since the edges incident to vertices from D₅ and D₆ and connected to vertices from the trivial cells D₁ D₂ D₃ D₄ are not included – only the edge (6,7) is included in Ch(C(D₅)) and (2,3) in Ch(C(D₆)).

![Fig. 1. Refinement algorithm RPB with a base cell B](image)

A channel graph of a partition Π (ChG) is an weighted graph with loops: each vertex of ChG corresponds uniquely to a cell of Π and its weight is the channel of the cell; each edge of ChG corresponds to a channel of the corresponding cells of Π and the weight of this edge is equal to the weight of this channel. Similar notion is a quotient graph in [44].

Selected non-trivial cell, SC(Π), of a partition Π is the cell Cᵢ, |Cᵢ|>1, that is selected by a defined criterion (often it is called *target cell*, for example in [12]). The procedure that finds the target cell is called *cell selector*. The selection of the target cell has strong influence on the search tree size (see the next section) and consequently, on the running time of the GA algorithms.

In algorithms Vsep, at given an equitable partition π we use the following 7 cell selectors:
1. CSL-1 (LCL_MAC in Vsep): (a) it selects the nontrivial cell C of π with maximal number of adjacent non-trivially joined cells to C, and (b) if there are several such cells it selects the first one of the smallest size;
2. CSL-2 (LCL_MAC1 in Vsep): it differs from (1) only in (b) selecting the first cell with largest size.
The partitions in the developed algorithms can be:

1. **Unit partition** (denoted by \( \Pi_0 = V = \{1, \ldots, n\} \)) - all its vertices are in one cell \( C_1 \) and the cell number is \( \text{NC}(i) = 1, i = 1, \ldots, n \).

2. **Equitable partition** - it is obtained as a result of the execution of the refinement procedure (RP) on given input partition (see the definition given above).

3. **Transformed partition** \( \Pi^T \) is obtained from a stable partition \( \Pi \) by separating from \( \text{SC}(\Pi) \) given vertex \( x \) in a singleton cell. The difference between \( \Pi^T \) and \( \Pi \) is that \( \text{SC}(\Pi) \) with cell label \( i \), is divided into two cells in \( \Pi^T \): cell \( C^i = \{x\} \) with label \( i \) containing vertex \( x \) and cell \( C''^i = \text{SC}(\Pi) \setminus \{x\} \) with label \( i+1 \) containing the other vertices of \( \text{SC}(\Pi) \). The transformation operation is denoted by \( \text{TR}: \Pi^T = \text{TR}(x, \Pi) \) and is called an **individualization** in some references.

   The output partition of RP could be:
   
   - **discrete (finite)**, when each of its cells is trivial - \( |C_j| = 1, j = 1, 2, \ldots, n \). We call it a numbering having in mind that in fact it’s a permutation that can be viewed as a graph vertices renumbering -vertex \( i \) corresponds to vertex \( x \) that is on the position \( i \) in the partition;
   
   - **intermediate (non-discrete)**, when it contains at least one non-trivial cell \( C_j, |C_j| > 1, 1 \leq j \leq n \).

The following theorem holds for the RP.

**Theorem 1**

*Given a graph \( G(V, E) \), two different equivalent partitions \( \Pi_1 \) and \( \Pi_2 \) on \( V \) under a non-trivial automorphism \( f \in \text{Aut}(G) \). Then, \( \text{NC}(x, \Pi_1) = \text{NC}(y, \Pi_2) \) for each pair \( x, y = f(x) \), where \( \Pi_a = \text{RP}(\Pi_1), \Pi_b = \text{RP}(\Pi_2) \).

In other words, RP gives output partitions where the similar vertices remain in cells with the same label.*

This theorem is equivalent to the Theorem 7.1 in [4] – for equivalent partitions under an isomorphism of two graphs and the statement that the RP is invariant under an automorphism [17]. This is the reason for not giving here the proof of the theorem.

**Corollary 1 of Theorem 1** Let \( \Pi \) be a partition on \( V \) of a graph \( G(V, E) \) with automorphism \( f \in \text{Aut}(G) \) and let for each pair of similar vertices \( x, y = f(x) \) the property \( \text{NC}(x, \Pi) = \text{NC}(y, \Pi) \) holds. Then, \( \text{NC}(x, \Pi_a) = \text{NC}(y, \Pi_b) \), where \( \Pi_a = \text{RP}(\Pi) \).

Corollary 1 means that the similar vertices in any cell of a given input partition remain in one cell of the resulting partition of RP.
Proof Let $\Pi=\Pi_1=\Pi_2$ in theorem 1. Then, we obtain $\Pi_3=\Pi_4=\Pi_5=\Pi_6=\Pi_7$ and $NC(\Pi_3)=NC(y,\Pi_3)$ is obtained by replacing $\Pi_3$ in $NC(\Pi_3)=NC(y,\Pi_3)$. ♦

Corollary 2 of Theorem 1 The refinement procedure $RP$ is invariant under the vertex orbits of a subgroup $H \subset A = Aut(G(V,E))$: if $Orb(x,H) \subseteq C(x,\Pi)$ for each vertex $x \in V$ of a given partition $\Pi$, then $Orb(x,H) \subseteq C(x,\Pi)$ for a partition $\Pi_{L}=RP(\Pi)$. (In other words, if each orbit of a given automorphism subgroup is a subset of a cell of the input partition $\Pi$, then the same is true for the output partition $\Pi_{L}=RP(\Pi)$. Obviously, this corollary holds for any stabilizer $A(x_{1},x_{2},...,x_{i})$ of the automorphism group.)

Proof The condition $Orb(x,H) \subseteq C(x,\Pi)$ means that $NC(\Pi_{x})=NC(y,\Pi_{x})$, $y=f(x)$ for each $f \in H$, i.e. the condition of Corollary 1 of Theorem 1 holds for each $f \in H$ and from it follows $NC(\Pi_{x})=NC(y,\Pi_{x})$, $y=f(x)$ for each $f \in H$, i.e. $Orb(x,H) \subseteq C(x,\Pi_{x})$. ♦

Corollary 3 of Theorem 1 $Orb(x,A) \subseteq C(x,\Pi_{1})$ holds for each vertex $x \in V$ of the initial partition $\Pi_{1}=RP(\Pi_{u})$ of the graph $G(V,E)$ where $\Pi_{u}$ is the unit partition.

Proof Let $H=A$ and $\Pi=\Pi_{u}$ for which obviously $Orb(x,A) \subseteq C(x,\Pi_{u})$. Then, $Orb(x,A) \subseteq C(x,\Pi_{1})$ follows from Corollary 2 where $\Pi_{1}=\Pi_{L}=RP(\Pi_{u})$. ♦

3. Auxiliary algorithms

3.1. Algorithm A1 for determining one discrete partition

The output of algorithm A1 (algorithm with successive selections of vertices) is a series of better partitions the last of which is discrete on given input partition $\Pi$. Using A1 we introduce new notions and prove a property used for speeding up our algorithms.

The following basic operations are performed in the algorithm A1: \{ $\Pi_{1}=RP(\Pi_{1}, L=1);$ \} determine $SC(\Pi_{L})$ by some cell selector; select any vertex $x_{L}$ in the $SC(\Pi_{L})$; $L:=L+1$; $\Pi_{L}:=IR(\Pi_{L-1}, X_{L-1})$; $L:=2, \ldots, LK$, where $\Pi_{LK}$ is discrete and $LK<n$.

Given any input partition $\Pi$ the initial partition $\Pi_{1}=RP(\Pi_{u})$ is determined first. In most cases we’ll consider that the starting input partition $\Pi_{1}$ is the unit partition, $\Pi_{1}=\Pi_{u}$.

A selection level is called the successive number $L$ of the refinement procedure $RP$ calls for obtaining the partition $\Pi_{L}$ in the algorithm A1. $\Pi_{L}:=\Pi(x_{1},x_{2}, \ldots, x_{L-1})$ denotes the partition that is obtained by making $L-1$ selections $x_{1},x_{2}, \ldots, x_{L-1}$ starting with the partition $\Pi_{1}$. The selected non-singleton cell in partition $\Pi_{L}$ is denoted by $SC(\Pi_{L})$ or $SC(x_{1},x_{2}, \ldots, x_{L-1})$. Five operations (rows 4, 5) are executed in the loop C: determining $SC(\Pi_{L})$, a selection of vertex $x_{L}$ in $SC(\Pi_{L})$, a move to next level (a forward move, $L+1$), obtain the transformed partition $\Pi_{T}:=TR(x_{L},\Pi_{L})$, $\Pi_{L}:=RP(\Pi_{L})$ (refinement with $RP$) – the last two operations are IR. Obviously, $\Pi_{L}$ is a stable partition. The determination of $SC(\Pi_{L})$ is made by some cell selector. This execution continues until a discrete partition $\Pi_{LK}$ is obtained – its level of selection $LK$ is called terminal or final. The process of obtaining the sequence $\Pi_{1}, \Pi_{2}, \ldots, \Pi_{LK}$ is called series of forward moves (SFM).

There is a class of connected graphs (we call it CLASS6) such that each graph from it holds the following property: The maximal value of $L$, $L_{max}$, in algorithm A1 for any graph from CLASS6 with number of edges $k \equiv n(n-1)/4$ is 6. (Shortly $L_{max}=6$).

Large set of graphs including the graphs of the projective planes hold this requirement. All experiments on thousands of graphs confirm this. We should note that this property holds only if the determination of $SC(\Pi_{L})$ (step 4) is done by some of the cell selectors described above. The property does not hold even for graphs of CLASS6 if the $SC(\Pi_{L})$ is the leftmost non-trivial cell – in this case $L_{max}$ is 37 for the graphs of projective planes of order 16.

Each partition $\Pi_{L}$, $L=1, 2, \ldots, LK$ is called a partition-child of $\Pi_{L-1}$ (partition-parent) and a successor of each of the partitions $\Pi_{L-1}, \Pi_{L-2}, \ldots, \Pi_{1}, \Pi_{0}$ (partitions-ancestors of $\Pi_{L}$).
The selected cells SC(L), L=1, 2, ..., L-1 for a given partition ПL are called supporting SC for ПL, and the selected vertices x1, x2, ..., xL-1 of ПL are called supporting vertices (or points) or a base of ПL.

A search tree (ST) is an oriented tree whose root represents the initial partition П1 = RP(П). Each node of the search tree corresponds to an equitable partition ПL. Each arc coming out of a vertex ПL corresponds to a selected vertex from the SC(ПL). Thus, the partition ПL+1 of a particular node q on a level L+1 could be obtained from the partition ПL (node p on a level L) by selecting a vertex x ∈ SC(ПL), x being depicted on the edge p-q in ST. Let r = |SC(ПL)|, then each node ПL = Π(x1, x2, ..., xL-1) with SC(ПL) = {a1, a2, ..., aL} has r nodes-children of level L+1: Π(x1, x2, ..., xL-1, a1), Π(x1, x2, ..., xL-1, a2), ..., Π(x1, x2, ..., xL-1, aL). Thus, each vertex in each SC(ПL), for each level L is selected in ST.

The just described search tree may be called full search tree in contrast to the reduced search tree RST, in which some vertices from SC(ΠL) are not selected according to a certain criterion. In the reduced search tree, for each orbit of a stabilizer AΛ := A(x1, x2, ..., xL-1) only one representative of the orbit (AΛ-1)εSC(ПL) is selected – this is the first orbits vertex met during the traversal of the SC(ΠL). This way of a selection of vertices is used in the algorithms Vsep. It is based on the theorems proved below.

The reduced search tree used in the algorithms Vsep is not explicitly presented in the algorithm – only the partitions of the path from the root to the current ПL are stored, i.e., the sequence П1, ..., ПL.

3.2. Algorithm A2 for generating the full search tree
Algorithm A2 (Fig. 3) generates all partitions of the search tree on a given partition П of graph G(V,E) and the selection of a vertex X1 ∈ SC(L) of the initial partition П1 = П. The leaf nodes of ST are discrete partitions. A new partition ПL (a new node of ST) is obtained after each execution of the instruction 10. In A2, each of the vertices in every SC(ПL) is successively selected and after that the algorithm continues with a forward move until a discrete partition is obtained. There are two loops in A2: the loop C1 (lines 4-15) performs a forward move and the loop C2 (lines 9-13) performs the backward move. In the forward move, as in the A1, we begin from the partition Пi (on a level L) and selected vertex xεSC(ΠL), and we obtain successively the partitions ПL+1, ПL+2, ..., ПLk (discrete). The backward move (L:=L-1) is made when all vertices in the SC(L) are selected.

We introduce a new notion – a level of the last backward move, denoted by LP and meaning the last value assigned to L by the instruction 10 (L:=L-1), i.e. LP is the level to which the last backward move is made. We call LP a working level and SC(ΠLP) - a working cell since the main operations of the algorithms are with the vertices in SC(ΠLP). The level LP is a significant notion for the algorithm Vsep-e. A sequence of forward moves (SFM) starts from the level LP. In fact, the algorithm A2 (as well as algorithm Vsep-e) generates the search tree in preorder – first visiting the root (a vertex εSC(ΠL)) then visiting the subtree of each vertex εSC(ΠL+1) from left to right [1,2].

A bouquet B(x1) or B(x1, x2, ..., xL) of a selected vertex x1εSC(ΠL) is called the set of all mutually non-equivalent discrete partitions derived from the partition ПL and the selection x1, i.e. obtained from П(x1, x2, ..., xL) = ПL+1. Only the first numbering obtained by the algorithm Vsep-e is stored from the set of equivalent discrete partitions and is used as a representative in B(x1). The bouquet B(x1, x2, ..., xL) consists of the bouquets of the orbits representatives of vertices in the SC(ΠL+i), i.e. it consists of the bouquets B(x1, x2, ..., xL, aL+i1), B(x1, x2, ..., xL, aL+i2), ..., B(x1, x2, ..., xL, aL+ip), where aL+i1, aL+i2, ..., aL+ip are...
Applying the corollary for \( L=1 \) we have \( f(x)=x \). Since both the base and the inductive step have been proved, it has now been proved by mathematical induction that \( NC(x, \Pi_L) = NC(y, \Pi_L) \) holds for all vertices \( x, y \in V \) of the graph \( G(V,E) \).

**Theorem 2** Given a graph \( G(V,E) \), a partition \( \Pi \) on \( V \), an automorphism \( f \in \text{Aut}(G, \Pi) \), \( NC(x, \Pi) = NC(y, \Pi) \) for each pair \( x, y=f(x) \) (a property of equal cell labels for each pair of similar vertices), two partitions \( \Pi_I=\Pi(a_1, a_2, \ldots, a_i, \ldots) \), \( \Pi=P(b_1, b_2, \ldots, b_i, \ldots) \) obtained by 2 series of executions of the algorithm A1 on the input partition \( \Pi \) and \( NC(a_i)=NC(b_i) \) for each pair \( x_i=f(a_i) \), \( i=1,2, \ldots, L-1 \) (equal cell labels of corresponding supports). Then, \( NC(x, \Pi_I) = NC(y, \Pi_I) \) for each pair \( x, y=f(x) \), \( x \in \Pi_L, y \in \Pi_L \) (the property holds for each pair of similar vertices).

**Proof** (by mathematical induction): 1. The base case: By assumption the property \( NC(x, \Pi_0) = NC(y, \Pi_0) \) holds for \( \Pi_0 \) and therefore it holds for \( \Pi_1=\Pi_0=RP(\Pi_0) \) as well (according to Corollary 1 of Theorem 1). In particular, \( NC(a_1, \Pi_1)=NC(b_1, \Pi_1) \).

2. The inductive step: Let the property holds for \( \Pi_I \): \( NC(x, \Pi_{I-1}) = NC(y, \Pi_{I-1}) \) for each pair \( x, y=f(x) \).

For \( \Pi_I^T \) in \( \Pi_I^T \), the property \( NC(x, \Pi_{I-1}^T) = NC(y, \Pi_{I-1}^T) \) holds since: supposedly \( NC(a_{i-1})=NC(b_{i-1}) \) for \( a_{i-1}, b_{i-1} \in f(a_{i-1}) \) is true. For all other vertices of the cells \( C(a_{i-1}) \) and \( C(b_{i-1}) \) the cell labels are equal: \( NC(a_{i-1})=NC(b_{i-1}) \). For the vertices \( x, y \in \Pi_{I-1} \) there is no change of cell labels. Hence, according to Corollary 1 of Theorem 1 the property also holds for \( \Pi_I=RP(\Pi_{I-1}^T) \). \( NC(x, \Pi_I) = NC(y, \Pi_I) \) holds since both the base and the inductive step have been proved, it has now been proved by mathematical induction that \( NC(x, \Pi_L) = NC(y, \Pi_L) \) holds for all vertices \( x, y \in \Pi_L \).

**Corollary of Theorem 2** Given a partition \( \Pi_L=\Pi(x_1, x_2, \ldots, x_{L-1}) \). Then, \( \text{Orb}(x, A_{L-1}) \subseteq C(x, \Pi_L) \) for each vertex \( x \in V \) of the graph \( G(V,E) \), \( L=1, \ldots, LK \). (In other words, the orbits of \( A_{L-1} \) are subsets of the cells of \( \Pi_L \)).

**Proof** Let \( b_i=a_i \), \( i=1,2, \ldots, L-1 \) in Theorem 2. Then, these \( L-1 \) vertices will be fixed points of automorphism \( f \) and \( \Pi_L=\Pi_L \). From \( NC(x, \Pi_L) = NC(y, \Pi_L) \) for each pair \( x, y=f(x) \) for each \( f \in A_{L-1}=A(a_1, a_2, \ldots, a_{L-1}) \) follows \( \text{Orb}(x, A_{L-1}) \subseteq C(x, \Pi_L) \).

Applying the corollary for \( L=1 \) we have \( \text{Orb}(x, A_0) = \text{Orb}(x, A(\Pi)) = C(x, \Pi_I) \). Applying it to \( L=LK \) we obtain \( \text{Orb}(x, A_{L-1}) \subseteq C(x, \Pi_L) \) and \( |\text{Orb}(x, A_{L-1})| = C(x, \Pi_L) | = 1 \) since \( \Pi_{LK} \) is discrete, i.e., \( |\text{Orb}(x, A_{L-1})| = 1 \).
Theorem 3  Given a graph \( G(V,E) \), \( n=|V| \), an automorphism \( f\in\text{Aut}(G) \) with fixed points \( a_1, a_2, ..., a_{j-1} \) and a partition \( \Pi=\Pi(a_1, a_2, ..., a_{j-1}) \), obtained after \((j-1)\) successive selections \( a_1, a_2, ..., a_{j-1} \) of the algorithm \( A1 \) with starting input partition \( \Pi_0 \) and vertices \( p, q\in SC(\Pi_0)\), \( q=f(p) \).

Then, each numbering

\[ \Pi'=\Pi(a_1, a_2, ..., a_{j-1}, p, a_{j+1}, a_{j+2}, ..., a_{|L_{K-1}|})=|x_1| |x_2| \ldots |x_i| \ldots |x_n|, \]

derivative of \( \Pi(a_1, a_2, ..., a_{j-1}, p) \) has a corresponding numbering

\[ \Pi''=\Pi(a_1, a_2, ..., a_{j-1}, q, b_{j+1}, b_{j+2}, ..., b_{|L_{K-1}|})=|y_1| |y_2| \ldots |y_i| \ldots |y_n|, \]

derived from \( \Pi(a_1, a_2, ..., a_{j-1}, q) \), such that \( y_i=f(x_i), i=1, 2, ..., n \) and \( NC(x_i, \Pi') = NC(y_i, \Pi'') \).

(Note: There is an equivalent theorem of B. McKay - Theorem 7.2 in [12]).

Proof Let us consider two executions (labeled I and II) of the algorithm \( A1 \) for graph \( G(V, E) \) with starting input partition \( \Pi \). The first \( j-1 \) selections \( a_1, a_2, ..., a_{j-1} \) are equal for both executions and the resulting partitions are equal to \( \Pi_j \). Under the conditions of the theorem, there are vertices \( p, q=f(p) \) in the cell \( SC(\Pi_j) \).

Let the \( j^{th} \) selection be \( p \) in the first execution, and the \( j^{th} \) selection be \( q \) in the second execution, i.e. the obtained partitions are: for execution I – \( \Pi=\Pi(a_1, a_2, ..., a_{j-1}, p) \), for execution II – \( \Pi''=\Pi(a_1, a_2, ..., a_{j-1}, q) \), for which the conditions of Theorem 2 hold: \( a_i=f(a_i) \) for \( i=1, 2, ..., j-1 \) and \( q=f(p) \). Therefore, according to Theorem 2, the similar vertices are in cells with the same label, and thus the vertex \( a_{j+1} \) in \( SC(\Pi_j) \) will correspond to the vertex \( b_{j+1}=f(a_{j+1}) \) in \( SC(\Pi_{j}) \).

So, the selection \( a_{j+1} \) is possible in execution I and the selection \( b_{j+1}=f(a_{j+1}) \) is also possible in execution II. The conditions of Theorem 2 also hold for these selections and at the \((j+2)^{th}\) selection similar vertices can be selected again, i.e. \( a_{j+2} \) in the execution I and \( b_{j+2}=f(a_{j+2}) \) in the execution II. This process continues until the last selections \( a_{|L_{K-1}|}, b_{|L_{K-1}|}=f(a_{|L_{K-1}|}) \) in both executions have been done – after these selections the partitions will be discrete. This means that each numbering

\[ \Pi(a_1, a_2, ..., a_{j-1}, p, a_{j+1}, a_{j+2}, ..., a_{|L_{K-1}|})=|x_1| |x_2| \ldots |x_i| \ldots |x_n|=\Pi' \]

has corresponding numbering

\[ \Pi(a_1, a_2, ..., a_{j-1}, q, b_{j+1}, b_{j+2}, ..., b_{|L_{K-1}|})=|y_1| |y_2| \ldots |y_i| \ldots |y_n|=\Pi'' \],

such that

\[ NC(x_i, \Pi') = NC(y_i, \Pi'') \], \( i=1, 2, ..., n \).

There are four obvious corollaries of Theorem 3:

Corollary 1 of Theorem 3  Under the conditions of Theorem 3 the discrete partitions of type \( \Pi'' \), successors of the partition \( \Pi(a_1, a_2, ..., a_{j-1}, q) \), do not find new automorphisms (new similar vertices). Consequently, it is not necessary to determine them if we preliminarily know the discrete partitions of type \( \Pi' \) - successors of the partition \( \Pi(a_1, a_2, ..., a_{j-1}, p) \).

Corollary 2 of Theorem 3  The bouquets of two similar vertices in a given \( SC(\Pi_{j}) \) are of the same size.

This statement is obvious because to each numbering of the one bouquet uniquely corresponds a numbering of the other bouquet.

Corollary 3 of Theorem 3  To determine whether two vertices \( X \) and \( Y \) in \( SC(\Pi_{j}) \) are similar we need to know the bouquet of one of the vertices, say \( B(L, X) \), and generate one numbering \( n_1 \) derived of a selection \( Y \) in \( SC(L) \) and compare \( n_1 \) with the numberings \( \epsilon B(L, X) \). Even more, \( B(L, X) \) should not contain equivalent numberings because of the transivity of the equivalence: if \( n_1 \) is equivalent to one of them it is equivalent to the another.

Corollary 4 of Theorem 3  The bouquet \( B(L, X) \) contains all bouquets derived from each representitave of an orbit in \( SC(\Pi_{L+1}) \).
Important conclusions follow from Theorem 3 and its corollaries. There are three possibilities to determine whether two vertices \( X \) and \( Y \) in \( SC(\Pi_1) \) are similar under \( A(x_1, \ldots, x_{l-1}) \):

(a) The bouquet \( B(L, X) \) of the vertex \( X \) should be stored and for the vertex \( Y \) we should generate only one numbering and compare it with the numberings \( \in B(L, X) \) - this version is used in algorithm Vsep-e.

(b) One numbering should be stored for vertex \( X \) and the whole bouquet for vertex \( Y \) should be generated. This version is used in Nauty [12] and in the most of the known algorithms;

(c) Two bouquets \( B(L, X) \) and \( B(L, Y) \) are partially generated and their numberings are compared for determining an automorphism (with a certain probability) that maps \( X \) to \( Y \). This probability might be near to 1 if we choose an appropriate selection of the bouquets size. This is the basis for the heuristic algorithms described in Section 5.

Let’s compare versions (a) and (b) (Table 1). Let \( m=|B(L, X)| \) and let’s consider that the numberings of the bouquets are stored in a hash table with a maximum number \( c \) of collisions of some hash function (characteristic of the numbering) we’ll explain below. Let’s also consider the worst-case – a rigid regular graph for \( L=1 \) and \( |SC(\Pi_1)|=q \) – in this case all vertices in \( SC(\Pi_1) \) are not similar each other. This is the worst-case since: (i) for \( L=1 \) the bouquets have the larger size than the bouquets for \( L>1 \) and (ii) the bouquets for rigid graphs are full – each vertex at each level is selected. The advantage of version (b) is a low storage – only one numbering is stored and the disadvantage of version (a) is the large required storage – the whole bouquet of size \( m \) for the first vertex \( x_1 \in SC(\Pi_1) \) is stored. Version (a) is faster since the number of the generated numberings is smaller: \( NG=m+q-1 \). In this case the bouquet of the first vertex \( x_1 \in SC(\Pi_1) \) is generated and stored and for each of the other \( q-1 \) vertices only one numbering is generated - totally \( NG=m+q-1 \). In case of version (b) for each vertex \( x \in SC(\Pi_1) \) all \( m \) numberings of bouquet \( B(I, x) \) are generated, i.e. \( NG=m.q \). We suppose that the size of each bouquet is \( m \) or \( m \) is the largest size. Since \( m.q >> m+q-1 \) version (a) is many times faster than version (b). The number (\( NC \)) of the comparisons of numberings is \( c.m(q-1) \) for both versions. In version (a) one numbering for each vertex in \( SC(1) \) is compared with \( c.m \) numberings of \( B(X_1) \). In version (b) the only stored numbering \( n_1 \) derived from the selection \( X_1 \) is compared with \( c.m \) numberings of each bouquet \( B(X), x \in SC(1), x \neq x_1 \).

| version | NS-number of stored numberings | NG-number of generated numberings | \( NC \) - number of comparisons of numberings |
|---------|--------------------------------|---------------------------------|--------------------------------------------|
| a       | \( m \)                        | \( m+q-1 \)                      | \( c.m(q-1) \)                              |
| b       | \( 1 \)                        | \( m+m(q-1) = q.m \)             | \( c.m(q-1) \)                              |

Table 1

Examples:
- Graph A29_1 (rigid regular graph from [24]): \( n=29, m=14 \) (this size is for each vertex in \( SC(\Pi_1) \), \( q=n=29; \) \( NG(a)=m+q-1=42, NG(b)=q.m=29.14=406 \) (in the brackets is the number of the version). We see the big difference between the numbers of generated numberings of the two versions.
- Graph G1275 (Rigid affine plane of order 25, received from R. Mathon in private communication):
  \( n=1275, \) bipartite graph with \( k=625*26=650*25=16250; m=8322060; q=625; NG(a)=m+q-1=83232060+625-1=83232684; NG(b)=q.m=625*8322060=5201287500. \) In this case the difference between \( NG \) (a) and \( NG \) (b) is impressive. The run time of version (a) for this graph is 9034.23 seconds for example and for version (b) should be approximately 625*9034.23 seconds = 65.35 days.

4. The exact algorithm Vsep-e
4.1. Basics of the algorithm
We need the following theorem for the reasoning of the algorithm Vsep-e.

**Theorem 4** Given: \( A=Aut(G(V,E)) \), an orbit \( Q=Orb(x_1,A) \) of vertex \( x_1 \in V \) and a generating set \( gen(A(x_1)) \) of a stabilizer \( A(x_1) \). Then, there is a tower of ascending subgroups of \( A \)
A(x_1)=A^{(i)} \subset A^{(2)} \subset \ldots \subset A^{(i)} \subset \ldots \subset A^{(m)}=A, such that: (a) A^{(i)} is a proper subgroup of A^{(i+1)}, 1 \leq i \leq m-1; (b) \text{gen}(A^{(i)})=\{ \text{gen}(A^{(i-1)}), \alpha_i \}, 2 \leq i \leq m, where the automorphism \alpha_i is such that (c) x_i=\alpha_i(x_1); (d) Orb(x_i, A^{(i)})\subset Orb(x_1, A^{(i)}); (e) Orb(x_1, A^{(i)}) \neq Orb(x_i, A^{(i)}); (f) |A^{(i)}| \geq 2, |A^{(i+1)}|, 2 \leq i \leq m; (g) \text{Orb}(x_i, A^{(i)}) \supseteq \text{Orb}(x_1, A^{(i)})\} |Orb(x_1,A^{(i)})|, 2 \leq i \leq m; (h) m is the minimal value of i such that \text{Orb}(x_i, A^{(m)})=Q. [Note: Evidently, the consequence of (b) is \text{gen}(A)=\text{gen}(A^{(m)})=\{\text{gen}(A(x_1)), \alpha_2, \alpha_3, \ldots, \alpha_m\}]

**Proof** (inductive, it follows the proof of Theorem 5 in [10]). Let’s construct a tower of ascending subgroups of A: \text{A(x_1)}=A^{(i)} \subset A^{(2)} \subset \ldots \subset A^{(i)} \subset \ldots \subset A^{(m)}=A, such that \text{A^{(i)}} is a proper subgroup of A^{(i+1)}, i=1, 2, \ldots, m-1; m is finite since A is a finite group. For i=1 we have \text{A^{(1)}}=A(x_1) and \text{gen}(A^{(1)})=\text{gen}(A(x_1)) is known. Assume inductively that \text{A^{(i)}} is a proper subgroup of A and let we have orbits Q=\text{Orb}(x_1, A^{(i-1)})\not\subset Q=\text{Orb}(x_i, A^{(i-1)}), Q', Q''\subset Q. Then, we’ll have an automorphism \alpha_i \in A^{(i-1)} such that x_i=\alpha_i(x_1) and \text{Orb}(x_i, \text{gen}(A^{(i)})) \supseteq Q' \cup Q''. Thus, \alpha_i is a generator of A and \text{A^{(i)}} since it does not belong to \text{A^{(i-1)}}, i.e. \text{gen}(A^{(i)})=\text{gen}(A^{(i-1)}) \cup \alpha_i and therefore \text{A^{(i)}} \supseteq \text{A^{(i-1)}} (since a new coset appear in the partitioning of A^{(i)} into cosets of A^{(i-1)} and \text{Orb}(x_1, \text{A^{(i)}}) \geq 2, |\text{Orb}(x_1, \text{A^{(i)}})| (from the Theorem ‘orbit-stabilizer’: |A^{(i)}|=|\text{Orb}(x_1, A^{(i)}), |A(x_1)|} and |A^{(i)}|=|\text{Orb}(x_i, A^{(i)}), |A(x_1)|}). The first value of i when \text{Orb}(x_1, \text{gen}(A^{(i)}))=Q and \text{A^{(i)}}=\emptyset is i=m and consequently \text{gen}(A)=\text{gen}(A^{(m)})=\{\text{gen}(A(x_1)), \alpha_2, \alpha_3, \ldots, \alpha_m\}.

Theorem 4 gives us the idea how to find the generators of a group if we know an orbit Q of the group and the generators of a stabilizer of a representative x_1 of this orbit. This is done by traversing the orbit step by step. At each step we find one new generator of a new subgroup of A knowing the generators and the orbits of the previous subgroup of A. Before the first step the previous subgroup is equal to A(x_1) with its orbits and generators. Visiting each vertex x of the orbit, \text{x_1} \not\in \text{x}, we select x only if x is not similar to x_1 under the previous subgroup. Thus a new automorphism-generator that maps x to x_1 and new orbits for a new subgroup are found. The new subgroup is a proper supergroup of the previous subgroup. Let us consider the orbit Q as an ordered set whose first vertex is x_1 and let \text{i(x)} denote the position of vertex x in the orbit Q. At each step the generators, orbits and order of the current group A (subgroup of A) are defined by the position of the selected vertex x, i.e. by the subset S(i(x)) of the orbit including the vertices from the beginning of the orbit to the x. S(i(x)) is the subset of the visited vertices. This process stops when the orbit of x_1 under the new subgroup becomes equal to the given orbit Q. The described process is presented in Table 2. The selected vertex x_i, i=2, \ldots, m is the first vertex after x_i-1 in Q that is not similar to x_1 under A^{(i-1)}. The position of x_i is i(x_i) \geq i(x_i-1). The generators of A(x_i) are called proper generators of A and the generators \alpha_2, \alpha_3, \ldots, \alpha_m are mutual generators of A. The following corollary is obvious:

**Corollary of Theorem 4** The number of the mutual generators of the graph automorphism group A toward the stabilizer A(x_1) is m-1=\log_2(\text{Orb}(x_1, A)]. Actually, Theorem 4 tell us that there is a generator x_i=\alpha_i(x_1) if x \not\in x_1 is not similar to x_1 under the current group but according to Theorem 3 to determine this generator we should know the bouquet \text{B(x_1)} and one numbering derivative of x and to compare them. Knowing the partition \text{P(x)} and \text{SC(P(x))} according to Theorem 4 to traverse the orbit Q we should traverse the SC(P(x)). Thus, we come to the idea of the Algorithm A3 (Fig. 4). We denote by \text{FRPO(X)} – all first representatives of the orbits of A positioned in \text{SC(P(x))} before the selected vertex X and by \text{BFROPO(X)} – the bouquets of \text{FRPO(X)}. Algorithm A3 determines \text{GOO(A)} of the graph automorphism group A=\text{Aut(G, P)} and the bouquet of each representative of an orbit \text{Orb}(A) \in \text{SC(P(x))} given \text{GOO(A(XF))} of a stabilizer A(XF) of a vertex XF \in \text{SC(P(x))} and the bouquet B(XF). Vertex XF is one of the root of the bouquets found so far, the vertices \text{Orb}(XF,A) are after XF in \text{SC(P(x))}. Thus we’ll traverse the orbit \text{Orb}(XF, A) traversing \text{SC(P(x))} since \text{Orb}(XF, A) \subset \text{SC(P(x))}. The bouquets \text{BFROPO(XF)} are known, i.e., the bouquet of each first representatives y of an orbit of \text{Orb}(A) in \text{SC(P(x))} with index i(y)<i(XF). Each representative y or XF has no similar vertices in a position in \text{SC(P(x))} before it.
According to Theorem 3 and 4 we’ll determine GOO(A) and the bouquet of each representative of an orbit
Orb(A) ∈ SC(Π_i) visiting each vertex x ∈ SC(Π_i) positioned after XF. Before the traversal of SC(Π_i) we
have GOO(A)=GOO(A(XF)). Each visited vertex x ∈ SC(Π_i) is selected if it is not similar to any previous
vertex x ∈ SC(Π_i) under the current group A. Then, we determine if there is an automorphism \( \alpha, x=\alpha(y), \)
where y is one of the roots FRPO(x). This is made (according to Theorem3) by comparing the first
numbering \( \Pi_{LK} \) derived from the selection x with the numberings \( \in \) BFRPO(x). Two cases are possible: (a)
If there is an automorphism \( \alpha \) then it belongs to a new subgroup of A since it unites the orbits of x and XF,
i.e., gen(A) = gen(A) \cup \{ \alpha \}; (b) If \( \Pi_{LK} \) is not equivalent to any numbering \( \in BFRPO(x) \) then x becomes a representative of a new orbit and a new search tree ST(x) is built - it determines gen(A(x)) and B(x). If
during the generation of ST(x) an automorphism is discovered and if it unites the orbits of A then, it is
also a generator for A since A(x) ⊆ A. Thus, in case (b) the number of the known bouquets of vertices
positioned before x increases by one and for the next selected vertex we should compare the numbering
\( \Pi_{LK} \) derived from the selection of x with the numberings of all known bouquets.
To determine the orbit of the vertex XF it is sufficient to do the above comparison only with the bouquet
B(XF) but we do this comparison with the numberings of all bouquets of FRPO(X) since we store them
and the earlier finding of a generator is better since we can use it earlier. If the found automorphism \( \alpha, \)
x=\( \alpha(y), y \neq XF \) unites orbits of the current A it is a generator of A.
After each of both cases has been handled the traversal of SC(Π_i) continue by selection of a new vertex x.
Thus, after the traversal of SC(Π_i) all vertices ∈ Orb(XF, A) will be visited and the bouquet of each first
representative \( x_i \in SC(\Pi_i) \) of an orbit of A and GOO(A) will be determined (according to Theorem 4).
During the execution of this algorithm we build implicitly (as in Theorem 4) a tower of ascending
subgroups of A: \( A(xI)=A^{(0)} \subset A^{(1)} \subset \ldots \subset A^{(i)} \subset \ldots \subset A^{(m)}=A \), such that \( A^{(i)} \) is a proper subgroup of \( A^{(i+1)} \),
\( 0 \leq i < m-I \).
Algorithm A3 can be applied for determining any GOO(A(X_{L-1})) and B(X_{L-1}), L=1, \ldots, LK under the
following requirements:
R1. GOO(A(XF_{L})), B(XF_{L}), \Pi_{L}, SC(\Pi_{L}) are known for a vertex XF_{L} ∈ SC(\Pi_{L});
R2. The position of the vertex XF_{L} in SC(\Pi_{L}) is such that it has no similar vertices under A(X_{L-1})) with a
position before it. This means that Orb(X_{L-1}, A(X_{L-1})) in SC(\Pi_{L}) is after XF_{L}, i.e. the vertices of the orbit
Orb(XF_{L}, A(X_{L-1})) should be with higher indices in SC(\Pi_{L}). Evidently, this condition holds when XF_{L}
is the first vertex in SC(\Pi_{L}). Thus, traversing SC(\Pi_{L}) we’ll traverse Orb(X_{L-1}, A(X_{L-1})) – this is the
requirement of Theorem 4;
R3. The bouquets BFRPO(XF_{L}) are known (if any);
R4. The first selected vertex is with index $i(x_F)+1$.

**Input:** a graph $G$; a partition $II=RP(II)$ for a given input partition $II$; $SC(II)$; $\alpha$ a vertex $XF \in SC(II)$ and its index $j$ in $SC(II)$; $GOO(XF)$: the generating set $gen(A(XF))$ of a stabilizer $A(XF)$, the orbits of $A(XF)$ and $|A(XF)|$ and the bouquet $B(XF)$; the bouquets $BFRPO(XF)$, i.e., the bouquet of each first representative $y$ of an orbit of $\text{Orb}(A)$ in $SC(II)$ with index $i(y)<i(XF)$; each representative $y$, $XF$ has no similar vertices in a position in $SC(II)$ before it.

**Output:** The generators, the orbits and the order (shortly GOO) of the graph automorphism group $A=\text{Aut}(G, II)$; the bouquet of each representative of an orbit of $A$ in $SC(II)$.

1. orbits of $A:=\text{orbits of } A(XF)$; $\text{gen}(A):=\text{gen}(A(XF))$;
2. $x:=x_i$;
3. do
4. select next $x \in SC(II)$; if there is no selected vertex $x$ then exit;
5. determine a numbering $n1$ by $\text{SFM}(x)$;
6. compare the numbering $n1$ with the numberings of the $BFRPO(x)$;
7. if $n1$ is equivalent to some numbering from $BFRPO(x)$, i.e. there is new automorphism $\alpha$ mapping $x$ to some vertex from $\text{FRPO}(x)$ then
8. $\text{gen}(A):=\text{gen}(A)\cup\alpha$; recompute the orbits of $A$; $|A|:=|\text{Orb}(XF)||A(XF)|$
9. else {$n1$ is not equivalent to any numbering from $BFRPO(x)$, i.e. there is no new automorphism mapping $x$ to some vertex from $\text{FRPO}(x)$}
10. build the search tree $ST(x)$ for determining $\text{GOO}(A(x))$ and the bouquet $B(x)$
11. end; {if}
12. enddo

**Fig. 4.** Algorithm A3

Algorithm A3 has a simplified version A3A that determines the mutual generators, the orbits and the order of the stabilizer $A(X_{L,i})$ and the bouquet of each representative of an orbit of $A(X_{L,i})$ in $SC(II)$ given a vertex $X_{F_L}\in SC(II)$ for which the bouquet $B(X_{F_L})$, the orbits $\text{Orb}(A(X_{F_L}))$, the order $|A(X_{F_L})|$ of a stabilizer $A(X_{F_L})$ and the bouquets $BFRPO(X_{F_L})$ are known.

4.2. The algorithm: cases CS1, CS2, CS3 and CS4

Let we have the starting series $\text{SFM}1$: $\Pi_1$, $\Pi_2$, . . . , $\Pi_{L_K}$. We can apply Algorithm A3 directly only to the partition $\Pi_{L_K}$ because for the other partitions the required input variables are not known. For the partition $\Pi_{L_K-1}$ we have $B(x_{L_K-1})=\Pi_{LK}$ and $\text{gen}(A(x_{L_K-1}))=\emptyset$, i.e., $|A(x_{L_K-1})|=1$ and discrete orbits of $A(x_{L_K-1})$. After the application of A3 to $\Pi_{L_K-1}$ we have determined correctly $B(X_{L_K-2})$ and $\text{gen}(A(x_{L_K-2}))$, the orbits and the order of $A(x_{L_K-2})$. Then, A3 can be applied to $\Pi_{L_K-2}$, i.e., a backward move is done from $L_K$ to $L_K-2$. Thus, applying A3 to the series $\Pi_{L_K-1}$, $\Pi_{L_K-2}$, . . . , $\Pi_2$, $\Pi_1$ we can determine $\text{GOO}(A)$. The lowest level to which a backward move has been made we denote by $\text{LMIN}$, i.e., $\text{LMIN}$ is the level for which we determine $\text{GOO}(A(X_{LMIN-1}))$. In Algorithm A3 the process of the backward moves is not included and the instruction 10 is not revealed. All this is taken into account in the algorithms PART1 and PART2 (Fig. 6 and 7, respectively) called from the main algorithm Vsep-e (Fig. 5) that determines $\text{GOO}(A)$ of the partition-wise stabilizer $A=\text{Aut}(G, II)$ given a graph $G(V,E)$ and the input partition $II$ on $V$. S3. Before calling PART1 and PART2 the algorithm Vsep-e determines (step S2) the orbits of $A$ by the heuristic algorithm $\text{HEURAUT}$ and select $X_1 \in SC(\Pi_1)$ as a representative of one of the smallest orbit of the vertices in $SC(\Pi_1)$. Experimental tests (Table 3) show with very rare exceptions that if the staring vertex $X_1$ is a representative of one of the smallest orbit of $A$ then the size of the bouquet $B(X_1)$ built by PART1 is the smallest and the running time is minimal. There are two exceptions from this rule in the table: $X_1=53$ and 534; $X_1=539$ and 273 for the graph DSFP. The algorithm PART1 (Fig. 6, the first part of the algorithm Vsep-e, line S4 in Fig. 5) can be considered as an application of the algorithm A3 with added the backward moves and revealed instruction 10 – all
| Graph name | Numbe of orbits | Orbit length | Starting vertex $X_1$ - representative of orbit | $|B(X_1)|$-size of the bouquet of the starting vertex (number of the numberings) |
|-----------|----------------|--------------|-----------------------------------------------|-------------------------------------------------|
| JOWK 258048 | 6              | 256          | 280                                           | 310942                                           |
|           |                | 224          | 136                                           | 269778                                           |
|           |                | 48           | 15                                            | 85794                                            |
|           |                | 14           | 540                                           | 40262                                            |
|           |                | 3            | 546                                           | 14568                                            |
|           |                | 1            | 273                                           | 10200                                            |
| DSFP 55296 | 8              | 256          | 463                                           | 1528328                                           |
|           |                | 192          | 161                                           | 1211376                                           |
|           |                | 48           | 261                                           | 343926                                           |
|           |                | 32           | 53                                            | 181188                                            |
|           |                | 12           | 534                                           | 186432                                           |
|           |                | 3            | 531                                           | 45606                                            |
|           |                | 2            | 539                                           | 23724                                            |
|           |                | 1            | 273                                           | 47600                                            |
| HALL 921600 | 6              | 256          | 398                                           | 155988                                           |
|           |                | 192          | 235                                           | 127512                                           |
|           |                | 80           | 15                                            | 46116                                            |
|           |                | 12           | 542                                           | 14232                                            |
|           |                | 5            | 539                                           | 6264                                             |
|           |                | 1            | 273                                           | 2856                                             |

Table 3

above requirements are implemented in it. The algorithm PART1 determines $\text{GOO}(A(x_1))$ and $B(x_1)$ given $\Pi_1$, $\text{SC}(\Pi_1)$ and $x_1 \in \text{SC}(\Pi_1)$. The algorithm PART2 (the second part of the algorithm Vsep-e, line S5 in Fig. 5) determines $\text{GOO}(A)$ given $\text{GOO}(A(x_1))$ and $B(x_1)$ obtained from the algorithm PART1. The algorithm PART2 can be considered also as an application of the Algorithm A3 to the partition $\Pi_1$ with replacing the instruction 10 by determining one derivative numbering $\Pi_{LK}$ of each selected vertex $x \in \text{SC}(\Pi_1)$ if $x$ is not similar to $x_1$ under the current $\text{Aut}(G)$. The algorithm PART2 may be also considered as a direct application of theorems 3 and 4 and its correctness follows from this – all requirements R1 to R4 hold. At the start $\text{GOO(\text{Aut}(G))} := \text{GOO(\text{Aut}(G,x_1))}$. We select (line B2) each vertex $x$ in $\text{SC}(\Pi_1)$ that is not similar to $x_1$ under the current $\text{Aut}(G)$ and we compare (line B5) the first numbering $\Pi_{LK}$ derived from the selection $x$ (line B4) with the numberings $\in B(x_1)$. If there is an automorphism $\alpha$ between some numbering $\in B(x_1)$ and $\Pi_{LK}$ then $\alpha$ is a generator for $A$ since it unites the orbits of $x$ and $x_1$. In both cases (existence or nonexistence of $\alpha$) we continue traversing $\text{SC}(\Pi_1)$ until its end. When the traversal of $\text{SC}(\Pi_1)$ completes, the generators and the orbits of $A$ are determined and we apply the ‘orbit-stabilizer’ theorem for determining $|A| = |\text{Orb}(x_1, A)| \cdot |A(x_1)|$ (line B3).

We’ll describe the algorithm PART1 considering an intermediate state of the search tree ST (Fig. 5) being build by the algorithm during its execution. The series of partitions $\Pi_L$, $L=2, \ldots, LK-1$ can be divided into three intervals: the first is from $\Pi_L$ to $\Pi_{\text{MIN},L-1}$, the second – from $\Pi_{\text{MIN},L}$ to $\Pi_L$ and the third – from $\Pi_L$ to $\Pi_{LK-1}$. The search tree is built in a preorder: first visiting the root (a partition $\Pi_L$) and then its subtrees (the partitions $\Pi_{L+1}$ derived from each selected vertex) in a defined order.

Let us give some formulae about the bouquets and the stabilizers in the search tree ST (Fig. 4). According to the definition of a bouquet we have

$$B(X_L) = \text{BFRPO}(X_{L+1}) + B(X_{L+1}), L=1,2, \ldots, LP-1;$$

(4.2.1)

Applying this formula to $B(X_{LP-1})$ we obtain
B(X_{LP}) = \text{BFRPO}(X_{LP}), \tag{4.2.2}

since B(X_{LP}) is not defined so far, i.e. B(X_{LP})=\emptyset.

Substituting (4.2.2) in (4.2.1) and substituting into recurrence we obtain

\[ B(X_L) = \sum_{L=1}^{LP} \text{BFRPO}(X_{L,1}) \tag{4.2.3} \]

From (4.2.3) for B(X_{LMIN-1}) we have

\[ B(X_{LMIN-1}) = \sum_{LMIN}^{LP} \text{BFRPO}(X_L) \tag{4.2.4} \]

Applying the algorithm A3 for determining \( \text{gen}(A(x_{L})) \) then we have:

\[ \text{gen}(A(x_L)) = \text{gen}(A(x_{L-1}^L)) \cup \text{MG}(x_{L-1,u}^L) \cup \text{gen}(A(x_{L-1})) \tag{4.2.5} \]

where \( \text{gen}(A(x_L)) \) is the generating set of the current stabilizer \( A(x_L) \), \( \text{gen}(A(x_{L-1}^L)) \) is the generating set of the stabilizer \( A(x_{L-1}^L) \), \( \text{MG}(x_{L-1,u}^L) \) is the set of the mutual generators of \( A(x_L) \) and \( \text{gen}(A(x_{L-1})) \) is the generating set of the current stabilizer \( A(x_{L-1}) \).

The values of the following variables for the search tree in Fig. 5 of the algorithm PART1 (Fig.6) are known:

C1: \( \Pi_1, \text{SC}(\Pi_1), X_L, L=1, 2, \ldots , LP; X_L \) is the current selected vertex in SC(\( \Pi_1 \)). Each selected vertex \( X_L \) is not similar to any previous vertex in the SC(\( \Pi_1 \)) under the current \( A(X_L) \), \( L=2, \ldots , LP; \)

C2: \( \text{LMIN}, LP, \text{LMINS} LP, LP \geq 2; \)

C3: GOO(X_{LMIN-1}), B(X_{LMIN-1}), \text{FRPO}(X_{LMIN}), gen(X_{LMIN}) for a vertex \( X_{LMIN} \in \text{FRPO}(X_{LMIN}); \)

C4: Orb(y, \text{A}(x_L)) for \( y=X_L \) and \( y \in \text{FRPO}(X_L), L=\text{LMIN}+1, \ldots , LP; \) Only the correctness of \( \text{Orb}(X_{LP}, \text{A}(X_{LP-1})) \) is not guaranteed;

C5: B(\text{FRPO}(X_L)), L=2, \ldots , LP;

C6: GOO(X_L)= GOO(X_{LMIN-1}), L=1, \ldots , \text{LMIN}-2;

C7: Each orbit \( \text{Orb}(x, \text{A}(x_{L})); \) for each \( x \in \text{FRPO}(X_L) \) \( L=\text{LMIN}, \ldots , LP \) is a subset of a different orbit of \( \text{A}(X_{LMIN-1}); \) this property holds for each selected vertex \( x= x_{L}, L=\text{LMIN}, \ldots , LP-1; \) It is not known that this property holds for the selected vertices \( x_{LP}, L \geq LP. \)

All above conditions can be considered as an invariant of the loop C1 of the algorithm PART1.

Let’s now describe the algorithm PART1. It calls the algorithms SFM1 (Fig. 8) and COMP (Fig. 11). At the start all of the searched variables are not known and for each partition \( \Pi_L, L=2, \ldots , \text{LK}-1 \) we select the first vertex \( X_L \in \text{SC}(\Pi_L) \) and obtain the partition \( \Pi_{L+1} \), i.e. the only action we do is a forward move (line I1) until a discrete \( \Pi_{L} \) is obtained. Thus, the conditions R1 to R4 hold only for \( \Pi_{L} \); Let’s now consider the above requirements R1 to R4 for determining \( \text{GOO}(A(X_{LP-1}))=\text{GOO}(A(x_1, \ldots , x_{LP-1})) \) and the bouquet \( B(X_{LP-1})=B(x_1, \ldots , x_{LP-1}) \) given the partitions \( \Pi_1, \Pi_1, \ldots , \Pi_{LP}; \) For \( \Pi_{LP}=\Pi(x_1, \ldots , x_{LP-1}) \) also \( \text{SC}(\Pi_{LP}) \) and the selected vertex \( X_{LP} \) are known. Besides, the requirements hold for the position of the current vertex \( X_{LP} \in \text{SC}(\Pi_{LP}); \) By the loop C1 (lines I1- I12) in algorithm PART1 each selected cell \( \text{SC}(\Pi_{LP}) \) is visited and the following three basic steps are performed:

A1 \{Selection\}: The selection of a vertex \( X_{LP} \) in \( \text{SC}(\Pi_{LP}) \) (line I3) is made starting from the position next to the current \( X_{LP} \). The vertex \( X_{LP} \) should not be similar to any previous vertex in \( \text{SC}(\Pi_{LP}) \) under the current \( A(X_{LMIN-1}); \) For each level \( L \) the position \( i(X_{L}) \) of the selected vertex \( X_L \) is stored and when a backward move to this level is performed then the selection of a new vertex starts from the next position, i.e. \( i(X_{L})+1. \) If there is no selected vertex in \( \text{SC}(\Pi_{LP}) \), i.e. the \( \text{SC}(\Pi_{LP}) \) has been traversed then, a backward move follows (step A4). If there is a selected vertex \( X_{LP} \) in \( \text{SC}(\Pi_{LP}) \) then, step A2 follows.

A2 \{Series of forward moves\}: A series of forward moves SFM1 is performed determining the partitions \( \Pi_{L}=\Pi_{L+1}, \ldots , \Pi_{LK} \) with discrete \( \Pi_{LK} \) (line I5). Each of these partitions the selected vertex \( X_L \) is the first vertex in \( \text{SC}(\Pi_{L}); \) This way the requirements hold for the orbit \( \text{Orb}(X_L, A(X_{L})); \)

A3 \{Comparison\}: A check if there is a new automorphism \( \alpha \) that not belong to the current subgroup of \( A(x_{LP-1}); \) and maps the vertex \( X \) to any vertex from \( \text{FRPO}(X) \) is made, i.e. if \( \alpha \) belongs to the next subgroup of \( A(x_{LP-1}); \) This check is made by comparing \( \Pi_{LK} \) with \( \text{BFRPO}(X) \) (line I6, algorithm COMP).

A4 \{Backward move\}: After the traversal of \( \text{SC}(\Pi_{LP}) \) is completed then \( \text{GOO}(A(x_{LP-1})) \) and \( B(x_{LP-1}) \) are
determined and a backward move \( LP := LP - 1 \) is made. Stop follows if \( LP = 1 \). Otherwise, a selection of a new vertex in \( SC(\Pi_{LP}) \) is made applying the step A1 to it.

Fig. 5.

If there is an automorphism \( \alpha \) then, it is a generator: \( \text{gen}(A(X_{LP-1})) = \text{gen}(A(X_{LP-1})) \cup \{ \alpha \} \) and the orbits and the order of \( A(X_{LP-1}) \) are recomputed. It is a generator also for \( A(X_1) \): \( \text{gen}(A(X_1)) = \text{gen}(A(X_1)) \cup \{ \alpha \} \) and the orbits and the order of \( A(X_1) \) are recomputed. If there is no \( \alpha \) mapping \( x \) to a vertex \( \in \text{FRPO}(X) \) then a move back to \( \text{LK} - 1 \) follows. This way the building of the tree \( ST(x) \) starts from \( \text{LK} - 1 \) performing the step A1 to \( SC(\Pi_{\text{LK-1}}) \). \( ST(x) \) is necessary since it determines the bouquet \( B(x) \) that belongs to \( B(X_{LP-1}) \).

After \( ST(x) \) has been built we continue with a selection of a new vertex in \( SC(LP) \) applying the step A1 to \( SC(\Pi_{LP}) \). The search tree is built in preorder traversal: first visiting the root (a partition \( \Pi_{LP} \)) and then its subtrees (the partitions \( \Pi_{LP+1} \) derived from each selected vertex) in a defined order.

For the selected vertex \( X_{LP} \) (line I3 – the start of \( ST(X_{LP}) \) building) by SFM1 (line I5) is built the first (leftmost) tree \( ST(X_{LP+1}), ST(X_{LP+2}), \ldots, ST(X_{LK-1}) \) for each previous subtree. Each of these subtrees is built in backward order. When the subtree \( ST(X_{LP+1}) \) has been built then the building of the subtree for the next selected vertex \( X_{LP+1} \) starts (\( X_{LP+1} \) should hold the requirements). When there is no selected vertex \( X_{LP+1} \) then a backward move \( LP+1 \) to \( LP \) is made – this means that the \( ST(X_{LP}) \) is built. If \( LP = 1 \) the algorithm stops.

4.2.1. Cases CS1 and CS3

Let us consider the cases when the numbering \( \Pi_{LK} \) (Fig. 4) does not form an automorphism with any numbering \( \in \text{BFRPO}(\Pi_{LP}) \). Knowing that \( |A(X_{LP-1})| \) is correct and supposing that each orbit \( \text{Orb}(X_L, A(X_{L-1})) \) for \( L = LP, \ldots, \text{LK-1} \) is also correct, and applying the Theorem ‘O-S’ we obtain
Input: Graph $G(V,E)$ and a partition $\Pi$ on $V$

Output: Generators, orbits and order of the partition-wise stabilizer $A=\text{Aut}(G, \Pi)$, denoted $\text{GOO}(A)$

S1. Initialization: $\Pi_1:=\text{RP}(\Pi_0, NCL)$; $|NCL|$-the number of the cells in $\Pi_1$

S2. if $NCL=\{\Pi_1\}$ then writeln(“Trivial group”); stop;

S3. CSLCh {cell selector chooser}; if the chosen cell selector is one of CLSL-5, CLSL-6, CLSL-7 then go to S4;

S3.1. CSLCh {cell selector chooser}; if the chosen cell selector is one of CLSL-5, CLSL-6, CLSL-7 then go to S4;

S3.2. New partition $\Pi_1a$ (with number of cells ncl1) is obtained by classifying the vertices $x$ of $\Pi_1$ by $S$ of $\Pi_1(x)$. If ncl1 > ncl then go to S4;

S3.3. Determine: (a) the orbits of $A$ by the heuristic algorithm TABLE, starting from discrete orbits; (b) SC$(\Pi_1)$; $X_1$:=a representative of the smallest orbit of the vertices in SC$(\Pi_1)$; Write vertex $x_1$ on the first position in SC$(\Pi_1)$; $A:=\{I\}$;

S4. PART1: Determine $\text{GOO}(A(x_1)), B(x_1)$ given $\Pi_1, SC(\Pi_1), x_1 \in SC(\Pi_1)$

S5. PART2: Determine $\text{GOO}(A)$ given $\text{GOO}(A(x_1)), B(x_1)$

Fig. 6. Algorithm Vsep-e

Input: $\Pi_1, SC(\Pi_1), x_1$

Output: $\text{GOO}(A(x_1)), B(x_1)$

I1: SFM1: Determine $\Pi_1, |A(X_{L_1})|=1, SC(L_1), L_1=2, \ldots, L_K$ given $\Pi_1, SC(\Pi_1), X_1$;

$LP:=LK-1; LMIN:=LP; \text{gen}(A(x_1)):=\emptyset; |A(x_1)|:=1; B(X_{L, K-1})=\{\Pi_{L, K}\};$

I2: do {loop C1: Visit each SC$(\Pi_{L, P})$}

I3: Select $X_{L, P}$ in SC$(LP)$;

I4: if $X_{L, P} \neq 0$ then {forward move}

I5: SFM1: Determine $\Pi_{L, P}, |A(X_{L, P})|, SC(L_{P}), L_{P}=L_{P}+1, \ldots, L_K$ given LP, $\Pi_{L, P}, SC(\Pi_{L, P}), X_{L, P}$;

I6: COMP: Compare $\Pi_{L, K}$ with the numberings $E_FRO(X_{L, P})$ for determining an automorphism $\alpha \in A(X_{L, P})$. Determine $\text{GOO}(A(X_{L_{MIN}})), LP$;

I7: else {backward move: SC$(LP)$ has been traversed}

I8: LP=LP-1;

I9: if LP=1 then return;

I10: if LP<LMIN then LMIN=LP; $X_{L_{MIN}}:=X_{L_{MIN}}; |Aut(X_{L_{MIN}})|:=|Aut(X_{L_{MIN}})|$

I11: enddo; {loop C1}

Fig. 7. Algorithm PART1 (instruction S4 of algorithm Vsep-e (Fig. 6))

Input: $L=LP, \Pi_{L, P}, SC(\Pi_{L, P}), X_{L}$

Output: $\Pi_{L, P}, |A(X_{L, P})|, L=LP+1, \ldots, L_K$

1. do

2. $L=L+1; \Pi_{L, P}:=TR(X_{L-1}, \Pi_{L-1}); \Pi_{L, P}:=RP(\Pi_{L-1}, \Pi_{L-1})$;

3. if NCL=0 then return

3. else determine SC$(L); X_i=$first vertex in SC$(L)$;

$|A(X_{L})|=|A(X_{L-1})|/|\text{Orb}(X_{L}, A(X_{L_{MIN}})) \cap SC(\Pi_{L})|$

5. enddo

Fig. 8. Algorithm SFM1 (instruction I2 of algorithm PART1 (Fig. 7))

$|A(X_{L_{P-1}})|/|\text{Orb}(X_{L_{P-1}}, A(X_{L_{P-1}}))|/|\text{Orb}(X_{L_{P-1}+1}, A(X_{L_{P}}))|/ \ldots /|\text{Orb}(X_{L_{K-1}}, A(X_{L_{K-2}}))|=|A_{L_{K-1}}|=1. \quad (4.2.1.1)$

However, the orbits in (4.2.1.1) are unknown and consequently we cannot use it. Instead, the sets $W=\text{COOr}(X_{L}, A(X_{L_{P-1}}))$ of the vertices in SC$(\Pi_{L})$ similar to $X_{L}$ under $A(X_{L_{P-1}})$ are known, i.e.

$W=\text{COOr}(X_{L}, A(X_{L_{P-1}}))=\text{Orb}(X_{L}, A(X_{L_{P-1}})) \cap SC(\Pi_{L})$. \quad (4.2.1.2)
The operations in the case CS3 may be considered as an error correction of the incorrect orbits of some separate orbit. Obviously, the invariant holds for the case CS3.

LMIN = LP, X invariant holds for LP = LK is denoted by CS1. If the case is CS1, then at the exit of the algorithm, i.e., each computed orbit is equal to the real one, then the sign in (4.2.1.4) is = and the case SC(1) is determined so far and the algorithm continues with a new top point: LP = LK. Thus, W can be considered as an union of orbits of A(XL1). We call this case non-separation of orbits (denoted by NSO) and the orbit U is called non-separated (non-partitioned).

Since the representatives of the orbits belonging to R are not known we can not select them during the traversal of the SC(ΠL1). Thus, the search tree of such a vertex cannot be built and its bouquet will not be determined. This is an unallowable error since these bouquets belong to B(XL1), B(XL2), . . . , B(X1) and they are needed (as we know from Algorithm A3) for determining GOO(A(XL2)), GOO(A(XL3)), . . . , GOO(A(X1)). If there is only one partition with non-separated orbit, then the sign in (4.2.1.4) is <, since the length of the computed orbit is greater or equal to the length of the real orbit – this is the condition to detect the presence of NSO. We call this case CS3. If there is no NSO in any partition, i.e. each computed orbit is equal to the real one, then the sign in (4.2.1.4) is = and the case is denoted by CS1. If the case is CS1, then at the exit of the algorithm COMP (line I6 in PART1) the invariant holds for LP = LK: only LP is changed, LMIN remains the same. When the case is CS3 we loose GOO(XLMIN−1) determined so far and the algorithm continues with a new top point: LP = LK, LMIN = LP, XLMIN−1 = XLK−1 is the first vertex in SC(LK−1) and A(XLMIN−1) = {1}, i.e., each vertex is put into a separate orbit. Obviously, the invariant holds for the case CS3.

The operations in the case CS3 may be considered as an error correction of the incorrect orbits of some A(XL1) determined by the moment since the algorithm interrupts its current execution and starts from the new top point for finding the correct orbits of A(XL1) and the bouquet B(XL1).

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**Fig. 9. Algorithm PART2 (instruction S5 of algorithm Vsep-e (Fig. 6))**

| Input: L=1, Π1, SC(Π1), X1, GOO(A(x1)), B(x1) |
| Output: GOO(A) |
| B1. Do |
| B2. Select next vertex X in SC(Π1); |
| B3. if X=∅  then |A|=|Orb(x1, A)|, return; |
| B4. SFM1A: Determine Π1K given L=1, Π1, SC(Π1), X∈ SC(Π1) |
| B5. Compare Π1K with the numberings of bouquet B(x1) for an automorphism α. If there is α then gen(A) = gen(A) ∪ α and recompute the orbits of A; |
| B6. enddo; |

**Fig. 10. Algorithm SFM1A (instruction B4 of algorithm PART2 (Fig. 9))**

| Input: L=1, Π1, SC(Π1), X ∈ SC(Π1) |
| Output: Π1K |
| 1. do |
| 2. L=L+1; Π1|=TR(XL−1, ΠL−1); ΠL=RP(ΠL−1, NCL); |
| 3. if NCL=n then return |
| 4. else determine SC(L); XL=first vertex in SC(L) |
| 5. enddo |

We call the set W ‘computed orbit’ to distinguish it from the real orbit U = Orb(XL, A(XL)). The following relation holds

$$U = \text{Orb}(x_L, A(x_{L-1})) \subseteq \text{Corb}(x_L, A(x_{L-1})) = W, \quad (4.2.1.3)$$

since $$A(x_{L-1}) \subseteq A(x_{L-1})$$. Considering (4.2.1.3) and applying the Theorem ‘O-S’ for the computed orbits we obtain

$$|A(x_{L-1})| |\text{Corb}(x_{L-1}, A(x_{L-1}))| |\text{Corb}(x_{L-2}, A(x_{L-1}))| \ldots |\text{Corb}(x_{L-k}, A(x_{L-1}))| = |A_{L-1}| \leq 1. \quad (4.2.1.4)$$

The computation on (4.2.1.4) is performed by the Algorithm SFM1 (Fig. 8) called from the instruction I5 of PART1. If the sign in (4.2.1.3) is = (i.e., the real and the computed orbit are equal), then we call the orbit Orb(xL, A(xL)) separated.

If the sign in (4.2.1.3) is <, then, obviously, W = U ∪ R, |R| > 1, i.e., W (and R) include vertices that belong to SC(ΠL) but are not similar to XL under A(XL). It can be proved that when W contains some vertex, then it contains the whole orbit of this vertex under A(XL). Thus, W can be considered as an union of orbits of A(XL). We call this case non-separation of orbits (denoted by NSO) and the orbit U is called non-separated (non-partitioned). Since the representatives of the orbits belonging to R are not known we can not select them during the traversal of the SC(ΠL). Thus, the search tree of such a vertex cannot be built and its bouquet will not be determined. This is an unallowable error since these bouquets belong to B(XL), B(XL), . . . , B(X) and they are needed (as we know from Algorithm A3) for determining GOO(A(XL2)), GOO(A(XL3)), . . . , GOO(A(X1)). If there is only one partition with non-separated orbit, then the sign in (4.2.1.4) is <, since the length of the computed orbit is greater or equal to the length of the real orbit – this is the condition to detect the presence of NSO.
Input: \( \Pi_L, SC(\Pi_L), X_L, |A(X_{L-1})|, L=2,3, \ldots, LK; LP, BFRPO(X_{LP}), \text{LMIN}, \text{GOO}(A(X_{\text{LMIN}-1})) \)

Output: \text{GOO}(A(X_{\text{LMIN}-1})), LP

1: Compare \( \Pi_{LK} \) with the numbering \( \in \text{BFRPO}(X_{LP}) \)
2: if \( \Pi_{LK} \) is not equivalent to any numbering \( \in \text{BFRPO}(X_{LP}) \)
3: then \{CS1 or CS3\}
4: if \( |A(X_{LK-1})| = 1 \)
5: then \{CS1\}
6: \( LP = LK-1 \); \( B(X_{LP}) = \{ \Pi_{LK} \} \); if \( LP < \text{LMIN} \) then \( \text{LMIN} = LP \)
7: else \{CS3\}
8: \( \text{LMIN} = LP \); \( A(X_{\text{LMIN}-1}) = \{1\} \); \( XF_{\text{LMIN}}= \) the current selected vertex in \( \text{SC}(\text{LMIN}) \); \( |\text{Aut}(X_{\text{LMIN}})| = 1 \)
9: endif
10: else \{CS2 or CS4: there is an automorphism \( \alpha \), \( X_{LP} = \alpha(U_{LP}) \), between \( \Pi_{LK} \) and some numbering \( \in \text{BFRPO}(X_{LP}) \) \}
11: Determine \( \text{GOO}(A(X_{\text{LMIN}-1})) \); \( \text{gen}(A(X_{\text{LMIN}-1})) = A(X_{\text{LMIN}-1}) \cup \{\alpha\} \); determine orbits of \( A(X_{\text{LMIN}-1}) \) and \( |A(X_{\text{LMIN}-1})| = |A(X_{\text{LMIN}})||\text{Orb}(X_{\text{LMIN}}, A(X_{\text{LMIN}}))| \)
12: for \( L = \text{LMIN}, \text{LMIN} + 1, \ldots, LP \) do
13: if \( \text{if } L = LP \) then \( X_L = U_{LP} \)
14: \( |A(X_L)| = |A(X_{L-1})| |\text{COrb}(X_L, A(X_{LMIN-1}))| \)
15: enddo \{loop for from line 15\}
16: \( \text{LMIN} = LP \); \( L = LK \); \( \text{gen}(\{\alpha\}) = \{\alpha\} \); the orbits of \( A(X_{\text{LMIN}-1}) = \text{cycles of } \alpha \)
17: \( |A(X_{\text{LMIN}-1})| = |\text{Orb}(U_{LP}, A(X_{\text{LMIN}-1}))| \); \( XF_{\text{LMIN}} = U_{LP} \); \( |\text{Aut}(X_{\text{LMIN}})| = 1 \);
18: \{the execution continues by starting selection of a vertex after the current position of \( X_L \)\}
19: else \{CS2 – all orbits and orders of the current path are correct\}
20: \{end if from line 2\}

**Fig. 11. Algorithm COMP (instruction I4 of algorithm PART1 (Fig. 7))**

### 4.2.2 Cases CS2 and CS4

Let’s consider the cases when there is an automorphism \( \alpha \) mapping \( X_{LP} \) to some vertex \( U_{LP} \in \text{FRPO}(X_{LP}) \), i.e., the numbering \( \Pi_{LK} \) forms an automorphism \( \alpha \) with some numbering \( \in \text{B}(U_{LP}) \). \( X_{LP} = \alpha(U_{LP}) \).

Then, there is a possibility of NSO for some orbits of vertices of the current path for the levels \( \text{LMIN} + 1 \leq L \leq LP \): we denote by CS2 the case when there is no NSO and by CS4 the case when there is at least one case of NSO in this interval. The automorphism \( \alpha \) is a generator of \( A(X_{\text{LMIN}-1}) \) since

\[
A(X_{LP-1}) \subseteq A(X_{\text{LMIN}-1}) : \text{gen}(A(X_{\text{LMIN}-1})) = \text{gen}(A(X_{\text{LMIN}-1})) \cup \{\alpha\}.
\]

Thus, the \( \text{Orb}(A(X_{\text{LMIN}})) \) and \( |A(X_{\text{LMIN}})| \) are changed and we denote by \( A^{\alpha}(X_L) \) the new value of \( A(X_L) \). Before \( \alpha \) each orbit and each order of the current stabilizers are correct:

\[
|A(X_L)| = |A(X_{L-1})| |\text{Orb}(X_L, A(X_{L-1}))| \text{ for each } X_L \in \text{SC}(L), L = \text{LMIN}, \ldots, LP.
\]

Then, we determine

\[
|A^{\alpha}(X_L)| = |A^{\alpha}(X_{L-1})| |\text{Orb}(X_L, A(X_{L-1}))| \text{ for each } X_L \in \text{SX}(L), L = \text{LMIN}, \ldots, LP, \text{ where } X_{LP} = U_{LP} \text{ if } L = LP.
\]

If \( |A^{\alpha}(X_L)| = 1 \) then the case is CS2 and each \( \text{Orb}(X_L, A(X_{L-1})) = \text{Orb}(X_L, A(X_{L-1})) \) – all orbits and orders of the stabilizers are correct. In the case CS2 we continue by selecting a new vertex from \( \text{SC}(\Pi_{LP}) \).

If \( |A^{\alpha}(X_L)| < 1 \) then the case is CS4 – this means that some of the above computed orbits and orders of the stabilizers are incorrect. Then we interrupt the current execution (as in case CS3) of the algorithm losing all found \( \text{GOO}(A(X_{\text{LMIN}-1})) \) but the found bouquets are saved. We continue with a new top point:
LP has not changed: $\text{LMIN} = \text{LP}$ and $\text{gen}(A(X_{\text{LMIN}})) = \{I\}$ and we select the vertex $Z$ from $\text{SC}(\Pi_{LP})$ repeating the building of its tree $\text{ST}(Z)$ – thus the requirements $R1$ to $R4$ hold for $\text{Orb}(Z, A(X_{LP}))$ after the tree $\text{ST}(Z)$ we’ll be built.

If $\text{LP} = \text{LMIN}$ then all orbits of $A^\alpha(X_{\text{LMIN}})$ in the cells of $\Pi_{LP}$ are correct ($\text{CS2}$ is the case) since each generator discovered so far has a base that is a superset of the base of $A^\alpha(X_{\text{LMIN}})$. Then, we continue by selecting a new vertex (line 3 in PART1) starting from the position after the current $X_{\text{LP}}$.

4.3. Examples

4.3.1. Simple example

Fig.12

Fig.13 illustrates the search tree (ST) of algorithm Vsep-e for the graph in Fig. 12. In each node of the ST for the first selection (vertex 4, $\text{LP}>1$) of $\text{SC}(\Pi_1)$ are given the following: $L$, $\Pi_1$, $\text{SC}(L)$, $|A_L|$ - the order of the subgroup of the stabilizer $A_L$ presented by 3 generators $\alpha_1 \alpha_2 \alpha_3$. For the other selections (vertices 5 and 6) in $\text{SC}(\Pi_1)$ ($\text{LP}=1$, PART2) only a series of forward moves is made, i.e. only one numbering is determined for each selected vertex: $\Pi_1 = [2,9,4,5,6,7,1,3,8,10]$; $\Pi_2 = \Pi(4) = [2,9,4,5,7,6,8,10,1,3]$; $\Pi_3 = \Pi(4,8) = [2,9,4,5,7,6,8,10,1,3]$; $\Pi_4 = n_1 = \Pi(4,8,1) = [2,9,4,5,7,6,8,10,1,3]$; $\Pi_4 = n_2 = \Pi(4,8,3) = [2,9,4,5,7,6,8,10,1,3]$; $\Pi_3 = \Pi(4,10) = [2,9,4,5,7,6,10,8,1,3]$; $\Pi_4 = n_3 = \Pi(4,10,1) = [2,9,4,5,7,6,10,8,1,3]$.

4.3.2. Example with all cases (CS1, CS2, CS3, CS4) (Fig.14): graph $G=B52$ (Mathon [24]), regular graph, $n=52$, degree=25, $|\text{Aut}(G)|=12$. Orbit lengths: $2*2+4*6+2*12$; Orbits: $(4,30)(24,5)$, $(17,36,16,42,10,43)(8,44,39,18,13,34)(26,35,28,2,9,52)(29,25,22,15,20,33,7,46,41,48,3,51)$.

We show in Fig.14 only the subtrees of the selections (4,11), (4,13), (4,14) and (4,24) of the search tree. The first selected vertex in $\Pi_1 = [1,2,\ldots,52]$ is the vertex 4 since it is from one of the smallest orbits – the orbits are found by the heuristic algorithm. We start the consideration from the selections (4,11,51) – this is the numbering n52: it is not equivalent to any numbering from B(4,2), B(4,3), B(4,10). Before these selections there were determined the bouquets of the representatives B(4,2), B(4,3), B(4,10). Before these selections there are found 4 generators of A(4), its order, orbits and some stabilizers. At the selections (4,11,51) the case CS3 has been discovered. That’s why the selected vertex 51 in $\text{SC}(\Pi_3)$, $\Pi_3 = \Pi(4,11)$ becomes a new starting point: all information about the stabilizer $A(4)$ obtained so far is lost and $A(4)=A(4,11)=A(4,11,51)=\{I\}$, $\text{LP}=\text{LMIN}=3$, $X_{\text{FMIN}}=51$, $|A(X_{\text{FMIN}})|=1$. The next selected vertex in $\text{SC}(\Pi_3)$ is 7. The numbering $\Pi(4, 11, 7)$ is equivalent to numbering n52.

Thus a new generator $\alpha_5$ for (4,11) and A(4) is found (this is case CS2), $\alpha_5 = (1,6)(2,52)(3,41)(4,5,45)(7,51)(8,39)(9,10,43)(11,12,21)(13,34)(14,23)(15,29)(16,17,36)(18,19,31)(20,22)(24)(25,33)(26,28)(27,32)(30,35)(37)(38,47)(40,49)(42)(44)(46,48)(50)$. Then, we compute $|A(X_{\text{LMIN}})| = |A(X_{\text{FMIN}})||\text{Orb}(X_{\text{FMIN}}, A(X_{\text{LMIN}}))|$, i.e., $|A(4,11)| = |\text{Orb}(51, A(4,11))||A(4,11,51)|=2*1=2$. The next selected vertex in $\text{SC}(\Pi_4)$ is 9 - the partition $\Pi_4 = \Pi(4, 11, 9)$ is not discrete: $|A(4, 11, 9)| = |A(4, 11)/\Pi(9, A(4, 11))|=2/|9|=2/1=2$. Then, the next selected vertex in $\text{SC}(\Pi_3)$ is 46 and $\Pi_5 = \Pi(4, 11, 9, 46)$ is discrete (numbering n53). The numbering n53 is not equivalent to the numbering n52 and $|A(4, 11, 9, 46)| = |A(4, 11, 9)/\Pi(46, A(4, 11))|=2/|46,48|=2/2=1$ – this is CS1. The vertex 48 is not selected in $\text{SC}(\Pi_3)$ since it is similar to the vertex 46 under A(4, 11, 9). Then, a backward move to L=3 and a selection of the vertex 10 are made. The partition n54 is discrete and not equivalent to any numbering in
Fig. 13. Search tree (ST) of the algorithm

| L=2 | L=3 | L=4 | L=3 | L=4 | L=3 | L=4 | L=3 | L=4 | L=3 | L=4 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| $\Pi(4)=\Pi_2$ | $\Pi(4,8)=\Pi_3$ | $\Pi(4,8,1)=\Pi_4$ | $\Pi(4,10)=\Pi_3$ | $\Pi(4,10)=\Pi_4$ | $\Pi(5)=\Pi_2$ | $\Pi(5,8)=\Pi_3$ | $\Pi(5,8,1)=\Pi_4$ | $\Pi(6)=\Pi_2$ | $\Pi(6,1)=\Pi_3$ | $\Pi(6,1,8)=\Pi_4$ |
| 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   |
| 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   |
| 9   | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 9   |
| 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   |
| 4   | 4   | 4   | 4   | 4   | 4   | 5   | 5   | 5   | 5   | 5   |
| 4   | 4   | 4   | 4   | 4   | 4   | 5   | 5   | 5   | 5   | 5   |
| 5   | 5   | 5   | 5   | 5   | 4   | 4   | 4   | 4   | 7   | 7   |
| 5   | 5   | 5   | 5   | 5   | 4   | 4   | 4   | 4   | 7   | 7   |
| 7   | 7   | 7   | 7   | 7   | 6   | 6   | 6   | 6   | 5   | 5   |
| 7   | 7   | 7   | 7   | 7   | 6   | 6   | 6   | 6   | 5   | 5   |
| 6   | 6   | 6   | 6   | 6   | 6   | 6   | 6   | 6   | 6   | 6   |
| 6   | 6   | 6   | 6   | 6   | 6   | 6   | 6   | 6   | 6   | 6   |
| 8   | 8   | 8   | 8   | 10  | 10  | 8   | 8   | 8   | 10  | 10  |
| 8   | 8   | 8   | 8   | 10  | 10  | 8   | 8   | 8   | 10  | 10  |
| 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  |
| 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  |
| 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 8   | 8   |
| 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   |
| $\alpha_1$ | $\alpha_2$ | $\alpha_2$ | $\alpha_3$ | $\alpha_3$ | $\alpha_3$ | $\alpha_3$ | $\alpha_3$ | $\alpha_3$ | $\alpha_3$ | $\alpha_3$ |

Table 4. The sequence of obtaining the partitions for the graph in Fig. 12 by Vsep-e (the cells with double lines are SC)
Due to the generators $\alpha_{18,34}\{14,19,23,27,31,32\}\{15,20,22,25,29,33\}\{16,17,36\}\{24\}\{26,28,35\}{30}{50}$, the number of $\Pi_1=\Pi(4,11,48,27)=n55$ is not equivalent to any numbering in $B(4,11)$:

$|A(4,11,48,27)|=|A(4,11)|/|Orb(48,A(4,11))|/|Orb(27, A(4,11,48))|=2/\{(46,48)\}/\{(27,32)\}=2/2/0.5<1$.

This is case CS3. So, the vertex 27 in $SC(2,11,48)$ becomes a new starting top point: all information about the stabilizer $A(4,11)$ is lost, $A(4,11,48)=A(4,11,48,27)=\{1\}$, $LP=LMIN=4$, $XF_{LMIN}=27$, $|A(XF_{LMIN})|=|A(4,11,48,27)|=1$. We omit the description of the next selections in $SC(2,11,48)=SC(2,11,41)$.

We only mention the occurrence of CS2: the generator $\alpha_{6,8}$ that leads to $gen(A(4,11))=\{\alpha_6, \alpha_8\}$, $|A(4,11)|=2$ and the orbits of $A(4,11)$ equal to the cycles of $A(4,11)$. After the $SC(2,11,41)$ has been traversed a backward move to $L=2$ follows: $LP=LMIN=2, B(4,11)\{n52,n52,\ldots,n64\}$, $B(4)\{n1,n2,\ldots,n63\}$, $XF_{LMIN}=11$, $|A(XF_{LMIN})|=|A(4,11)|=2$. The next selected vertex in $SC(2,11)$ is 13: the pattern $\Pi_1=\Pi(4,13)$ is not discrete, we do forward move to $L=3$ and choose the vertex 3 in $SC(3)$. The numbering $\Pi_1=\Pi(4,13,3)$ (n65) is not equivalent to any numbering in $B(4)$. The order of its stabilizer is $|A(4,13,3)|=|A(4)|/|Orb(13, A(4))|/|Orb(3,A(4,13))|=2/\{(13,34)\}/\{(3)\}=2/2/1=1$ (CS1). After the selection 47 in $SC(3)$ and 31 in $SC(3)$ we obtain the numbering $n66=\Pi_1=\Pi(4,13,47,31)$ it's not equivalent to n65 and $|A(4,13,47,31)|=|A(4)|/|Orb(13,A(4))|/|Orb(47,A(4,13))|/|Orb(31,A(4,13,47))|=2/\{(13,47)\}/\{(47)\}/\{(31)\}=2/1/1/1$ (CS1). After the selection 14 in $SC(3)$ we have the numbering $\Pi(4,13,47,14)$, $LP=4$, $LMIN=2$. Numerating $\Pi(4,13,47,14)$ is equivalent to previous one n65. Thus, a new generator $\alpha_7=(1,49)\{(2,9)(3,46)(4,50)(6,45)(7,41)(8,44)\}/\{11,38\}/\{12,37\}/\{13\}/\{14,31\}/\{15,33\}/\{16,17\}/\{18,34\}/\{19,32\}/\{20,29\}/\{21\}/\{22,25\}/\{23,27\}/\{24\}/\{26\}/\{28\}/\{35\}/\{30\}/\{36\}/\{39\}/\{42\}/\{43\}/\{47\}/\{48,51\}/\{50\}/\{52\}$ for $A(4)$ is found and the new orbits are: $Orb(A(4))\{1,5,6,40,45,49\}/\{2,3,2,52\}/\{3,7,41,46,48,51\}/\{4\}/\{8,39,44\}/\{10,42,43\}/\{11,38,47\}/\{12,21,37\}/\{13,18,34\}/\{14,19,23,27,31,32\}/\{15,20,22,25,29,33\}/\{16,17,36\}/\{24\}/\{26,28,35\}/\{30\}/\{50\}$ and the order of the stabilizer $A(4)=|A(4)|/|Orb(11,A(4))|=2=6 (XF_{LMIN}=11)$. Then, a check for CS2/CS4 follows (LMIN<LP). We check for NRO for each vertex $Z_4\in SC(3)$ and $Z_4\in FRPO(X_4)$, $L=LMIN+1$, $LP=3,4$, i.e., if there are changes of the orders $|A(4,13,3)|$ and $|A(4,13,47,31)|$. The order of $|A(4,13,3)|$ before $\alpha_7$ is $|A_{\alpha_7}(4,13,3)|=|A_{\alpha_7}(4)|/|Orb(13,A_{\alpha_7}(4))|/|Orb(3,A_{\alpha_7}(4,13))|=2/2/1=1$ and after $\alpha_7$ it is $|A(4,13,3)|=|A(4)|/|Orb(13,A(4))|/|Orb(3,A(4,13))|=6/\{13,18,34\}/\{13,46,51,48\}=6/3/4/0.5$. This difference $|A_{\alpha_7}(4,13,3)|\neq|A(4,13,3)|, l=0.5$ shows that the orbit $Orb(3,A(4,13))=\{3,13,46,51,48\}$ under $A(13,43)$ is incorrect, it is united orbit, i.e., the case is CS4. (As we'll see later, the correct orbits are $\{3,46\},\{51,48\}$). Hence, the check for $A(4,13,47,31)$ is not necessary. As the case is CS4 we set $LP=4$ (not changed), $LMIN=LP$, $gen(A(XF_{LMIN})=gen(A(4,13,47))=\{\alpha_7\}$; $Orb(A(4,13,47))=cycles$ of $\alpha_7$ and $|A(4,13,47)|=2$ (the least multiple of the cycle lengths of $\alpha_7$). We also set $XF_{LMIN}=31$ and we start the selection of a new vertex from the current $XF_{LP}=14$ and since it is the last vertex in $SC(4)$ we make a move back to the level $L=3$ selecting the vertex 46. We omit the following actions of the algorithm. We only mention the last generators

$\alpha_8=(1,5)(2,51)(3,46)(4,60)(7,46)(8,9,52)(10,42)(11,47)(12)(13,18)(14,32)(15,22)(16,36)(17)(19,23)$

$(20,33)(21,37)(24)(25,29)(26,35)(27,31)(28)(30)(34)(38)(39,44)(41,48)(43)(45,49)(50)$ and $\alpha_9=(1,45,40)(2,52,9)(3,7,48,4)(5,6,49)(8,39,44)(10,42,43)(11,38,47)(12,21,37)(13,18,34)$

$(14,19,23,27,31,32)(15,20,22,25,29,33)(16,17,36)(24)(26,28,35)(30)(50)$ and $|A(4)|=|Orb(XF_{LMIN},A(4))|=6=6$. Where $XF_{LMIN}=14$. The last generator found by PART2 is $\alpha_{10}=(1,27,2,28,3)(29,4,9,30)(5,31)(6,32)(7,33)(8,34)(9,35)(10,36)(11,37)(12,38)(13,39)$

$(14,40)(15,41)(16,42)(17,43)(18,44)(19,45)(20,46)(21,47)(22,48)(23,49)(24,50)(25,51)(26,52)$. The orbits of $A$ due to the generators $\alpha_8, \alpha_9$ and $\alpha_{10}$ are given at the beginning of this section and $|A|=|A(4)||Orb(A,4)|=6\times2=12$. Thus, the output is: $|A|=12, Orb(A)$ and generators $\alpha_8, \alpha_9$ and $\alpha_{10}$. 

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Fig. 14. The search tree ST for the graph B52
4.3.3. Example of rigid graph: A50, Mathon [24], n=50, regular bipartite graph, k=105=15*7+35*3, Fig.15.). The bouquet |B(1)|=168, |SC(Π2)|=14, each selected cell SC(Π3) has size |SC(Π2)|=12. The search tree is full.

Fig.14. The search tree ST for the graph B52 (continued)
4.4. Coding the partitions and storing the bouquets

We propose new coding of a partition of the graph vertices. The partition code is a number depending on the labels, sizes of the partition cells and the number of the edges between the cells. The coding is used for reducing required storage in the graph isomorphism and automorphism algorithms. The code of a given partition can be computed directly from the partition and the graph representation or from the code of the parent partition and the differences between the partition and its parent partition.

In our algorithms a large number of discrete partitions (numberings) of graph vertices are generated and stored. The length of each partition is \( n \) (\( n \) is the number of the graph vertices). One way of reducing storage requirements is the coding of partitions. To every partition is assigned a code (a number, characteristic value). The codes of two partitions are compared (instead of comparing the corresponding partitions) and if they are equal then the partitions are compared to determine if they form an automorphism. In this case the partitions have to be regenerated using the stored base of the partition (the cardinality \( p \) of the base is \( p<6 \) for graphs CLASS6, i.e. \( p \) is many times less than \( n \)) and then applying the IR algorithm. Let consider the storing of the successive derived partitions \( \pi_0, \pi_1, \pi_2, \ldots, \pi_L \) obtained from the start partition \( \pi_0 \) by applying the IR algorithm successively. This means that the stored information is \( p+1 \) numbers (one code and \( p \) numbers for regenerating the partition). This way the amount of the stored information is reduced from \( n \) to \( p+1 \) numbers, where \( p \ll n \). Or, if we use a polynomial code for the base of the partition then we have to store for the partition 2 numbers – the partition code and the code of the base.

The requirements for the code are:

i) the codes of the equivalent partitions have to be equal;

ii) The splitting ability of the code has to be maximal. This means that the number of not equivalent partitions with equal codes have to be minimal (minimum collisions);

iii) The computation of the code should have minimal number of operations (easy to compute);

We have examined few versions of coding and the code with the best satisfaction of the requirements is the following:

\[
\text{Code}(\pi) = \sum_{(x,y) \in E} L(C(x)).L(C(y)), \text{ where:}
\]

\[
(4.4.1)
\]
\[ \pi \] - the adjacency refinement partition of the vertices of graph G(V,E), \((x,y)\)- an edge of the graph, \(C(x), C(y)\) – the cells of the vertices \(x, y \in V\) and \(L(C(x)), L(C(y))\) – the labels of the cells \(C(x), C(y)\). The label of a cell is the index of the first vertex in the cell representing a partition as an array.

Evidently, the time complexity of computing the code by (4.4.1) is \(T=k=O(n^2)\) multiplications (\(k\)-the number of the graph edges) since \(k=O(n^2)\). The code of \(\pi\) can be computed directly by (4.4.1) or indirectly by the code of the parent partition of \(\pi\). The maximal value of the code \(\text{Max}\{\text{Code}(\pi)\}\) is obtained for a discrete partition \(\pi\) of a complete graph on \(n\) vertices (in this case there is an edge between each two vertices):

\[
\text{Max}\{\text{Code}(\pi)\} = \frac{n(n-1)(n+1)(3n+2)}{24} = \sum_{i=1}^{n-1} i(i + 1 + i + 2 + \ldots + n - 1 + n) \quad (4.4.2)
\]

**Example:** Let’s consider the graph in Fig.16 and a series of partitions:

![Diagram](Image 126x536 to 283x608)

\(\pi_0 = \pi(0) = 1, 2, 3, 4, 5, 6, 7, 8\) = \(C_0^1\); \(\text{Code}(\pi_0) = 12\); \(\pi_1 = \pi(1) = \text{RP}\{1|2, 3, 4, 5, 6, 7, 8|\} = 1|7, 8|5, 6|3, 4|2\) = \(C_1^1 C_2^1 C_3^1 C_4^1\); \(\text{Code}(\pi_1) = 208\); \(\pi_2 = \pi(1, 7) = \text{RP}\{1|7|8|5, 6|3, 4|2\} = 1|7|8|5, 6|3, 4|2\) = \(C_1^2 C_2^2 C_3^2 C_4^2 C_5^2\)

\(\text{Code}(\pi_2) = 218\); \(\pi_3 = \pi(1, 7, 5) = \text{RP}\{1|7|8|5|6|3, 4|2\} = 1|7|8|5|6|3, 4\) = \(C_1^3 C_2^3 C_3^3 C_4^3 C_5^3 C_6^3 C_7^3\)

\(\text{Code}(\pi_3) = 234\). In table 5 we illustrate only how \(\text{Code}(\pi_1)\) is computed.

| edge \((x,y)\) | 1,2 | 1,3 | 1,4 | 2,3 | 2,4 | 3,5 | 4,6 | 5,7 | 5,8 | 6,7 | 6,8 | 7,8 | Code(\(\pi_1\)) |
|----------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------------|
| \(L(C(x)), L(C(y))\) | 1,8=8 | 1,6=6 | 1,6=6 | 8,6=48 | 8,6=48 | 6,4=24 | 6,4=24 | 4,2=8 | 4,2=8 | 6,2=12 | 6,2=12 | 2,2=4 | 208 |

| Table 5 |

4.5. Correctness of the algorithm
We do not formally prove the algorithm correctness by invariants. The correctness of the algorithm follows from the description of the algorithm. If the bouquets of each representative of an orbit in \(SC(\Pi_L)\) are correct and the whole orbit of each selected vertex in \(SC(\Pi_L)\) is traversed then according to Theorem 4 \(\text{GOO}(A(X_{L-1}))\) and \(B(A(X_{L-1}))\) will be determined correctly. The main problem is to guarantee the correctness of the bouquets but this we proved in the description of the cases CS1, CS2, CS3, CS4. The traversal of the whole orbit of each selected vertex in \(SC(\Pi_L)\) is also guaranteed (Fig. 7).

4.6. Algorithm complexity
For determining both complexities (space and time) we will consider the worst-case for the algorithm – a rigid graph when |Aut(G)|=1: there is no non trivial automorphisms, each vertex in each SC is selected (the search tree is complete), the size of bouquets is largest and the number of comparisons of numberings is maximal (see Fig. 15 for example of the search tree of rigid graph). We’ll consider connected graphs \(G\) with \(k \leq n(n-1)/4\). If \(k \geq n(n-1)/4\) we use the complement graph as it has the same automorphism group. We’ll consider the case when for each level \(L\) the sizes of \(SC(\Pi_L)\) are equal, i.e., for each selected vertex from \(SC(\Pi_L)\) the sizes of \(SC(\Pi_L)\) are equal. We call this kind of a tree **level-regular tree**. All rigid graphs we tested hold this property. Otherwise, we transform the search tree to such a case considering all sizes of \(SC(\Pi_L)\) equal to the maximum size of \(SC(\Pi_L)\) – this way we overestimate the both complexities. We
compute Big-Oh complexities and since Big-Oh is an upper bound we should never underestimate the complexities.

For the analysis we use the following notations: \( b(L) \) for \( |B(L)| \) - the size of all bouquets derived from the selection of each vertex in \( SC(\Pi_L) \), \( e(L) \) for \( |SC(L)| \), \( s(L) \) for the number of all comparisons of numberings derived from the selection of each vertex in \( SC(L) \), \( r(L) \) for the number of the calls of RP for generating all partitions derived from the selection of each vertex in \( SC(\Pi_L) \). The complexities of the heuristic algorithm are determined in Section 7.

### 4.6.1. Space complexity

By definition for the bouquet we have

\[
B(X_L) = \bigcup_{j=1}^{d(L+1)} B(X_{L,j}), \quad L=1, 2, \ldots, LK-1, \text{ where } B(X_L) \text{ is the bouquet of a selected vertex } X_L \text{ in } SC(\Pi_L) \text{ and } B(X_{L,j}) \text{ is the bouquet of } j\text{-th vertex in } SC(\Pi_{L+1}). \]

Then,

\[
|B(X_L)| = \sum_{j=1}^{d(L+1)} |B(X_{L,j})|.
\]

If \( |B(X_{L,j})| = |B(X_{L+1,j})| = \ldots = |B(X_{L+1})| \) then,

\[
|B(X_L)| = |SC(L+1)||B(X_{L+1})|. \]

Otherwise, we may use the maximal size of the bouquet

\[
|B(X_{L+1})|_{\text{max}} = \max(|B_{L+1}^1|, \ldots, |B_{L+1}^{d(L+1)}|) \text{ and then we obtain}
\]

\[
|B(X_L)| \leq |SC(L+1)||B(X_{L+1})|_{\text{max}}.
\]

Thus,

\[
|B(X_L^i)| \leq |SC(2)||SC(3)|\ldots|SC(LK-1)|.
\]

Considering that the partition \( \Pi_L \) has \( L-1 \) selected vertices (in separate cells) then the largest non-singleton cell may have maximum \( n-(L-1) \) vertices, i.e., \( |SC(L)| \leq n-L+1 \). This means that the sizes of \( SC \) for levels \( L=1, 2, \ldots, LK-1 \) are:

\[
|SC(\Pi_L)| \leq n, |SC(\Pi_2)| \leq n-1, |SC(\Pi_3)| \leq n-2, \ldots, |SC(\Pi_{LK-1})| \leq n-LK-2.
\]

Then,

\[
|B(X_L^i)| \leq (n-1)(n-2)\ldots(n-LK+1) = O(n^{LK-2}).
\]

For the graphs of Class6 we have \( LK \leq d=6 \) and

\[
|B(X_L^i)| = O(n^{d-2}) = O(n^4) - \text{this means polynomial space complexity for Class6}.
\]

We also store the intermediate partition for each level \( \Pi_1, \Pi_2, \ldots, \Pi_{LK-1} \). The storage for these partitions is at most \( n.(LK-1) \) but it is negligible compared to \( |B(X_L)| = O(n^{d-2}) \). There are no stored numberings in the algorithm PART2.

### 4.6.2. Time complexity

Let’s first consider the time complexity of the basic operations of the algorithm \( (n, k - \text{the number of graph vertices and edges respectively}) \):

1. The time complexity \( ta(n) \) of RP (see Section 2) is \( ta(n)=O(k.log(n))=O(n^2.log(n)) \) since \( k=O(n^2) \);

2. The time complexity \( tb(n) \) of the comparison of two numberings: for each corresponding vertices \( x \) and \( y \) and the numberings we check for each adjacent vertex \( u \) of \( x \), whether its corresponding vertex \( w \) is adjacent to \( y \). The maximum number of these checks is equal to the maximal vertex degree \( \maxdeg \leq n-L \). Thus all checks we made are \( tb(n)=n.maxdeg \leq n(n-1) = O(n^2) \);

3. The time complexity \( tc(n) \) of determining the code of a numbering: one multiplication of the cell labels (positions) of \( x \) and \( y \) for each edge \( (x,y) \) is made. Thus the number of all multiplications is \( tc(n) = k \leq n(n-1)/2 = O(n^2) \);

4. The time \( td(n) \) for restoring a numbering when given a level \( L \) and the selected vertices \( x_{L_1}, x_{L+1}, \ldots, x_{LK-1} \), \( LK-L \) calls to RP are made. Thus, the time is \( td(n)=(LK-L).O(n^2.log(n))=O(n^2.log(n)) \) since \( LK-L \) is at most \( LK \) and \( LK \) is constant.

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5. The time for te(n) selecting a cell with maximal partitioning ability is te(n) = O(n^2) since the maximal length of a partition is n-1, i.e. the pass through all cells of the partition has maximum n-1 steps and for one vertex x in a cell we check for each adjacent vertex of x to define its cell label. The number of these checks is O(n) since the number of adjacent vertices of a vertex is O(n).

6. For each selected vertex x in SC(L) we do a forward move (FM): (a) obtaining the transformed partition \( \Pi_{L+1} = TR(x, \Pi_L) \); (b) refining this partition \( \Pi_{L+1} = RA(\Pi_{L+1}) \); (c) selecting SC(\( \Pi_{L+1} \)) (d) selection of a vertex \( X_{L+1} \) in SC(L+1). The times for these operations are respectively: (a) O(n); (b) \( O(n^2 . \log(n)) \); (c) O(n^2) and (d) O(n).

We simplify the analysis considering only the most time consuming operations. The total time complexity of the algorithm is T(n) = T1(n) + T2(n) where T1(n) is the time of all forward moves (calls of RP) for generating all partitions needed in the algorithm and T2(n) is the time for comparing the numberings. The number of the selected vertices, i.e. the number of forward move operations (denoted NR) is NR=NR1+NR2, respectively for the first (NR1) and for the second (NR2) part of the algorithm. NR1 includes 1 call for starting partition, 1 call for the first selected vertex \( X_1 \) in SC(1), NR1(2) for the selected vertices in SC(2) = |SC(2)|+ |SC(2)|.NR1(3). For any SC(L) we have the recurrence equation NR1(L)= |SC(L)|+ |SC(L)|.NR1(L+1)= |SC(L)|+(1+ NR1(L+1)), since for each SC(L) we select each vertex, i.e. [SC(L)] selections and for each selection in SC(L) we have NR1(L+1) selections, derived from each selection in SC(L+1).

The solution of this equation is

\[
NR1(L)= |SC(L)|+ |SC(L)|.NR1(L+1)= |SC(L)|+(1+ |SC(L)|. . . . +|SC(L)|. ). .
\]

Considering that |SC(L)| ≤ n-L+1 we obtain

\[
NR1(L) ≤ (n-1) + (n-2) + (n-3) + . . . . + (n-LK+3) (1+n-LK+2) . . . . ) = O(n^{LK-2})
\]

Obviously NR2 = (|SC(1)| - 1)(LK – 1) – for each vertex from SC(1) excluding \( X_1 \) we have maximum LK-1 selected vertices and LK-1 forward moves. Thus, NR=NR1+NR2= O(n^{LK-2}) + (|SC(1)| - 1)(LK – 1) ≤ O(n^{LK-2}) + (n-1) (LK-1) = O(n^{LK-2}) and T1(n)=NR. O(n^2 . \log(n))= O(n^{LK-2}).O(n^2 . \log(n))= O(n^{LK}. \log(n)) - polynomial time complexity.

The above formula is not changed if we consider the time for computing the code of each numbering of the bouquet B(X_1).

For each level L we have:

- \( b(L)=b(L+1).c(L+1), L=LK-2, . . . . , 1; b(LK-1)=1 \), where \( b(L) \) is the bouquet size of one selected vertex from SC(L). It follows from the definition of \( b(L) \).

- \( s(L)=\frac{c(L)(c(L)-1)}{2}.b(L)+c(L).s(L), L=LK-1, . . . . , 2; s(LK)=1 \), where \( s(L) \) is the number of all comparisons of numberings derived from a selection of each vertex in SC(L). The first member \( c(L).c(L-1)b(L)/2 \) of the above formula is the number of all comparisons of the first numbering derived from vertex \( x \) in SC(L) with the bouquets of the vertices in SC(L) positioned before vertex \( x \). The sizes of these bouquets are: \( b(L) \) for the vertex on position 2, 2b(L) – for position 3, (i-1). b(L) – for position i and (c(L)-1).b(L) – for position c(L). Consequently, the total number of these comparisons is \( c(L).c(L-1)b(L)/2 \).b(L/2). The second member \( c(L).s(L+1) \) of the above formula is the number \( s(L+1) \) of all comparisons of numberings made for level L+1 when each vertex from SC(L) is selected.

Now, we’ll do Big-O estimation of these two equations for each level L:

- \( b(L)=b(L+1).c(L+1), b(LK-2)=c(LK-1).b(LK-1)=c(LK-1)=O(n), b(LK-3)=c(LK-2).b(LK-2)=c(LK-1), c(LK-2)=O(n^2), . . . . , b(L)=\prod_{i=LK-2}^{L} c(i) = O(n^{LK-L-1}) \) since \( c(L)=O(n) \).

- \( s(L)=c(L).c(L-1)b(L)/2+c(L).s(L+1), s(L)=O(n^2), s(LK-2)=O(n^{LK-L-1})+O(n), s(LK-1)=O(n^{LK-L-1})+O(n), s(LK)=O(n^2), \)

\( s(LK-1)=O(n^2)+O(n), s(LK)=O(n^2)+O(n)=O(n^2), \)

\( s(LK-2)=O(n^2)+O(n), s(LK-1)=O(n^3)+O(n). O(n^2)=O(n^3) \).
s(LK-3)=O(n^4)+O(n).s(LK-2)=O(n^4)+O(n). O(n^2)=O(n^4),...,s(L)=O(n^{LK-L+1}), s(2)=O(n^{LK-1}).

Then, T2″=s(2).O(n^2)=O(n^{LK+1}).

For the second part of the algorithm we have T2″″=|SC(L)|.b(1).O(n^2)=(c(1)-1).b(1).O(n^2)=n-1).O(n^{LK-1}). In the analysis for the comparisons of numberings we don’t consider the effect of the coefficient reducing the number of the comparisons only between those with equal codes. This effect does not influence the asymptotical estimation but it is considerable on real program implementation. Our experimental tests on very large number of graphs confirm this.

Finally, T2=T2″+T2″″=O(n^{LK+1})+O(n^{LK+1})=O(n^{LK+1}) and

T=T1+T2=O(n^{LK}.log(n))+O(n^{LK+1})=O(n^{LK+1}).

This means that T=O(n^5) for the graphs of Class6 with LK ≤ 6. The experiments showed that the running time of the algorithm is quite less than O(n^5) because O(n^5) is overestimated. For the general case LK=O(n), T=O(n^{O(n)}), i.e. exponential time complexity.

4.6.3. A note on the time complexity of the algorithm for an arbitrary undirected graph

We proved that Algorithm Vsep-e has polynomial time complexity for any graph G∈Class6. We do not consider here the algorithm called VsepARN1 for determining GOO(G) of any undirected graph, connected or disconnected. It is known [11] that the automorphism group Aut(G) for the graph G whose connected components consist of n1 copies of G1, . . . , ni copies of Gi, where G1, . . . , Gi are pairwise non-isomorphic, is defined as

```
Aut(G) = (Aut(G1) o S_n1) x ... x (Aut(Gi) o S_ni),
```

where x is for the direct product of two permutation group and o is for the wreath product of ni copies of a permutation group Gi[11].

We’ll do some considerations about the time complexity of VsepARN1 when it is applied to a connected graph G ∈ Class6. In this case we take the complement \( \overline{G} \) and find its connected components C1, . . . , Cn and for each component C_i we find its complement \( \overline{C_i} \) and its connected components. This process continues until a state when all connected components of G are in Class6. Then, we apply Vsep-e to each component and the graph isomorphism algorithm called ISOM for each two components C_i, C_j, j>i. This takes \( p(p+1)/2 \) execution of Vsep-e and ISOM in the worst case when each pair are non-isomorphic. We do not describe here the graph isomorphism algorithm ISOM since it is very similar to Vsep-e and has the same time and space complexity. The same operations are performed for an arbitrary undirected graph. Both operations (determining \( \overline{G} \) and connected components of a graph) takes \( O(n^3) \) steps. Thus, the time complexity of VsepARN1 is polynomial since the number of the new operations needed for G ∈ Class6 and the operations themselves are polynomial.

5. The heuristic algorithms (Vsep-H1, Vsep-h2)

They are based on Theorem 3. For determining whether two vertices x and y are similar two partial bouquets are built for both vertices and then, some automorphisms between the numberings of these bouquets are determined. To determine certainly that x and y are similar one of the bouquets should be full. Consequently, the probability to find at least one automorphism mapping x to y is less than 1 if we use the algorithm with partial bouquets. This makes the algorithms inexact. Instead, less time is needed for bouquets building and less storage is needed for them because of their smaller sizes. We describe two heuristic algorithms (Vsep-H1, Vsep-h2) in this section.

5.1. Algorithm Vsep-H1

It has two main steps S1 and S2:

S1) Determine the orbits Orb(G, Π) by an heuristic algorithm TABLE (fig. 18) applied with a parameter LB = 1;

S2) Use the algorithms PART1, PART2 to determine GOO(G, ΠORB) of the orbit partition ΠORB found in S1.
TABLE does not guarantee the computation of the exact orbits of GOO(G, Π) and consequently Vsep-H1 is an heuristic algorithm - it does not guarantee the computation of the exact GOO(G, Π). But if the parameters of Vsep-H1 are selected in proper way the probability of the exact computation of GOO(G, Π) is very close to 1.

5.2. Algorithm Vsep-h2
In the heuristic algorithm Vsep-h2 (Fig. 17) a highway of partitions for levels (called basic) LB=1, 2, . . . , LK-1 is built. The generators and the orbits of the stabilizer \( A_{LB-1} = A(x_1, x_2, \ldots, x_{LB-1}) \) are determined for each basic level LB by the heuristic algorithm TABLE (Fig. 18). Then, SC(LB) is determined and a vertex from the first minimal orbit of \( A_{LB-1} \) is selected in it and a forward move is made (LB=LB+1). The same is done for the new level LB – it continues until a discrete partition is obtained. Then, the determination of \( |A| \) by the orbit-stabilizer Theorem follows:

\[
|A_{LB}| = |\text{Orb}(x_{LB+1}, A_{LB})| = |A_{LB+1}| \quad \text{for} \quad LB = \text{LK-2, LK-3, . . . , 1, 0}; \quad |A| = |A_0| = |\text{Aut}(G)|;
\]

1. The heuristic algorithm TABLE (Fig. 19) starts from a state where each vertex is in a separate orbit. After that, the algorithm makes a fork for SC(LB), i.e. each vertex is selected, a SFM1 is made and each new numbering is compared with the previous numberings for determining new automorphisms that unite orbits. Each new automorphism that unites orbits for the level LB is stored in separate section for this level.

2. A regular selection tree (RST) is built for each representative of a given number \( nm1 \) of minimal orbits from SC(LB), i.e. a forward move is made and in each SC(L), L> LB, a fixed number of vertices is selected and a forward move is made again for each vertex until a discrete partition is obtained which, afterwards, is compared with the previous numberings for determining new automorphisms and orbits. If the determined automorphism unites orbits for the level LB then it is stored in separate section for this level as in step S2. Besides, it is checked if the given automorphism unites orbits for lower levels L< LB and in case there is such an union a backward move to the level L is made;

3. The building of RST is performed for the next orbit representative if there was a union of orbits from the RST for the previous orbit representative. If there was no such a union the building of RST is performed for each of the next orbit representatives \( nm1 = k1.nmorb \) times (\( nmorb \) – the current number of the orbits, \( 0 < k1 \leq l \)) or for all orbit representatives if \( nm1 > brorb \). Most often in practice \( 0.3 \leq k1 \leq 0.4 \);

4. The number \( nm2 \) of the vertices that are selected in SC(L) is usually 5 or 6 in a regular tree. These vertices are selected successively, starting from the beginning of SC(L) by step \( \geq 1 \). The experiments show that when these vertices are evenly distributed in SC(L) the results are more correct compared with other ways of distribution.

The automorphisms found in (1) and (2) are generators for \( A_{LB+1} \) if they unite orbits for the level LB. The generating set is determined in the following order:

\[
gen(A(x_{L1,1})) \subseteq gen(A(x_{L1,2})) \subseteq \ldots \subseteq gen(A(x_2)) \subseteq gen(A(x_1)) \subseteq gen(A).
\]

Starting with discrete orbits and \( gen(A) = \emptyset \) each generator from \( gen(A(X_{LB})) \), LB= LK-1, LK-2, . . . , 1, 0 is included into \( gen(A) \) if it unites the current orbits Orb(A).

The heuristic algorithm has been tested for the most known ‘difficult’ graphs of projective planes of different orders (9, 16, 25, 27, 49) with the corresponding number of vertices \( n=182, 546, 1302, 1514 \) and 4902. The results of these tests for minimum \( T_{\text{min}} \) and maximum \( T_{\text{max}} \) runtime are shown on Table 8 and Fig.19 and 20 in Section 6. These times are many times less than the times of the exact algorithm. These results show that the experimental time complexity is of order \( O(n^2) \). Even more, the computed by this algorithm orbits and order of the automorphism group on all tested graph are correct – this fact shows that the algorithm is almost exact.
Input: Graph $G(V,E)$ and a partition $\Pi$ on $V$
Output: Generators, orbits and order of the partition-wise stabilizer $A=\text{Aut}(G, \Pi)$, denoted $\text{GOO}(A)$

S1. Initial settings: $L:=1; \ Pi_{L}:=[1,2,3, \ldots , n]; \ Pi_{L}:=\text{RP}(\Pi_{L}, \text{BRCL}); \{\text{BRCL}-number of \ Pi_{L} \text{ cells}\};$
S2. if $\text{BRCL}=\Pi_{1}$ (\Pi_{1} \text{ is discrete}) then begin writeln('Asymmetric graph'); exit end;
S3. LB:=1; \{ LB is a basic level\}
S4. repeat
S5. TABLE (LB, Orb(LB), L) – an heuristic algorithm for determination of orbits of a stabilizer $A_{LB}=A(x_{1}, x_{2}, \ldots , x_{LB-1})$; Orbits for each level LB are stored in a row LB of two-dimensional array. If there is an orbits union for level L < LB from the found automorphisms for LB, then LB:= L; goto S5 – this is a move back;
S6. Forward move: Determine SC(LB ); Select vertex $X_{LB}$ – a representative of the minimal orbit in SC(LB ); $LB:=LB+1; \ Pi_{LB}^{T}=\text{TR}(x_{LB}, \Pi_{LB-1}); \ Pi_{LB}:= \text{RP}(\Pi_{LB}^{T})$
S7. until $\Pi_{LB}$ becomes discrete;
S8. Determine $|A|$ by the orbit-stabilizer theorem : $|A_{LK}|=1$;
\[
|A_{LB}| = |\text{Orb}(x_{LB+1},A_{LB})| \ast |A_{LB+1} | \text{ for } LB= LK-2, LK-3, \ldots , 1, 0, \text{ where } |A_{0}| = |A|=|\text{Aut}(G)|;
\]
Starting with discrete orbits and $\text{gen}(A)=\emptyset$ each generator from $\text{gen}(A(LB))$, $LB= LK-1, LK-2, \ldots , 1, 0$ is included into $\text{gen}(A)$ if it unites the orbits $\text{Orb}(A)$.

Fig. 17. Heuristic algorithm Vsep-h2

5.3. Complexity of Vsep-h2
Again we’ll consider the worst-case complexity – a rigid graph when each vertex in each SC is selected and consequently both complexities are the worst. We again consider a search tree as a level-regular tree (see Section 4.6)

5.3.1. Space complexity
At each basic level LB at most the following numberings are generated: (a) $n-L+1$ for the fork; (b) $k_{1}(n-L+1)b^{2Lk-1}$, where $k_{1}(n-L+1)$ is the number of the selected vertices in SC(L) and $b^{2Lk-1}$ is the number of the numberings of the regular selection tree RST(L). The total number of the generated numberings for all levels $L=1, \ldots , LK-1$ is

\[
\sum_{L=1}^{LK-1}(n-L+1)+k_{1}(n-L+1)b^{2Lk-1} = (LK-1)\frac{2n-LK+2}{2} + k_{1}b^{2Lk-1}((n+1)\sum_{L=1}^{LK-1}b^{2L} - \sum_{L=1}^{LK-1}Lb^{2L}) = \]

$= O(n)$, since there are only two members of the formula that depends linearly on $n$ considering $LK$ as a constant.

5.3.2. Time complexity
A) Let’s first determine the number $r=r_{1}+r_{2}$ of numberings comparisons, $r_{1}$-for the operation fork, $r_{2}$-for the level-regular tree.
For each level L for SC(L) the following comparisons are made : vertex x on position i in SC(L) is compared with all vertices on position less than i in SC(L), i.e. for the SC(L) the number of comparisons is $\sum_{i=2}^{L}(i-1) = \frac{c(L)(c(L)-1)}{2}$ and for all levels we have

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\[
rl = \sum_{L=1}^{LK-1} \frac{c(L)(c(L)-1)}{2} \quad \text{and since } c(L) \leq n-L+1 \text{ we have } \quad rl \leq \sum_{L=1}^{LK-1} \frac{(n-L+1)(n-L)}{2} = O(n^2). \quad \text{Then,} \quad T1=r1.O(n^2)=O(n^4).
\]

**Input:** a level LB  
**Output:** Generators and orbits of the stabilizer \(A(x_1, x_2, \ldots, x_{LB-1})=A(LB-1)\);  

**T1. Initialization:** Set \(\text{Orb}(A(LB-1))\) to discrete orbits; \(\text{gen}(A(LB-1))=\emptyset\).  

T2. Generate one numbering for each vertex \(x_{\text{SC}(LB)}\) by series of forward move and compare it for an automorphism \(\alpha\) with the previous numberings: \(\text{gen}(A(LB-1))=\text{gen}(A(LB-1)) \cup \{\alpha\}\). We call this operation a *fork*. It determines the automorphisms that make unions of orbits for level LB. If there is an orbits union for level \(L<LB\) then follows exit  

T3. A forest of regular search trees (FRST) is built for a number \(nm1\) of representatives of the orbits in \(\text{SC}(LB)\) determined so far and sorted in increasing order of their lengths starting from the smallest one - \(nm1=kl.nmorb\) where \(nmorb\) is the number of orbits for the level LB and \(k1\) is a given coefficient, \(0<k1\leq1\). Each representative \(x\) of the orbit is a root of the tree. The regular search tree (denoted \(\text{RST}(LB, x)\)) is built for each \(x \in \text{SC}(LB)\). The depth of the RST is \(D\). Each node of the RST corresponds to selection level \(L, LB < L \leq LB+D\) and a target cell \(\text{SC}(L)\). In each \(\text{SC}(L)\) a fixed number \(nm2\) of vertices \(y\) are selected, then a forward move to next level is made for each \(y\). In the level LB+D only a series of forward moves SFM is made for each selected vertex until a discrete partition is obtained. The number \(nm2\) is usually 5 or 6 – it may be regarded as out-degree of the node. These vertices in \(\text{SC}(L)\) are selected successively by step \(w \geq 1\) starting from the beginning of \(\text{SC}(L)\), i.e. they are evenly distributed in \(\text{SC}(L)\). For determination of an automorphism \(\alpha\) and orbits each numbering is compared with the previous numberings: \(\text{gen}(A(LB-1))=\text{gen}(A(LB-1)) \cup \{\alpha\}\). Algorithm stops when: (a) the number of coincidences of the number of the found orbits for different RSTs becomes equal to \(nm1\); (b) RSTs are generated for all representatives of the found orbits; (c) there is an orbits union for a level \(L<LB\).

**Fig. 18. Algorithm TABLE**

Now \(r2=?\) Each first numbering derived from the selection of each vertex \(x\) in \(\text{SC}(L)\) is compared with the bouquets of the vertices preceding \(x\) in \(\text{SC}(L)\), i.e. for the second vertex the number is \(b(L+1)\), for the third \(-2.b(L+1), \ldots, \) for the vertex in position \(c(L)-(c(L+1)-1).b(L+1)\), i.e. totally for a given \(\text{SC}(L)\) we have \(b(L+1)\sum_{i=1}^{c(L)-1} i = \frac{c(L)(c(L)-1)}{2}b(L+1)\).

For all levels we have

\[
r2 = \sum_{L=1}^{LK-1} \frac{c(L)(c(L)-1)}{2}b(L+1) \leq \sum_{L=1}^{LK-1} \frac{(n-L+1)(n-L)}{2}k1(n-L+1)b2^{LK-L-2} = O(n^3).
\]

Then, \(T2=2.O(n^3)=O(n^5)\).

B) The time for the forward move – we have to determine the number \(r=r3+r4\) of selections of vertices, where \(r3\) is for the number of selections in fork operation and \(r4\)- for the number of selections during the generating the level-regular trees. Respectively, T3 and T4 are the times for these cases.

\(r3=?\) For each vertex in \(\text{SC}(L)\) the number of selections is \(LK-L\) for obtaining a discrete partition and for the whole \(\text{SC}(L)\) the number is \(c(L)(L-L)\). For all levels we have

\[
r3 = \sum_{L=1}^{LK-1} c(L)(LK-L) \leq \sum_{L=1}^{LK-1} (n-L+1)(LK-L) = O(n)\text{. Then,} \quad T3=r3.O(n^2.\log(n))=O(n). \quad O(n^2.\log(n))=O(n^3.\log(n)).
\]
Now \( r_4 = ? \)
For a given \( SC(L) \) we have number of selections \( ns = k_1.c(L) + k_1.c(L).b_2^{LK-L-1} \)
where \( k_1.c(L) \) is the number of selections made in the basic cell \( SC(L) \) and \( k_1.c(L).b_2^{LK-L-1} \) is the number of selections made during the generation of the level-regular trees.

For all levels we have
\[
r_4 = \sum_{L=1}^{LK-1} k_1.c(L)(1 + b_2^{LK-L-1}) \leq k_1 \sum_{L=1}^{LK-1} (n - L + 1)(1 + b_2^{LK-L-1}) = O(n).
\]

Then, \( T_4 = r_4.O(n^2 \cdot \log(n)) = O(n) \). \( O(n^2 \cdot \log(n)) = O(n^3 \cdot \log(n)) \).

Thus the total time complexity of the heuristic algorithm is
\[
T = T_1 + T_2 + T_3 + T_4 = O(n^3) + O(n^3) + O(n^3 \cdot \log(n)) + O(n^3 \cdot \log(n)) = O(n^5).
\]

This time complexity is overestimated since many important coefficients for the algorithm are not considered. That why the experimental time complexity is less than \( O(n^5) \). Of course, the time complexity of the heuristic algorithm is less than the time complexity of the exact algorithm.

6. Experimental results
In this section we present experiments that compare the performance of our algorithms with Traces (from nauty2.5r7 [41]) – one of the most competitive known tool for the worst cases. The most difficult graphs for our algorithms are the graphs with \( |Aut(G)| = 1 \) or with small \( |Aut(G)| \). It is known that none of the known algorithms outperform others for all graphs. For each algorithm there are difficult and easy graph families. Given graph family maybe easy for one algorithm and very difficult for another. The same is for Vsep and Traces. Even more, for Vsep different cell selectors give different running times – none of the cell selectors outperform others. The chooser of cell selectors does not always choose the optimal cell selector. For each result we show the cell selector for which it is obtained. The experiments were carried out on a laptop Dell, CPU: Intel(R) Core (TM) i5-3317U @ 1.7 GHz, Memory: 8 GB, OS: 64 bit Microsoft Windows 7 Ultimate. For the experiments, we have used all the benchmark graphs of nauty&Traces page [41], which include a variety of graph families with different characteristics. We show mostly the results for the graphs that are worst cases for either of the compared tools and cell selectors for which they are obtained (only for Vsep). It is evident from table below that Vsep outperforms Traces considerably for the graphs tnn(39)_1014-1 and chh_cc(7-7)_1078-1. On the other side Traces outperforms Vsep considerably for the graphs of projective planes (pp-16-14, 15, 22, pp-25-90, 116), had-176 and latin-sw-112. There are no essential differences between Vsep and Traces on the other graphs on the table! Traces is slow for the graphs with large order of the automorphism group and large number of generators – my experience show that this is maybe due to the use of Schreier-Sims method. The main disadvantage of Vsep-e is the storing of the whole bouquet of the first selected vertex- millions of words for some graphs. For some of the graph families the heuristic version Vsep-H1 is exact and gives the same running time as the exact one, for others it is many times faster and at correctly chosen parameters gives the correct results. Only some of the worst cases for the exact algorithm Vsep-e are also difficult cases for Vsep-h1 – for example, the graphs had-176 and latin-sw-30-1. The heuristic version Vsep-h2 has also hard cases (the results are not shown in the table) – the graphs for which the maximal selection level LMAX is very large - for example, LMAX ≥ 38 for graphs tnn(7)_181-1 and larger in the family tnn.

7. Concluding remarks and open problems
Three new algorithms for determining the generators, orbits and order of the graph automorphism group are presented: one exact (Vsep-e) and two heuristic (Vsep-h1, Vsep-h2). A new method for developing algorithms is used in the exact algorithm: if during its execution some of the searched or intermediate variables obtain a wrong value then the algorithm continues from a new start point losing some of the results determined so far (cases CS3, CS4). The new start point is such that the correct results can be obtained. The worst case time complexity of Vsep-e for an arbitrary graph is exponential but for Class6 it is polynomial. The main difference of the exact one and the well-known tools is the storing of the whole bouquet of the first selected vertex in the first level. Seven cell selectors are used in the algorithms and a
The worst cases made requirements for memory are very small. The chooser of optimal cell selector is presented. Some of the cell selectors are new, namely CSL-4, CSL-5, CSL-6 and CSL-7. Experimental comparison of the proposed algorithms with the algorithm Traces is made - it shows their worst and best cases. A disadvantage of the algorithm Vsep-e is its higher requirements for memory (for some worst cases several millions of numbers are stored. The worst cases for the algorithm Vsep-e are the graphs with smaller order |Aut(G)|, especially the rigid graphs. The heuristic algorithms Vsep-h1, Vsep-h2 are extremely fast (with some exceptions) compared with the exact one and are almost exact - for all tested thousands graphs they give correct results. Practically, their requirements for memory are very small.

| Graph, n*,minval,* Maxval* | [Aut(G)] | norb* | T in seconds |
|----------------------------|---------|-------|--------------|
|                            |         |       | Traces | Vsep-e*, CSL*, Bouquet size* | Vsep-h1*, CSL |
| tmn(39)_1014-1, 1014, 4, 312 | 6.314790834154e174 | 12 | 4 runs: 1183.08, 2900.09, 7681.50, 4261.06 | 1.34, CSL-4, 1 | 1.34, nink |
| cmz-50, 1200, 2.5 | 1.267650600228e32 | 8 | 0.01 | 0.51, CSL-6, 1 | 0.51, nink2 |
| ag-49, 4851, 49,50 | 2.710632960000e10 | 2 | 0.06 | 0.156, CSL-5, 2 | 0.17, nink1 |
| cif-200,2000, 3, 3 | 2.535301200456e30 | 800 | 0.16 | 1.42, CSL-1, CSL-2, 1 | 1.42, 1 to 2 |
| chh_cc(7-7)_1078-1 1078,3,45 | 4.907372642035e71 | 8 | 5859.28 | 0.57, CSL-1, 1, 15836 | 0.37, 1 |
| Had-112 448,113,113 | 1677312 | 1 | 0.08 | 130.07, CSL-4, 31994 | 148.39, 4 |
| Had-176, 704,177,177 | 15257088 | 1 | 0.05 | 747.73, CSL-1, 21210 | 741.52, 3 |
| Had-256, 1024,257,257 | 1.401962828716e24 | 1 | 0.03 | 0.61,(all CSL but CSL-6),1 | 0.686,1,1, 0.62,1,1 |
| latin-30,dre, 900,87,87 | 43200 | 1 | 0.00 | 0.468, CSL-2 0.92, CSL-1,1512 | 1.59,1 |
| Latin-sw-30-1, 900,87,87 | 900 | 1 | 0.17 | 14.21, CSL-1, 1,812 | 14.24, 1 |
| had-sw-112, 448,113,113 | 224 | 2 | 1.84 | 326.70, CSL-4, 519624 | 4.25,3 5.76,3 |
| lattice-30,dre, 900,58,58 | 1.407181592771e65 | 1 | 0.12 | 0.11, CSL-1,1 | 0.1404, 1 |
| 10cube, 1024,10,10 | 3.715891200e9 | 1 | 0.17 | 0.6200E-01 CSL-1,1 | 0.1248, 1 |
| paley-461,dre, 461,230,230 | 1.06030e5 | 1 | 0.00 | 0.1092, CSL-1,1 | 0.1248, 1 |
| pg2-49, 4902,50,50 | 1.328752276992e14 | 1 | 0.20 | 1.61, CSL-1,121 | 1.61, 1 |
| pp-16-14, 546,17,17 | 2304 | 14 | 1.19 | 65.3, CSL-4, 420960 | 0.20, 3 |
| pp-16-22, 546,17,17 | 9216 | 10 | 0.59 | 17.21, CSL-4, 117264 | 0.357,3 0.343,4 |
| pp-25-1, 1302,26,26 | 609336000000 | 2 | 0.03 | 0.22, CSL-4,10 | 0.09, 3 |
| pp-25-90, 1302,26,26 | 1000 | 40 | 40.00,60.83, 111.56,90.62 | 2621.00, CSL-4, 5016276 | 6.08, 3 |
| pp-25-116, 1302,26,26 | 500 | 64 | 150.73, 58.34, 180.85 | 5951.08, CSL-4, 10784808 | 7.39, 3,4 |

Table 5. * n - number of vertices, norb-number of orbits, vsep-e (prgrarn t5j12c), vsep-e1 (program ef5), cs: cell selector, minval, maxval - minimal and maximal degree of a vertex of the graph, Bouquet size – number of the stored nonequivalent discrete partitions
The future work on developing Vsep algorithms will include: a) use of the Schreier-Sims algorithm in some suitable parts of the Vsep algorithms; b) search for a new cell selector that will reduce the size of the search tree; c) search for a new chooser of a cell selector; d) develop a new algorithm that unites the three Vsep algorithms; e) conduct a comparison of Vsep algorithms with other known GAG algorithms.

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