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Algebraic Combinatorics in Mathematical Chemistry.  
Methods and Algorithms.  
II. Program Implementation of the Weisfeiler-Leman Algorithm

Preliminary Version

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Abstract

The stabilization algorithm of Weisfeiler and Leman has as an input any square matrix $A$ of order $n$ and returns the minimal cellular (coherent) algebra $W(A)$ which includes $A$.

In case when $A = A(\Gamma)$ is the adjacency matrix of a graph $\Gamma$ the algorithm examines all configurations in $\Gamma$ having three vertices and, according to this information, partitions vertices and ordered pairs of vertices into equivalence classes. The resulting construction allows to associate to each graph $\Gamma$ a matrix algebra $W(\Gamma) := W(A(\Gamma))$ which is an invariant of the graph $\Gamma$. For many classes of graphs, in particular for most of the molecular graphs, the algebra $W(\Gamma)$ coincides with the centralizer algebra of the automorphism group $\text{Aut}(\Gamma)$. In such a case the partition returned by the stabilization algorithm is equal to the partition into orbits of $\text{Aut}(\Gamma)$.

We give algebraic and combinatorial descriptions of the Weisfeiler–Leman algorithm and present an efficient computer implementation of the algorithm written in C. The results obtained by testing the program on a considerable number of examples of graphs, in particular on some chemical molecular graphs, are also included.
1 Introduction

The fundamental problem of graph symmetry perception arises in numerous areas of chemistry and physics. In this context molecules are modelled by graphs where the vertices represent atoms and the edges represent bonds. The aim is to find equivalence classes of “elements” (e.g. vertices, edges, pairs of vertices, subgraphs etc.) of the graph, or more rigorously, the orbits of the action of the automorphism group Aut(Γ) of the graph Γ on the set of all “elements” of a considered “mode” (for example the orbits of Aut(Γ) on the set of vertices). It is clear that in order to use such a statement one has to get at some intermediate stage a convenient description of Aut(Γ).

However, usually chemists avoid the computation of Aut(Γ), preferring to use certain invariants in order to get a classification of “elements” of the graph.

Let us express the above claim more accurately for the case of vertices. A vertex invariant in a graph Γ is a property or a parameter of vertices which is preserved by any of its automorphisms, i.e. the property does not depend on the labelling of the graph. Let φ be a function which is defined on the set of all vertices of Γ. Then φ is an invariant of vertices if φ(x) = φ(x’) whenever the vertices x, x’ belong to the same orbit of Aut(Γ).

Let us now consider a certain invariant (a set of invariants). Then we may define that two vertices belong to the same equivalence class if and only if they have the same value of the invariant (invariants) being taken into account. Whatever the classification approach, the resulting partition cannot be finer than the partition into the orbits of the automorphism group (the automorphism partition).

From an algorithmical point of view the main goal in classification of vertices is to find an algorithm which ensures to produce the automorphism partition of a graph and which is known to be theoretically efficient (this means that the running time is restricted by a polynomial in the size of the input). However, all known polynomial time methods for the automorphism partitioning problem yield heuristic solutions, i.e. they result in partitions where the equivalence classes are orbits or unions of orbits.

It is well known (see e.g. [ReaC77], [Pon94c]) that the automorphism partitioning problem (which is strongly related to the problem of graph symmetry\(^1\)) is algorithmically equivalent to the graph isomorphism problem (the problem of graph identification) in the following sense. Assume that a polynomial algorithm is given solving one of the two problems. Then it is possible to construct from this algorithm a second polynomial algorithm which solves the other problem. However, both problems seem to be hard from a computational point of view. Therefore heuristic approaches are still considered as practically helpfull.

\(^1\)In this paper we are not interested in finding the automorphism group of a graph (what is commonly meant by solving the problem of graph symmetry) but rather in finding the automorphism partition.
The simplest of these approaches are restricted to a classification of vertices (in chemical terms they determine atom equivalence only) and are based on different techniques, often applied iteratively, using the valencies of the vertices. The major weakness of these methods is that they will not give any partition for regular graphs (graphs where all vertices have the same valencies). For that reason it seems quite natural to extend these techniques to a classification of vertices and edges (i.e. atoms and pairs of atoms). Now, not only configurations of two vertices (which define the valencies) but also configurations consisting of three vertices have to be considered. This is exactly the basic idea of the algorithm of Weisfeiler and Leman. It partitions all vertices and ordered pairs of vertices of a graph by examining all ordered triples of vertices. This approach turns out to be the most powerful method in some class of graph symmetry perception algorithms.

The algebraic object which is constructed in this way and which has been introduced by Weisfeiler and Leman in [Wei68] is a cellular algebra. It is an invariant of the underlying graph. Under a different point of view (without any relation to the automorphism partitioning problem) this object has also been found and called coherent configuration by Higman in [Hig70]. In greater detail, Weisfeiler-Leman's approach was described (in English) in [Wei76]. However, during approximately twenty years, their ideas were completely unknown and neglected in mathematical chemistry. Nowadays, the approach itself and its interrelations with the identification and symmetry perception of graphs are rather familiar to the experts in algebraic combinatorics (see e.g. [Hig87], [Fri89], [FarL90], [Pon93b], [Pon94b], [FarKM94]), however a careful investigation of its abilities still remains a topical problem.

More or less the same as Weisfeiler-Leman's approach was independently elaborated by G. Tinhofer (partly in joint work with his student J. Hinteregger) in [Tin75] and [HinT77], however without explicitly describing the resulting algebraic object. In 1989, Ch. and G. Rücker (a chemist and a mathematician) realized the necessity of having a method for the partition of atom pairs, and produced a heuristic computer program for that purpose by simple reasoning without using any group theoretical machinery [RueR90a], [RueR90b], [RueR91].

The main purpose of our paper is not only to draw attention to the algorithm of Weisfeiler and Leman but, mainly, to present a good and practical program implementation. To our knowledge, no such implementation exists up to now. Only few attempts were made in the past. A first version of our program has been described by I.V. Chuvaeva, M. Klin and D.V. Pasechnik in [ChuKP92]. By means of a very careful revision we now realized all advantages and disadvantages of this implementation. Recently, L. Babel established in [Bab95] the theoretical complexity of the Weisfeiler-Leman algorithm and, using these considerations, also created a computer program. A detailed description is given in [BabBLT97]. Our common experiences (including some important suggestions of Ch. Pech) enabled us to modify the version of the program by Chuvaeva et al. into a very fast program implementation. A comparison with the program of Babel et al. shows that our program, although inferior with respect to theoretical complexity, is much more efficient from a practical point of view.

This paper is organized as follows. In Section 2 we introduce the standard terminology and some basic definitions. After that a brief survey on previous approaches to graph stabilization is given in Section 3. Section 4 contains the definitions of a cellular algebra and related algebraic
objects, states some important properties and interpretations and introduces the cellular algebra which is associated to a given graph. In Section 5 an algebraic description of the algorithm of Weisfeiler and Leman is presented, followed in Section 6 by a more illustrating combinatorial interpretation. Thus, the algorithm is exposed from two different points of view, the first using matrix notation, the second using graph theoretical notation. Sections 7 and 8 give a description of the program implementation and an estimation of its complexity. Furthermore, in a brief excursion we present the main ideas of the complexity considerations and of the implementation of Babel's algorithm. Finally, in Section 9, extended testing of our program on a large number of examples is documented in order to demonstrate its capability. We conclude with a discussion in Section 10.

This work is the second contribution in a series of papers [KliRRT95], [FurKT] concerning different aspects of algebraic combinatorics with emphasis on applications in mathematical chemistry. The series introduces the basic concepts of algebraic combinatorics and presents some of the main features and tools for perception of symmetry properties of combinatorial objects. Those readers who are not familiar with mathematical standard definitions and notations such as matrix, group, basis, equivalence class, etc. are referred to the first paper [KliRRT95] in this series. However, we tried to make this work as self-contained as possible and hope that it should be understandable for readers with a rather limited knowledge of mathematics.
2 Preliminaries

An undirected graph is a pair $\Gamma = (\Omega, E)$ consisting of finite sets $\Omega$ and $E$, the vertices and the edges. Each edge connects two different vertices $u$ and $v$ from $\Omega$ and is denoted by $\{u, v\}$. This means that each element from $E$ is an unordered pair of different vertices from $\Omega$. A directed graph is a pair $\Delta = (\Omega, R)$ with vertex set $\Omega$ and arc set $R$, where each arc, denoted by $(u, v)$, links two different vertices $u$ and $v$ and additionally is assigned a direction, namely from $u$ to $v$. Each element of $R$ is an ordered pair of different vertices from $\Omega$. If a vertex $u$ belongs to an edge or an arc then $u$ is said to be incident to the edge or arc. Often it is convenient or useful to consider an undirected graph $\Gamma$ as a directed graph $\Delta$ with each edge $\{u, v\}$ replaced by two arcs $(u, v)$ and $(v, u)$.

Usually, a directed or undirected graph is given either by its diagram or by its adjacency matrix. A diagram is a drawing on the plane consisting of small circles which represent the vertices and lines between pairs of vertices which represent the edges. An arc $(u, v)$ is indicated by an arrow starting in vertex $u$ and ending in vertex $v$. A more abstract representation is the $(0,1)$-adjacency matrix $A = (a_{uv})$. In order to make evident that the matrix $A$ represents a graph $\Gamma$, we will also write $A(\Gamma)$. The rows and columns of $A$ are indexed by the elements of $\Omega$, which for sake of simplicity are often numbered by $1, 2, \ldots, n$ with $n = |\Omega|$ (or, as for example in the computer package COCO, see below, by numbers $0, 1, \ldots, n - 1$). Thus, $A$ is a $n \times n$-matrix. The entry $a_{uv}$ is equal to 1 if the edge $\{u, v\}$, respectively the arc $(u, v)$, exists and 0 otherwise. Note that the $(0,1)$-adjacency matrix of an undirected graph is symmetric with respect to the main diagonal, whereas in general this is not the case for directed graphs.

Sometimes it is necessary to deal with (undirected or directed) multigraphs. In a multigraph each pair of vertices may be connected by more than one edge or arc. The number of edges resp. arcs between two vertices is called the multiplicity of the edge resp. arc. In the diagram multiple edges are drawn as parallel lines, multiple arcs as parallel arrows, in the adjacency matrix the entry $a_{uv}$ denotes the multiplicity of the edge or arc connecting $u$ and $v$.

The complete directed graph is the graph with $n$ vertices where all $n(n - 1)$ arcs are present.

For certain purposes it is more convenient to consider graphs with loops. A loop is an arc connecting a vertex with itself. In this sense, a complete directed graph with loops has $n^2$ arcs. In particular, there is one additional arc $(u, u)$ for each vertex $u$. The main advantage is that vertices can be identified with the corresponding loops, which considerably simplifies our notation.

The most general notion of a graph is the colored graph.

In a colored complete directed graph $\Delta$ all vertices and all arcs are assigned colors in such a way that the colors of the vertices are different from the colors of the arcs. Assume that $\{0, 1, \ldots, s - 1\}$ are the colors of the vertices and let $\Omega_j$ denote the vertices which are assigned color $j$. Then $\Omega = \Omega_0 \cup \Omega_1 \cup \ldots \cup \Omega_{s-1}$ is a partition of the vertex set of $\Delta$. Similarly, if $\{s, s + 1, \ldots, r - 1\}$ are the colors of the arcs and $R_k$ denotes the arcs of color $k$ then $R =$
$R_s \cup R_{s+1} \cup \ldots \cup R_{r-1}$ is a partition of the arc set of $\Delta$. Each colored complete directed graph can be represented by its adjacency matrix $A = (a_{uv})$ which contains in the $u$th row and $v$th column the color of the arc $(u,v)$, that means $a_{uv} = k$ if and only if $(u,v) \in R_k$. The entry in the $u$th row and $v$th column is the color of the vertex $u$, thus $a_{uu} = j$ if and only if $u \in \Omega_j$.

Obviously, any undirected or directed graph can be considered as a colored complete directed graph with three colors. The vertices are assigned color 0, the edges (arcs) and nonedges (nonarcs) are assigned colors 1 and 2. In the case of a multigraph, different colors of arcs correspond to different multiplicities. In this sense, any chemical structure can be seen as a colored complete graph. The colors $a_{uv}$ can be interpreted as modes of vertices, for example names of atoms in a molecular graph, the colors $a_{uv}$ reflect the multiplicity of bonds or symbolize certain chains of atoms. Figure 1 shows a chemical structure and the adjacency matrix $A$ of the corresponding colored complete directed graph (interesting properties of this compound are discussed in [DunB95]) is given below; here 0, 1, 2, 3 stands for the atoms of C, N, O, H respectively, 4 denotes usual bond, 5 double bond, all other pairs of atoms are denoted by 6, upper superscripts denote the labels of atoms.

![Diagram](image)

**Figure 1**
A permutation $f$ acting on a finite set $\Omega$ is a bijective mapping from $\Omega$ onto itself. For each permutation $f$ we denote by $v = u^f$ the image $v$ of an element $u \in \Omega$. Let $S_n$ be the symmetric group of degree $n$, i.e. the group of all permutations acting on the set $\Omega$ with $n = |\Omega|$. Each subgroup $G$ of $S_n$ is called a permutation group of degree $n$. The notation $(G, \Omega)$ indicates that the permutation group $G$ acts on the set $\Omega$.

An automorphism of a colored complete directed graph $\Delta = (\Omega, R)$ is a permutation $g$ on $\Omega$ which preserves the colors of the vertices and arcs, i.e. which fulfills $u \in \Omega_j \Leftrightarrow u^g \in \Omega_j$ and $(u, v) \in R_k \Leftrightarrow (u^g, v^g) \in R_k$ for all $u, v \in \Omega$ and all colors $j, k$. It is easy to realize that the set of all automorphisms of a graph $\Delta$ forms a group. This group is called the automorphism group of $\Delta$ and is denoted by $Aut(\Delta)$. Clearly, $G = Aut(\Delta)$ is a permutation group acting on $\Omega$.

Let $(G, \Omega)$ be a permutation group acting on $\Omega$. We define a binary relation $\approx$ on $\Omega$ in such a way that $u \approx v$ holds for two elements $u, v \in \Omega$ if and only if there exists a permutation $g \in G$ with $v = u^g$. Since $(G, \Omega)$ is a group, the relation $\approx$ is an equivalence relation on $\Omega$, its equivalence classes are called orbits (or 1-orbits) of $(G, \Omega)$. The set $1-orb(G, \Omega)$ of the orbits of $(G, \Omega)$ forms a partition of the set $\Omega$.

The automorphism partition of the vertex set $\Omega$ of a colored complete directed graph $\Delta$ is the set $1-orb(Aut(\Delta), \Omega)$ of the orbits of its automorphism group. Obviously, if two vertices $u$ and $v$ belong to the same 1-orbit, then there is an automorphism $g$ which maps $u$ onto $v$. The automorphism partitioning problem is the problem of finding the automorphism partition of a graph.
To give an example, the bijective mapping \( g \) on \( \Omega = \{1, 2, \ldots, 19\} \) defined by

\[
\]

is an automorphism of the colored complete directed graph \( \Delta \) which belongs to the structure in Figure 1. The automorphism partition of \( \Delta \) is

\[
\{\{1\}, \{2, 6\}, \{3, 5\}, \{4\}, \{7, 8\}, \{9\}, \{10, 11, 12, 13\}, \{14, 15\}, \{16\}, \{17, 18\}, \{19\}\}.
\]

A graph \( \Delta \) is called \textit{vertex-transitive} if for any two vertices \( u \) and \( v \) there exists at least one automorphism such that \( v = u^g \). Obviously, if a graph is vertex-transitive then its automorphism partition is trivial, meaning that there is exactly one orbit containing all vertices from \( \Omega \).

Commonly, a permutation \( f \) on \( \Omega \) is represented by a so called \textit{permutation matrix} \( M(f) = (m_{uv}) \). This \( n \times n \)-matrix has entries 0 and 1 with \( m_{uv} = 1 \) if and only if \( v = u^f \). It is easy to see that a permutation matrix has exactly one entry equal to 1 in every row and in every column, all other entries are 0. In fact, this property is a necessary and sufficient condition for a matrix to be a permutation matrix. Now the property of a permutation to be an automorphism of a graph can be reformulated in terms of matrices. Namely, a permutation matrix \( M \) determines an automorphism \( g \) of \( \Delta \) if and only if \( M \) commutes with the adjacency matrix \( A \) of \( \Delta \). This means that the equality

\[
M \cdot A = A \cdot M
\]

holds. For example, let \( \Gamma \) be the undirected graph depicted in Figure 2.

![Figure 2](image-url)

Then

\[
A = \begin{pmatrix}
0 & 1 & 2 & 1 \\
1 & 0 & 1 & 1 \\
2 & 1 & 0 & 1 \\
1 & 1 & 1 & 0
\end{pmatrix}
\]
is the adjacency matrix of the corresponding colored complete directed graph $\Delta$. The permutation $g$ of $\Omega = \{1, 2, 3, 4\}$ defined by $1^g = 3$, $2^g = 4$, $3^g = 1$ and $4^g = 2$ is an automorphism of $\Delta$ with associated permutation matrix

$$M = \begin{pmatrix}
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0
\end{pmatrix}.$$

Given a permutation group $(G, \Omega)$, let us now consider the set of permutation matrices $M(G) = \{ M(g) \mid g \in G \}$. A graph $\Delta$ is called invariant with respect to the permutation group $(G, \Omega)$ if and only if its adjacency matrix commutes with all permutation matrices from $M(G)$. Let us further consider the set $V(G, \Omega)$ of all $n \times n$-matrices $B$ which commute with matrices from $M(G)$, i.e.

$$V(G, \Omega) = \{ B \mid M(g) \cdot B = B \cdot M(g) \quad \text{for all} \quad g \in G \}.$$

$V(G, \Omega)$ is called the centralizer algebra of the permutation group $(G, \Omega)$ (the notation $V(G, \Omega)$ stems from the German word “Vertauschungsring”, the use of which goes back to I. Schur and H. Wielandt). It is easy to realize that the set of nonnegative integer matrices $B$ from $V(G, \Omega)$ coincides with the set of adjacency matrices of multigraphs which are invariant with respect to $(G, \Omega)$. A centralizer algebra $V(G, \Omega)$ is known to have the following main properties:

(i) $V(G, \Omega)$ can be considered as a linear space with basis $A_0, A_1, \ldots, A_{r-1}$, where each $A_i$ is a $(0, 1)$-matrix.

(ii) $\sum_{i=0}^{r-1} A_i = J$, where $J$ is the matrix with all entries equal to 1.

(iii) For every matrix $A_i$ there exists a matrix $A_j$ with $A_i^T = A_j$, where $A_i^T$ denotes the transposed matrix of $A_i$.

To each permutation group $(G, \Omega)$ we can associate a new induced permutation group $(G, \Omega^2)$, where for $f \in G$ and $(u, v) \in \Omega^2$ we define

$$(u, v)^f = (u^f, v^f).$$

Let $2$-orb$(G, \Omega)$ be the set of orbits of the induced action of $G$ on $\Omega^2$. This partition of the set of all ordered pairs of elements of $\Omega$ is called the partition into $2$-orbits of $(G, \Omega)$. Each member $R_i \in 2$-orb$(G, \Omega)$ of this partition defines a graph $\Gamma_i = (\Omega, R_i)$ with the adjacency matrix $A_i = A(\Gamma_i)$. It turns out that the matrices $A_0, A_1, \ldots, A_{r-1}$ mentioned in (i) coincide with the latter adjacency matrices.

More precisely, the basis matrices $A_0, A_1, \ldots, A_{r-1}$ of the centralizer algebra $V(G, \Omega)$ correspond to the $2$–orbits of the permutation group $(G, \Omega)$ in the following manner. The $(u, v)$–entry of the basis matrix $A_i$ is equal to 1 if and only if $(u, v)$ belongs to the $i$-th $2$–orbit. In this sense, the set of all $2$–orbits can be represented very conveniently by a single matrix of the form

$$A = \sum_{i=0}^{r-1} i \cdot A_i.$$ 

This means that two pairs $(u, v)$ and $(u', v')$ belong to the same $2$–orbit if and only if the corresponding entries in the matrix $A$ are equal.
Let us consider as an example the set
\[ G = \{(1)(2)(3)(4)(5), (1,2,3), (1,3,2), (1,2)(4,5), (1,3)(4,5), (2,3)(4,5)\} \]
of permutations acting on the set \( \Omega = \{1,2,3,4,5\} \). It can be easily proved that \((G, \Omega)\) is a permutation group (cf. 4.16 in [KliRRT95]). Now consider the corresponding set of permutation matrices
\[
M(G) = \left\{ \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix} \right\}.
\]

It turns out (cf. 5.4 in [KliRRT95]) that the centralizer algebra \( V(G, \Omega) \) has the basis
\[
A_0 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad A_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad A_3 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix},
\]

\[
A_4 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \end{pmatrix}, \quad A_5 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}
\]

thus we obtain
\[
A = \begin{pmatrix} 0 & 2 & 2 & 4 & 4 \\ 2 & 0 & 2 & 4 & 4 \\ 2 & 2 & 0 & 4 & 4 \\ 5 & 5 & 5 & 1 & 3 \\ 5 & 5 & 5 & 3 & 1 \end{pmatrix}.
\]

To our knowledge, B.Yu. Weisfeiler and A.A. Leman were the first to consider the more general problem (in comparison with the automorphism partition) of finding the set of 2–orbits of \((\text{Aut}(\Delta), \Omega)\) for a given graph \( \Delta \). In this setting the automorphism partition of a graph is a byproduct of the determination of the 2–orbits: the 1–orbit of a vertex \( u \) is simply the 2–orbit of the pair \( (u, u) \) (for brevity, we will sometimes speak about the orbits of a graph, of a vertex, etc., instead of the orbits of the automorphism group of the graph).

In the following it will be our goal to determine the 2–orbits of a given graph or, equivalently, to find the 2–orbit matrix \( A \).
3 Stabilization Procedures

First attempts to attack the automorphism partitioning problem date back approximately thirty years. All these approaches try to find the 1–orbits of a given graph. Usually, the classical paper [Mor65] by H.L. Morgan is considered to be the first procedure for graph stabilization. Given an undirected graph \( \Gamma = (\Omega, E) \), the idea is to start with a partition of the vertex set \( \Omega \) according to the valencies. The valency of a vertex \( u \) is the number of edges which are incident to \( u \). Two vertices \( u \) and \( v \) are put into the same class of the partition if and only if they have equal valencies. Then this partition is refined iteratively using the extended valencies. The extended valency of \( u \) is defined as the sum of the previous extended valencies of all neighbours of \( u \), i.e. of all vertices which are connected with \( u \) by an edge. Again two vertices are put into the same class of the partition if and only if they have equal extended valencies. This iteration procedure terminates as soon as the stable partition is reached, that is the next partition coincides with the previous one.

Years later it has been recognized that Morgan's approach is just a special case of stabilization of depth 2. This technique works as follows. Assume that we have a partition \( \Omega_0, \Omega_1, \ldots, \Omega_{s-1} \) of the vertex set \( \Omega \) of \( \Gamma \) according to the valencies. Assume further that this partition is numbered such that \( \Omega_0 \) contains the vertices of smallest valency, \( \Omega_1 \) the vertices of second smallest valency, etc. Now for each vertex \( u \in \Omega \) we compute a list of length \( s \) which contains the valencies of \( u \) with respect to each class \( \Omega_j \) (that means the number of edges connecting \( u \) with vertices from \( \Omega_j \)), \( j = 0, 1, \ldots, s - 1 \). Each class \( \Omega_j \) may now be partitioned into subclasses, each consisting of vertices with equal lists. In this way we may eventually obtain a refinement of the original partition. If this is the case, then the subclasses are numbered according to the lexicographical ordering of the corresponding lists. Then we restart the same proceeding with the refined partition. If in each class the lists of the vertices are identical, then no further refinement is obtained and the procedure stops.

The resulting partition of \( \Omega \) is commonly called the total degree partition of the graph \( \Gamma \) (see e.g. [Tin86]). It is the coarsest partition \( \Omega_0, \Omega_1, \ldots, \Omega_{s-1} \) of \( \Omega \) with the property that every two vertices belonging to the same cell \( \Omega_j \) have the same valencies with respect to any other cell \( \Omega_k \), \( k = j \) included (the coarsest equitable partition of \( \Gamma \) in the sense of [God93]).

The total degree partition cannot be finer than the automorphism partition, since, obviously, a necessary condition for two vertices \( u \) and \( v \) to belong to the same 1–orbit of \( \text{Aut}(\Gamma) \) is that they belong to the same class of the total degree partition. In fact, every class of the total degree partition is a union of 1–orbits. Figure 3 shows a graph where the total degree partition consists of one class only, namely \( \Omega \), but which is not vertex-transitive, i.e. the automorphism partition consists of more than one 1–orbit. This example makes evident the weakness of the above kind of stabilization. The method will not give any partition for regular graphs (graphs where all vertices have the same valencies), not even in the case when \( \text{Aut}(\Gamma) \) is the trivial group consisting of the identity only (what means that each 1–orbit consists of a single vertex).
The reader will recognize in Figure 3 "cuneane", cf. 4.26 and 5.8 in [KliRRT95].

![Figure 3](image)

As already mentioned in the introduction, the problem of the recognition of graph symmetry can be made more precise in mathematical language as an automorphism partitioning problem; the problem of graph identification corresponds to an isomorphism problem. Let us give a precise mathematical statement of the latter problem.

An isomorphism from a graph \( \Gamma = (\Omega, E) \) to a graph \( \Gamma' = (\Omega', E') \) is a bijective mapping \( h \) from \( \Omega \) to \( \Omega' \) such that \((u, v) \in E\) if and only if \((u^h, v^h) \in E'\). If such a mapping exists then \( \Gamma \) and \( \Gamma' \) are called isomorphic. Obviously, if \( \Gamma = \Gamma' \) then an isomorphism coincides with an automorphism. The isomorphism problem is the problem of deciding whether two graphs are isomorphic or not. Similarly as for the automorphism problem there is also a matrix formulation for the isomorphism problem. Namely, two graphs \( \Gamma \) and \( \Gamma' \) with adjacency matrices \( A \) resp. \( A' \) are isomorphic if and only if there exists a permutation matrix \( M \) with

\[ M \cdot A = A' \cdot M. \]

If this equality is multiplied from the left with the inverse \( M^{-1} \) of \( M \) then, using the fact that \( M^{-1} = M^t \) holds for each permutation matrix \( M \), we obtain

\[ A = M^t \cdot A' \cdot M. \]

This modified equality can be interpreted in the following way. The matrix \( A \) is obtainable from the matrix \( A' \) by permuting simultaneously rows and columns. This corresponds just to a renumbering of the vertices.

G. Tinhofer has found a very interesting algebraic characterization of total degree partitions. He first relaxed the notion of an isomorphism between two graphs \( \Gamma \) and \( \Gamma' \) using doubly stochastic matrices. A matrix \( X \) is doubly stochastic if the entries of \( X \) are nonnegative and the sum of
the entries in each row and in each column is equal to 1. Note that every permutation matrix is doubly stochastic. Now let again $A$ and $A'$ be the adjacency matrices of $\Gamma$ resp. $\Gamma'$. Then the two graphs are called doubly stochastic isomorphic if and only if there exists a doubly stochastic matrix $X$ fulfilling the equality $$X \cdot A = A' \cdot X.$$ Of course, two isomorphic graphs are also doubly stochastic isomorphic, however, the converse direction is not true in general. For example, the graphs $\Gamma$ and $\Gamma'$ of Figure 4 are doubly stochastic isomorphic (choose $X = 1/6 \cdot J$), but they are not isomorphic.

![Diagram of graphs $\Gamma$ and $\Gamma'$](image)

Figure 4

Tinhofer proved in [Tin86] that two graphs are doubly stochastic isomorphic if and only if they have identical total degree partitions. To be more precise, the total degree partitions $\Omega_0, \Omega_1, \ldots, \Omega_{s-1}$ of $\Gamma = (\Omega, E)$ and $\Omega'_0, \Omega'_1, \ldots, \Omega'_{s'-1}$ of $\Gamma' = (\Omega', E')$ are identical, if $s = s'$, $|\Omega_j| = |\Omega'_j|$ and, for each pair of vertices $u \in \Omega_j$ and $u' \in \Omega'_j$, the valency of $u$ with respect to $\Omega_k$ is equal to the valency of $u'$ with respect to $\Omega'_k$, $j, k \in \{0, 1, \ldots, s - 1\}$.

The shortcoming of the total degree partition, as pointed out above, motivated the construction of more powerful algorithms for graph stabilization. A well known approach is to apply the refinement technique, which has already been used for the computation of the total degree partition, by replacing the valencies of the vertices by other invariants of the graph. For example, for each vertex $u$ we may count the number of cycles of a given length which contain $u$, the number and sizes of cliques containing $u$, etc. However, finding cycles or cliques in a graph is an extremely difficult task which, in general, requires time exponential in the size of the graph. Therefore, we should use a criterion which is easy to check. A reasonable approach is to consider not only configurations consisting of two vertices, i.e. the edges and nonedges (which define the valencies), but to examine also configurations consisting of three vertices, i.e. all triples of vertices. This procedure is commonly called stabilization of depth 3. The algorithm of Weisfeiler and Leman, which will be formulated and discussed in great detail in Sections 5 and 6, is based on that principle.

We have seen above that stabilization of depth 2 can be associated with a certain combinatorial object, namely with the total degree partition of the graph under consideration. This immediately implies the question whether there is a similar object which belongs to stabilization of depth 3. It turns out that such an object really exists. Moreover, this object has not only a
combinatorial but also a very interesting algebraic description. The details are exposed in the next section.
4 Cellular Algebras

A matrix algebra of degree \( n \) is a set of \( n \times n \)-matrices which is closed under matrix addition, matrix multiplication and multiplication of a matrix by a scalar, i.e. if \( X \) and \( Y \) belong to the matrix algebra and \( z \) is any real number, then also \( X + Y, X \cdot Y \) and \( z \cdot X \) belong to the matrix algebra.

A cellular (or coherent) algebra is a matrix algebra which additionally is closed under Schur-Hadamard (=componentwise) multiplication of matrices and under matrix transposition, and which contains the identity matrix \( I \) and the matrix \( J \) all entries of which are equal to 1. We will denote the Schur-Hadamard product of two matrices \( X \) and \( Y \) by \( X \circ Y \). Thus, if \( X = (x_{uv}) \) and \( Y = (y_{uv}) \) then \( X \circ Y = (x_{uv} \cdot y_{uv}) \). Each cellular algebra \( W \) has a basis \( A_0, A_1, \ldots, A_{r-1} \) (basis of the vector space \( W \)) consisting of \((0,1)\)-matrices which is called standard basis of \( W \), \( r \) is the rank of \( W \). It is not hard to see that a standard basis \( A_0, A_1, \ldots, A_{r-1} \), if suitable numbered, satisfies the following properties:

(i) \[ \sum_{i=0}^{r-1} A_i = J \]

(ii) \[ \sum_{i=0}^{q-1} A_i = I \quad \text{for some } q \text{ with } q \leq r \]

(iii) \[ A_i \odot A_j = 0 \Leftrightarrow i \neq j, \ i, j \in \{0, 1, \ldots, r-1\} \]

(iv) for each \( i \in \{0, 1, \ldots, r-1\} \) there is a \( j \in \{0, 1, \ldots, r-1\} \) such that \( A_i^j = A_j \)

(v) for each pair \( i, j \in \{0, 1, \ldots, r-1\} \) we have

\[ A_i A_j = p_{ij}^0 A_0 + p_{ij}^1 A_1 + \ldots + p_{ij}^{r-1} A_{r-1}. \]

A cellular algebra \( W \) with standard basis \( A_0, A_1, \ldots, A_{r-1} \) can be represented in a very convenient way using the matrix \( A(W) = \sum_{i=0}^{r-1} i \cdot A_i \), called the adjacency matrix of the cellular algebra \( W \). This matrix is unique up to the numbering of the basis matrices.

The nonnegative integers \( p_{ij}^k \) are called the structure constants of \( W \). These numbers have a very nice geometric interpretation. We consider the colored complete directed graph \( \Delta = (\Omega, R) \) which belongs to the adjacency matrix of \( W \). For our purposes, it is very convenient to identify each vertex \( u \) in \( \Delta \) with the corresponding loop \((u, u)\), i.e. we deal with the complete directed graph with loops. Then the matrices \( A_k \) correspond in a natural way to the arc sets \( R_k \) of color \( k \) (the first \( q \) matrices of the standard basis virtually represent the vertices of \( \Delta \); the induced partition of the vertex set is called the standard partition\(^3\) of the graph). An arc \((u, v)\) has color \( k \) if and only if the matrix \( A_k \) has entry 1 in the \( u \)th row and \( v \)th column. The entry \((u, v)\) in

\[^3\] More rigorously, we should speak about standard partition of depth 3 in order to emphasize that the partition is induced by stabilization of depth 3. In the following, we briefly call it the standard partition.
the matrix $A_i \cdot A_j$ is the number of directed paths of length 2 from vertex $u$ to vertex $v$, such that the first step is an arc of color $i$ and the second step is an arc of color $j$. The decomposition (v) implies that for any arc $(u, v)$ of a fixed color $k$ the number of paths of length 2 from $u$ to $v$, such that the first step is of color $i$ and the second step is of color $j$, is the same and equal to $p_{i,j}^k$ (see Figure 5). In fact, if $A_0, A_1, \ldots, A_{r-1}$ fulfill (i)-(iv), then this condition is sufficient for these matrices to be the standard basis of a cellular algebra.

![Figure 5](image)

It is not hard to see (see [KliRRT95]) that each centralizer algebra is also a cellular algebra (therefore, the matrix $A$ given at the end of Section 2 represents a cellular algebra of rank 6 with standard basis $A_0, A_1, \ldots, A_3$). Let $W$ be a cellular algebra. If a group with the centralizer algebra $W$ exists then the cellular algebra $W$ is called Schurian, after I. Schur, who was the first to investigate cellular algebras (actually he was using a different terminology of group rings, see [KliRRT95] for details). The importance of Schurian cellular algebras stems from the fact that, as already indicated in Section 2, its basis matrices correspond to the 2−orbits. Moreover, the diagonal matrices of the basis correspond to the 1−orbits.

Given any $n \times n$−matrix $X$, the cellular algebra $W(X)$ generated by $X$ is defined to be the smallest cellular algebra which contains $X$. It is important to know that this definition is rigorous, that means the resulting algebra is well defined and unique (for a detailed explanation see [KliRRT95]). As a consequence, we are able to associate with each graph $\Gamma$ a matrix algebra, namely the cellular algebra $W(A)$ which is generated by the adjacency matrix $A$ of $\Gamma$. We will also write $W(\Gamma)$ in order to indicate that the cellular algebra corresponds to the graph $\Gamma$.

There are a number of graph classes whose associated cellular algebras are Schurian (for example graphs with a simple spectrum [Pon94a]). For those graphs the automorphism partition can be immediately deduced from the cellular algebra. Namely, in this case the automorphism partition coincides with the standard partition. Unfortunately, this is not the case in general. Simplest counterexamples can be found among strongly regular graphs. An undirected graph is called strongly regular (see [HesH71]) if the standard basis of the associated cellular algebra consists only of 3 matrices. First such examples of non-Schurian cellular algebras of rank 3 were found by H. Wielandt [Wie64], L.C. Chang [Cha59], S.S. Shrikhande [Shr59] and G.M. Adel'son-Velskii et al. [AdeWLF69]. All these graphs have rather large automorphism groups. Later
on, collaborators of Weisfeiler found an example with the identity automorphism group (see [Wei76]).

Nevertheless, although we cannot guarantee that we get the 1–orbits and 2–orbits for each graph, extended practical experience indicates that the results obtained by the cellular algebras are sufficient, in particular for practically all chemical graphs. This is confirmed by the computational results which are presented in Section 9.

The representation of a cellular algebra as a colored complete directed graph and the interpretation of the structure constants \( p_{i,j}^k \) shows that in a cellular algebra implicitly all configurations of a graph consisting of three vertices are considered. In other words, the cellular algebra is the algebraic object which is associated to stabilization of depth 3.

At the end of this section, let us give a precise statement of the problem which now has to be solved. Given a graph \( \Gamma \), we actually deal with two closely related problems.

**Problem 1**: Compute the basis \( A_0, A_1, \ldots, A_{r-1} \) of the cellular algebra \( W(\Gamma) \) (or in other words the colored complete graph \( \Delta \) which is associated to the cellular algebra \( W(\Gamma) \)).

**Problem 2**: Construct the colored complete graph \( \Delta \) with the structure constants \( p_{i,j}^k \).

In the next section we give an algebraic description of the algorithm of Weisfeiler-Leman which settles Problem 1. In Section 6 we present a very illustrative graph theoretical interpretation which solves Problem 2.
5 Algebraic Description of the Algorithm

B. Weisfeiler and A. Leman were the first to show that the cellular algebra of a graph can be computed in polynomial time. The proposed method, firstly described in Russian language in the paper [WeiL68], has as input any matrix \( A \) (the adjacency matrix of a graph \( \Gamma \)) and as output a basis of the cellular algebra \( W(A) \) generated by \( A \). The initial description of the algorithm was too sophisticated, clearer ones are given in the English written book [Wei76], also in [Fri89] and [Hig87]. We will first explain the main features of the algorithm by combining all these ideas, illustrate it by an example, and then present a formal description.

The construction of the cellular algebra \( W(A) \) proceeds iteratively. We start with the adjacency matrix \( A = (a_{uv}) \) of an undirected or directed graph \( \Gamma \) (the diagonal entries are set to be different from the nondiagonal entries). This matrix can be written in the form \( A = \sum_{i=0}^{r-1} i \cdot A_i \) where \( A_i \) are \((0,1)\)-matrices with \((u,v)\)-entry equal to 1 if and only if \( a_{uv} = i \). At the end of each iteration we obtain a new set of \((0,1)\)-matrices \( A'_0, A'_1, \ldots, A'_{r-1} \) which fulfills the properties (i)-(iv) of a cellular algebra as stated in Section 4, but which may fail property (v). In particular, this means that \( A'_0, A'_1, \ldots, A'_{r-1} \) is the basis of a linear subspace \( S \) which is closed under Schur-Hadamard multiplication and transposition and which contains the identity matrix \( I \) and the all 1 matrix \( J \). Note that this also holds at the beginning of the procedure in case \( A \) is symmetric and the values of the diagonal entries are different from all other entries.

Initially, the linear subspace \( S \) with basis matrices \( A_0, A_1, \ldots, A_{r-1} \) will not fulfill property (v) of a cellular algebra, i.e. \( S \) will not be closed with respect to matrix multiplication. It is easy to see that \( S \) contains all products of matrices from \( S \) if and only if it contains all products \( A_i \cdot A_j \) of basis matrices. Therefore, we consider in each iteration the linear subspace which is generated by all these products \( A_0 A_0, A_0 A_1, \ldots, A_{r-1} A_{r-1} \) and compute a basis of \((0,1)\)-matrices for it. This process is repeated until it is stable, this means the basis of the actual iteration coincides with the basis of the previous iteration (up to the numbering of the basis matrices). In that case the subspace \( S \) is closed under matrix multiplication, property (v) is satisfied and, consequently, \( S \) is a cellular algebra.

A straightforward method to construct the basis \( A'_0, A'_1, \ldots, A'_{r-1} \) of a linear subspace \( S \) which is generated by some set of matrices \( \{B_0, B_1, \ldots, B_{r-1}\} \) (in our case this is just the set \( \{A_0, A_0 A_1, A_1 A_2, \ldots, A_{r-1} A_{r-1}\} \) and which is closed under Schur-Hadamard multiplication is described in the paper [Hig87]. Let \( B = B_0 \). If \( B = 0 \) then set \( B_i = B_{i+1} \) for \( i = 0,1,\ldots,p-1 \) and repeat the procedure. Assume that \( B = (b_{uv}) \neq 0 \) and let \( t \) be a nonzero entry of \( B \). Set \( D = (d_{uv}) \) to be the \((0,1)\)-matrix such that \( d_{uv} = 1 \) if and only if \( b_{uv} = t \). Let \( B = D \circ B_1 \). If \( B \neq 0 \) then let \( D = \) a \((0,1)\)-matrix as constructed above. Now let \( B = D \circ B_2 \) and repeat the procedure. If \( B = 0 \) then let \( B = D \circ B_3 \) and repeat the procedure. The last \((0,1)\)-matrix \( D \) will be the first element \( A'_0 \) in the basis of \( S \). Let \( B_i = B_i - B_i \circ A'_0, i = 0,1,\ldots,p-1 \) and repeat the procedure. In this way we obtain a set \( A'_0, A'_1, \ldots, A'_{r-1} \) of \((0,1)\)-matrices fulfilling property (iii).

This procedure can be formulated in a more compact and convenient way (which in fact was the original way used by Weisfeiler-Leman) by introducing indeterminates \( t_i, i = 0,1,\ldots,r-1 \), which can be considered to represent the different entries of an adjacency matrix. In this sense,
the matrix $D = \sum_{i=0}^{r-1} t_i A_i$ represents the adjacency matrix. Since matrix multiplication is a noncommutative operation, it is important in the following to assume that the indeterminants are noncommuting with respect to multiplication, i.e. $t_i t_j \neq t_j t_i$. Now compute the product $B = D \cdot D = \sum_{i=0}^{r-1} \sum_{j=0}^{r-1} t_i t_j A_i A_j$. Each entry of this matrix is a sum of products $t_i t_j$. In order to obtain the basis of $S$ we replace equal entries in $B$ by new indeterminates $t_i'$. Now it is not hard to verify that the $(0, 1)$-matrices $A_0', A_1', \ldots, A_{r-1}'$ of the resulting matrix $A' = \sum_{i=0}^{r-1} t_i A_i'$ are exactly the basis matrices of $S$.

The following very simple example will illustrate this procedure. Consider the graph $\Gamma$ which is depicted in Figure 6.

![Figure 6](image)

Here superscripts denote the numbers from $\Omega = \{1, 2, 3, 4, 5, 6\}$ associated to atoms which form the molecule of ethene. Let $A$ be the adjacency matrix of the colored graph $\Gamma$ associated to the molecular graph depicted in Figure 6 (here 0 stands for carbon atom, 1 for hydrogen atom, 2 for usual bond, 3 for double bond and 4 means that there is no bond between corresponding atoms),

$$A = \begin{pmatrix}
0 & 3 & 2 & 2 & 4 & 4 \\
3 & 0 & 4 & 4 & 2 & 2 \\
2 & 4 & 1 & 4 & 4 & 4 \\
2 & 4 & 4 & 1 & 4 & 4 \\
4 & 2 & 4 & 4 & 1 & 4 \\
4 & 2 & 4 & 4 & 4 & 1 \\
\end{pmatrix}.$$

Then we get that

$$D = \begin{pmatrix}
t_0 & t_3 & t_2 & t_2 & t_4 & t_4 \\
t_3 & t_0 & t_4 & t_2 & t_2 & t_2 \\
t_2 & t_4 & t_1 & t_4 & t_4 & t_4 \\
t_2 & t_4 & t_1 & t_4 & t_4 & t_4 \\
t_4 & t_2 & t_4 & t_1 & t_4 & t_4 \\
t_4 & t_2 & t_4 & t_4 & t_4 & t_1 \\
\end{pmatrix},$$

20
\[
B = \begin{pmatrix}
  x_0 & x_2 & x_3 & x_4 & x_4 \\
  x_2 & x_0 & x_4 & x_4 & x_3 \\
  x_5 & x_6 & x_1 & x_7 & x_8 \\
  x_5 & x_6 & x_7 & x_1 & x_8 \\
  x_6 & x_5 & x_7 & x_8 & x_7 \\
\end{pmatrix},
\]

where

\[
\begin{align*}
x_0 &= t_0^2 + 2t_2^2 + t_3^2 + 2t_4^2, \\
x_1 &= t_1^2 + t_2^2 + 4t_4^2, \\
x_2 &= t_0t_3 + 2t_2t_4 + t_3t_0 + 2t_4t_2, \\
x_3 &= t_0t_2 + t_2t_1 + t_2t_4 + t_3t_4 + 2t_4^2, \\
x_4 &= t_0t_4 + 2t_2t_4 + t_3t_2 + t_4t_1 + t_4^2, \\
x_5 &= t_1t_2 + t_2t_0 + t_4t_2 + t_4t_3 + 2t_4^2, \\
x_6 &= t_1t_4 + t_2t_5 + t_4t_0 + 2t_4t_2 + t_4^2, \\
x_7 &= t_1t_4 + t_2^2 + t_4t_1 + 3t_4^2, \\
x_8 &= t_1t_4 + t_2t_4 + t_4t_1 + t_4t_2 + 2t_4^2.
\end{align*}
\]

Now we proceed with the matrix \( A' \),

\[
A' = \begin{pmatrix}
0 & 2 & 3 & 3 & 4 & 4 \\
2 & 0 & 4 & 4 & 3 & 3 \\
5 & 6 & 1 & 7 & 8 & 8 \\
5 & 6 & 7 & 1 & 8 & 8 \\
6 & 5 & 8 & 8 & 1 & 7 \\
6 & 5 & 8 & 8 & 7 & 1
\end{pmatrix}.
\]

We suggest the reader to repeat the process with the matrix \( A' \) instead of \( A \) and to check that the matrix \( A'' \) resulting from the second iteration coincides with \( A' \). This means that \( A' \) is in fact the desired result of the stabilization, namely, the adjacency matrix \( A(W(\Gamma)) \). The reader can easily find that the order of the automorphism group \( G = \text{Aut}(\Gamma) \) of our graph \( \Gamma \) is equal to 8 and the matrix \( A' \) represents the set of 2-orbits of \((G, \Omega)\). Hence in this case \( W(\Gamma) \) is really a Schurian cellular algebra.

Here is a formal description of the algorithm (which will be denoted in the following by the initials of the authors).

**Algorithm WL**

Input: the adjacency matrix \( A = A(\Gamma) = (a_{uv}) \) of colored graph \( \Gamma \).
Output: a standard basis $A_0, A_1, \ldots, A_{r-1}$ of the cellular algebra $W(G)$, or more exactly the adjacency matrix $A(W(G))$.

(0) Let \{0, 1, \ldots, s - 1\} be the set of different entries of $A$.
   For $k = 0, 1, \ldots, s - 1$ do
   Define $A_k = (a(k))_{uv}$ to be the matrix with
   $a(k)_{uv} = 1$ if $a_{uv} = k$ and $a(k)_{uv} = 0$ otherwise.
   Let $r := s$.

(1) Let $D = \sum_{k=0}^{r-1} t_k A_k$,
   where $t_0, t_1, \ldots, t_{r-1}$ are distinct indeterminates,
   which are noncommuting with respect to multiplication.

(2) Compute the matrix product $B = (b_{uv}) = D \cdot D$.
   Each entry $b_{uv}$ of $B$ is a sum of products $t_i t_j$.

(3) Determine the set \{d_0, d_1, \ldots, d_{s-1}\}
   of different expressions among the entries $b_{uv}$.

(4) If $s > r$ then
   For $k = 0, 1, \ldots, s - 1$ do
   Define $A_k = (a(k))_{uv}$ to be the matrix with
   $a(k)_{uv} = 1$ if $b_{uv} = d_k$ and $a(k)_{uv} = 0$ otherwise.
   $r := s$. Goto (1).

(5) STOP.

As already indicated in the previous section, it follows from the representation of a cellular algebra by a colored complete directed graph that algorithm WL implicitly considers all configurations consisting of three vertices in the graph. There are other methods (see e.g. the references in [Rue90b]) for perception of graph symmetry which also use configurations of three vertices. The main advantage of algorithm WL over them is the fact that the cellular algebra contains exhaustive information which is obtainable from subgraphs of at most three vertices. Thus, the resulting partitions of the vertices and pairs of vertices are the finest among the partitions which can be deduced using these configurations.

An interesting method which is rather close to algorithm WL is described in [Rue90b]. It is based on raising the adjacency matrix to its higher powers, evaluating the entries and partitioning the atoms and pairs of atoms into equivalence classes. Indeed, this procedure considers subgraphs consisting of three vertices. However, some information can get lost such that the resulting partitions are coarser than those obtained by algorithm WL. In particular, an “orientation”
of edges cannot occur. Note that this is possible even if the algorithm WL is applied to an undirected graph. Consider for example the graph \( \Gamma \) in Figure 7.

![Diagram of graph \( \Gamma \)]

\[
\begin{pmatrix}
0 & 2 & 2 & 2 \\
3 & 1 & 4 & 4 \\
3 & 4 & 1 & 4 \\
3 & 4 & 4 & 1
\end{pmatrix}
\]

Figure 7

The edge \( \{1, 2\} \), for instance, can be considered to be oriented (in the sense that its endvertices are situated differently according to the whole graph). Algorithm WL applied to this graph yields not only a coloration, but also an orientation of the edges, i.e. in the colored complete directed graph, which represents the cellular algebra, the arcs \( (1, 2) \) and \( (2, 1) \) have different colors (the colored complete directed graph is given above by its adjacency matrix). The cellular algebra of \( \Gamma \) is of rank 5. The standard basis consists of the following matrices:

\[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix},
\begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix},
\begin{pmatrix}
0 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0
\end{pmatrix},
\begin{pmatrix}
0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0
\end{pmatrix},
\begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 1 & 1 \\
0 & 1 & 0 & 1 \\
0 & 1 & 1 & 0
\end{pmatrix}
\]

Note that for the same graph the algorithm which was described in [Rue90b] will get as the output the symmetric matrix

\[
\begin{pmatrix}
0 & 2 & 2 & 2 \\
2 & 1 & 3 & 3 \\
2 & 3 & 1 & 3 \\
2 & 3 & 3 & 1
\end{pmatrix},
\]

hence two antisymmetric basic matrices of \( W(\Gamma) \) will be merged.
6 Graph Theoretical Interpretation

In the previous sections, we already indicated that each cellular algebra \( W \) with basis \( A_0, A_1, \ldots, A_{r-1} \) can be represented by a colored complete directed graph \( \Delta = (\Omega, R) \), the graph whose adjacency matrix is the matrix \( A(W) = A(\Delta) = \sum_{i=1}^{r-1} t_i A_i \) (with indeterminates \( t_i \) standing for the colors \( i \)). This matrix sometimes is called generic matrix of \( W \). For convenience, the vertices in \( \Delta \) have been identified with the corresponding loops. In this sense, the basis matrix \( A_k \) corresponds to the arc set \( R_k \) of color \( k \), and \( R = \{ R_0, R_1, \ldots, R_{r-1} \} \). The number of colors in \( \Delta \) is equal to the rank of \( W \). More generally, to each linear subspace \( S \) with linear basis \( A_0, A_1, \ldots, A_{r-1} \) satisfying the properties (i)-(iv) of a cellular algebra, we can associate a colored complete directed graph \( \Delta = (\Omega, R) \), the graph which belongs to the generic matrix \( \sum_{i=0}^{r-1} t_i A_i \) of \( S \).

With this representation, the main idea of the algorithm described above can be sketched in a more illustrative manner. In each iteration of the algorithm, the coloring of the underlying complete directed graph is modified by means of Schur-Hadamard multiplication and matrix multiplication. These two operations may be interpreted as follows. Given generic matrices \( X = (x_{uv}) \) and \( Y = (y_{uv}) \) of two colored complete directed graphs \( \Delta' \) and \( \Delta'' \) with indeterminates representing the colors, the Schur-Hadamard product \( X \circ Y = (x_{uv} \cdot y_{uv}) \) corresponds to the generic matrix of a new colored complete directed graph \( \Delta \) where the color of arc \((u, v)\) is the ordered mixture of the colors of both arcs in the original graphs. In the case of the matrix product \( X \cdot Y \), the color of the arc \((u, v)\) in the new graph \( \Delta \) depends on the number and colors of paths of length 2 starting in \( u \) and ending in \( v \) such that the first step in the path is an arc of \( \Delta' \) and the second step is an arc of \( \Delta'' \). The \((u, v)\)-entry \( \sum_w x_{uw} y_{wv} \) of \( X \cdot Y \) completely describes the set of these paths.

In the following we present a slightly different procedure leading to our main goal, namely an efficient computer program for graph stabilization. The method is based on the computation of the structure constants \( p_{ij}^{k} \) which have been defined and interpreted in Section 4. To recall the main result, a basis \( A_0, A_1, \ldots, A_{r-1} \) of a cellular algebra \( W \) must fulfill

\[
A_i A_j = p_{ij}^{0} A_0 + p_{ij}^{1} A_1 + \ldots + p_{ij}^{r-1} A_{r-1}
\]

for each pair \( i, j \in \{0, 1, \ldots, r-1\} \). In the colored graph \( \Delta \), this means that each arc \((u, v)\) of a given color \( k \) is the basis arc of exactly \( p_{ij}^{k} \) triangles with first nonbasis arc of color \( i \) and second nonbasis arc of color \( j \) (a triangle consists of three not necessarily distinct vertices \( u, v, w \) and arcs \((u, v), (u, w) \) and \((w, v)\)). The arc \((u, v)\) is called the basis arc, the other arcs are the nonbasis arcs of the triangle; see Figure 5).

The idea of the algorithm can be described informally as follows. One iteration includes the round along all arcs of the given graph \( \Delta \). For each arc \((u, v)\) of a fixed color \( k \) we count the number of triangles with basis arc \((u, v)\) and nonbasis arcs of color \( i \) and \( j \), respectively, \( i, j = 0, 1, \ldots, r-1 \) (equivalently, we count the number of paths of length 2 such that the first arc \((u, w)\) is of color \( i \) and the second arc \((w, v)\) is of color \( j \)). These numbers should be equal for all arcs. If this is true, then these numbers are just the structure constants \( p_{ij}^{k} \). If not, then the arc set \( R_k \) of color \( k \) has to be partitioned into subsets \( R_{k'_0}, R_{k'_1}, \ldots, R_{k'_{k-1}} \), each consisting
of arcs with the same numbers. This step is performed for all colors \( k \in \{0, 1, \ldots, r - 1\} \). Then the graph \( \Delta \) is recolored, i.e., we identify color \( k_0 \) with the old color \( k \) and introduce the new colors \( k_1, \ldots, k_{t-1} \) (in algebraic language, recoloring \( \Delta \) means to replace the basis matrix \( A_k \) by new basis matrices \( A_{k_0}, A_{k_1}, \ldots, A_{k_{t-1}} \)).

The next iteration is performed for the recolored graph \( \Delta \). If in some iteration no new colors are introduced, then the process is stable and we can stop. In this case, the graph \( \Delta \) with the final stable coloring represents the required cellular algebra \( W \). Here is a more formal description of the algorithm.

**Algorithm STABIL**

**Input:** the adjacency matrix \( A(\Gamma) = (a_{uv}) \) of a colored graph \( \Gamma \).

**Output:** a complete directed graph \( \Delta = (\Omega, R) \) with a stable coloring and the structure constants \( p_{ij}^k \).

(0) Let \( \{0, 1, \ldots, s - 1\} \) be the set of different entries of \( A(\Gamma) \) and \( \Delta = (\Omega, R) \) the colored complete directed graph belonging to \( A(\Gamma) \). Determine the arc sets \( R_0, R_1, \ldots, R_{s-1} \) of colors \( 0, 1, \ldots, s - 1 \).

Let \( r := s \).

(1) For \( k = 0, 1, \ldots, r - 1 \) do

For all \( (u, v) \in R_k \) do

Compute the numbers \( p_{ij}^k \) of triangles with basis arc \( (u, v) \) and nonbasis arcs of colors \( i \) and \( j \), respectively, \( i, j \in \{0, 1, \ldots, r - 1\} \).

Collect all arcs having the same parameters \( p_{ij}^k \), i.e., all arcs which belong to the same number of triangles of any colors, and assign them to new sets \( R_{k_0}, R_{k_1}, \ldots, R_{k_{t-1}} \).

Replace \( R_k \) by \( R_{k_0}, R_{k_1}, \ldots, R_{k_{t-1}} \), i.e., recolor the arcs of color \( k \) using the old color \( k_0 = k \) and the new colors \( k_1, \ldots, k_{t-1} \).

(2) Let \( s \) be the number of colors used to recolor \( \Delta \).

If \( s > r \) then

\( r := s \). Goto (1).

(3) STOP.

Let us illustrate this method by a small example, namely we consider again cuneane, see Figure 3.
Here

\[
A = \begin{pmatrix}
1 & 2 & 3 & 3 & 3 & 3 & 2 & 2 \\
2 & 1 & 2 & 2 & 3 & 3 & 3 & 3 \\
3 & 2 & 1 & 2 & 3 & 3 & 3 & 2 \\
3 & 2 & 2 & 1 & 2 & 3 & 3 & 3 \\
3 & 3 & 3 & 2 & 1 & 2 & 2 & 3 \\
3 & 3 & 3 & 3 & 2 & 1 & 2 & 2 \\
2 & 3 & 3 & 3 & 2 & 2 & 1 & 3 \\
2 & 3 & 2 & 3 & 3 & 2 & 3 & 1
\end{pmatrix}
\]

is the adjacency matrix of the corresponding colored graph;

\[
B = \begin{pmatrix}
1 & 2 & 3 & 4 & 4 & 3 & 2 & 2 \\
2 & 1 & 5 & 5 & 4 & 6 & 4 & 3 \\
3 & 5 & 1 & 5 & 4 & 4 & 6 & 2 \\
4 & 5 & 5 & 1 & 2 & 4 & 4 & 4 \\
4 & 4 & 4 & 2 & 1 & 5 & 5 & 4 \\
3 & 6 & 4 & 4 & 5 & 1 & 5 & 2 \\
2 & 4 & 6 & 4 & 5 & 5 & 1 & 3 \\
2 & 3 & 2 & 4 & 4 & 2 & 3 & 1
\end{pmatrix}
\]

is the result after the first iteration,

\[
C = \begin{pmatrix}
1 & 2 & 3 & 4 & 4 & 3 & 2 & 5 \\
6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 \\
13 & 8 & 7 & 9 & 10 & 12 & 11 & 6 \\
14 & 15 & 15 & 16 & 17 & 18 & 18 & 14 \\
14 & 18 & 18 & 17 & 16 & 15 & 15 & 14 \\
13 & 11 & 12 & 10 & 9 & 7 & 8 & 6 \\
6 & 12 & 11 & 10 & 9 & 8 & 7 & 13 \\
5 & 3 & 2 & 4 & 4 & 2 & 3 & 1
\end{pmatrix}
\]

is the result which we get after the second iteration (it in fact coincides with the final result).
7 Program Implementation

The presented algorithm STABIL has been coded in programming language C and was tested on a SUN-Sparcstation. The program requires as an input a file containing the number of colors, the vertex number $n$ and the adjacency matrix $A(\Gamma)$ of an arbitrary graph $\Gamma$, and provides as an output the number of colors (i.e. the rank), the number of cells in the standard partition, the adjacency matrix of the cellular algebra $W(\Gamma)$, and (if requested) the structure constants of $W(\Gamma)$.

In the following we will give some information about the implementation. The adjacency matrix of the graph $\Gamma$ is stored in a $n \times n$-matrix. After each iteration of the program, this matrix will contain the adjacency matrix of the actual colored complete graph $\Delta$. In the final state it contains the adjacency matrix of $W(\Gamma)$.

During any iteration of the program, except the last one, the number of colors increases and some arcs of $\Delta$ are recolored. Arising of new colors implies a new iteration, while absence of new colors during some iteration gives the sign for finishing the program. In the latter case a new iteration will not change the coloring of $\Delta$.

Any iteration includes the following two imbedded loops: the loop around the colors and the loop around the arcs of a fixed color. To handle the loop around all arcs of a fixed color, we introduce an additional data structure representing the graph $\Delta$, namely lists which store the arcs $(u, v)$ of a given color. Each element of a list contains the entries $u$ and $v$, i.e. the number of the row and column of the arc in the adjacency matrix, and a pointer to the information concerning the next arc of the given color.

The following actions with one arc $(u, v)$ of color $k$ form an elementary step of the program, except the last one:

(i) Computing the structure constants\footnote{We stress the reader's attention that the term "structure constants" has a rigorous meaning only after the fulfillment of the program. Currently the structure constants are just the numbers of triangles with the prescribed properties.} $p_{ij}^k$ for $(u, v)$. Since $i, j \in \{0, 1, \ldots, r - 1\}$, i.e. $\Delta$ is colored by $r$ colors, there are $r^2$ such numbers.
(ii) Saving the nonzero structure constants $p_{ij}^k$ for $(u, v)$ as the sequence of triples $(i, j, p_{ij}^k)$ at the end of a vector MEMORY.
(iii) Assigning the color to the arc $(u, v)$. This is done by examining whether the last sequence in MEMORY is a new sequence (then a new color is introduced), or the same sequence already appears in MEMORY for some other arc of the actual color $k$.

Let us consider these actions in some more detail.

*Computation of the structure constants.* As mentioned above, each arc is characterized by a set of $r^2$ numbers, called structure constants. The geometrical meaning of these numbers has been described, too. In order to calculate the numbers $p_{ij}^k$ for a given arc $(u, v)$, we examine
all triangles with basis arc $(u, v)$ (see Figure 5). Note that there are $n$ such triangles. If for some vertex $w$ the arc $(u, w)$ has color $i$ and the arc $(w, v)$ has color $j$, then we increase $p_{ij}^k$ by 1 (initially all $p_{ij}^k$ are set equal to 0). Thus the number of nonzero $p_{ij}^k$ does not exceed $n$.

If we compute simultaneously all $r^2$ structure constants for an arc and store them in a straightforward way using an $r \times r$-matrix, then we will soon get storage overflow, since the existence of a matrix with $r^2$ elements in the program is impossible already for comparatively small $n$. However, since there are at most $n$ nonzero structure constants for each arc, we can use instead of a matrix CONST with $r^2$ entries a data structure whose size is proportional to $n$. This data structure consists of lists whose elements contain the information $i$, $p_{ij}^k$ and a pointer to the next nonzero structure constant in the column $j$ of the matrix CONST. Additionally we need a vector with $r$ elements to save the pointers to the columns (the described technique, called hashing, is a well known tool to treat efficiently set manipulation problems; see [AhoHU74]).

Saving of the structure constants for arcs of a given color. In view of the forthcoming manipulations, it is more adequate to save the structure constants as a sequence of triples $i, j, p_{ij}^k$. The maximal number of such triples in the sequence of a given arc is $n$. During the pass along the arcs of a given color $k$, we have to save all sequences of structure constants belonging to the arcs of this color. Therefore the length of the vector MEMORY should be about $3n^2$ (note that the number of arcs of color $k$ is restricted by $n^2$).

The search along MEMORY and recoloring of an arc. The nonzero structure constants for a given arc $(u, v)$ of color $k$ are saved at the end of the vector MEMORY. Then we should examine whether we have a new sequence or whether an identical sequence has been saved in MEMORY before. We use the partial ordering of the sequences by their lengths. So, if we search for an identical sequence, in the case of equal lengths we come to an element by element comparison, in the case of nonequal lengths we pass to the next sequence.

As mentioned before, the main problem in the program is to find memory for the structure constants. For graphs with a comparatively large number of vertices, it is impossible to save all these constants for a given color $k$. Therefore we decided to save only the nonzero numbers as triples $i, j, p_{ij}^k$ in the vector MEMORY. Now, some graphs may initially produce a very large number of different sequences $i, j, p_{ij}^k$ and the corresponding massive storage requirements may exceed the available memory capacity of small computers. Therefore we start the program with a simple preprocessing procedure which aims to increase in advance the number of colors, before starting the main program.

In the first step of this preprocessing we classify the vertices of the (colored) graph $\Gamma$ in the following way. Two vertices are put into the same cell if and only if they are incident to the same number of edges of each color. Then we can recolor the edges according to the new coloring of the vertices. If two edges, which initially have the same color, connect two different colored pairs of vertices, then the edges are assigned different colors, too.

Some additional practically important details about the current version of the program implementation of algorithm STABIL may be found in Section 9.
8 Estimation of the Complexity

The question of the theoretical complexity\(^1\) of the WL-stabilization was not considered for a long time. Weisfeiler and Leman only stated that the complexity is polynomial in the vertex number \(n\) of the graph, without giving any explicit time bound. A first attempt for an estimation was done by S. Friedland. In [Fri89] he pointed out that the required time is restricted by \(O(n^{10})\). I.N. Ponomarenko [Pon93a] improved the time bound to \(O(n^3 \log n)\). Very recently, L. Babel showed in [Bab95] that the algorithm can be implemented to run in time \(O(n^3 \log n)\).

8.1. Before we are going to determine the worst case complexity of our implementation, let us once more stress that we are dealing with two different problems, depending on the point of view. The first problem is to find the standard basis of the cellular algebra \(W(\Gamma)\) belonging to some graph \(\Gamma\). The second problem, which many times appears in framework of algebraic combinatorics, is to compute the structure constants \(p^k_{ij}\) and a stable coloring of the complete directed graph \(\Delta\) representing the cellular algebra \(W(\Gamma)\). Our implementation solves the second problem whereas the implementation of the above-mentioned algorithm by Babel solves the first problem.

Let us now analyze the complexity of algorithm STABIL. We only have to examine step (1), the initializing step (0) and step (2) obviously can be performed in time \(O(n^2)\). We have seen in the previous section that an elementary step of (1) consists of three actions which are performed for each of the \(n^2\) arcs of the graph.

In action (i) the \(n\) triangles with basis arc \((u, v)\) have to be found. This can be done in time \(O(n)\) by inspecting the \(u\)th row and the \(v\)th column of the adjacency matrix \(A = (a_{uv})\) of the graph. Note that for each vertex \(w\) there is one triangle with basis arc \((u, v)\), the entries \(a_{uw}\) and \(a_{wv}\) of \(A\) are the colors of the nonbasis arcs \((u, w)\) and \((w, v)\). For each triangle the value of some parameter \(p^k_{ij}\) is actualized. To be more precise, let \(a_{uv} = k\). Then the value of \(p^k_{ij}\) must be increased by 1 if \(a_{uw} = i\) and \(a_{wv} = j\). In order to find the actual value of \(p^k_{ij}\) we have to pass through the corresponding list in the data structure (containing the information \(i, p^k_{ij}\)). Since the length of this list is at most \(n\), this requires time \(O(n)\) for each triangle. Thus, action (i) requires total time \(O(n^2)\) for one arc. Since there are at most \(n\) nonzero structure constants for each arc, action (ii), namely saving the sequence of structure constants in the vector MEMORY, can be executed in time \(O(n)\). The most time consuming part is action (iii). In order to compare the sequence of triples \(i,j,p^k_{ij}\) for one arc \((u, v)\) with all such sequences already stored in MEMORY, we eventually have to pass through the whole vector MEMORY. Since this vector may be of length \(3n^3\), this requires time \(O(n^3)\). (We stress that the current implementation does not use any storage/search technique, see also 8.5).

This shows that the complexity of one elementary step is \(O(n^3)\). Since \(n^2\) arcs are treated, one iteration of step (1) requires time \(O(n^5)\). Now it remains to give a bound on the number

---

\(^1\)Readers who are not familiar with complexity considerations of algorithms are referred to the standard book [AhoHU74].
of iterations. If only one color is added during each iteration, then there are \( n^2 \) iterations. Altogether, this results in a worst case time bound of \( O(n^7) \).

Remarks

(i). Similar reasonings were done less carefully in [ChuKP92] and thus resulted in the evaluation \( O(n^8) \).

(ii). In fact, the number of iterations in the WL-stabilization is less than \( n^2 \) ([Ade95]), however such an opportunity to improve the evaluation will not be used in this paper.

(iii). In the worst case, if \( W(\Gamma) \) coincides with the full matrix algebra of order \( n \), there are \( n^2 \) basis matrices and therefore \( n^6 \) structure constants (most of them are zero). This information may help the reader to realize the difference between the statements of Problems 1 and 2.

The crucial point in the implementation concerning both running time and space requirement is the vector MEMORY. In order to make the program applicable also for relatively small computers, it is favourable to restrict the length of MEMORY to \( O(n^2) \)\(^1\). With this modification, it may be impossible to store all the different sequences of structure constants. In that case, new sequences are not saved and all the corresponding arcs are assigned the same color. This color will be split during the next iteration of the program (note that this procedure may increase the number of iterations which are needed to obtain the stable coloring).

8.2. As mentioned above, the implementation of the algorithm presented in [Bab95] has a considerably lower worst case complexity. We will very briefly indicate the main ideas of that implementation. Compared to algorithm STABIL, there are two main modifications, one decreases the number of triangles which are examined in one iteration, the other involves some sophisticated sorting techniques.

In each iteration of algorithm STABIL, all \( n^3 \) triangles of the colored graph \( \Delta \) are examined. However, it is not really necessary to inspect the whole set of triangles. One can restrict to a certain subset. Roughly sketched, the procedure is the following. Let a colored complete directed graph \( \Delta \) be given. In each iteration some arcs of the graph will keep their colors, others are assigned new colors (which have not been used in the previous iteration). More concrete, the arc set \( R_k \) is split into subsets \( R_{k_0}, R_{k_1}, \ldots, R_{k_{r-1}} \), where one of the colors \( k_0, k_1, \ldots, k_{r-1} \) is equal to \( k \) and the others are new colors. The basic idea is to inspect only those triangles which contain at least one arc of a new color. Denote by \( T_M \) the set of these triangles. Further let \( R_M \) denote the set of arcs which are basis arcs of triangles from \( T_M \). Now, step (1) of algorithm STABIL is modified in the following way. Each arc \( (u, v) \in R_M \) is the basis arc of some (in general less than \( n \)) triangles from \( T_M \). For \((u, v) \in R_M \) list the colors of the nonbasis arcs of these triangles. Now, each arc from \( R_M \) is associated a multiset of some ordered pairs \((i, j)\). Collect arcs with equal multisets and assign them the same color, i.e. replace each arc set \( R_k \)

\(^1\)In the actual version of the program, we defined MEMORY to be of length \( 3n^2 \), see also additional remarks in next section
by suitable subsets $R_{k_0}, R_{k_1}, \ldots, R_{k_{t-1}}$. One of these subsets, say $R_{k_0}$ (which may be empty), consists of all arcs from $R_k$ which do not belong to $R_M$. The procedure stops if no new colors are generated.

It is not yet designated which one of the colors $k_0, k_1, \ldots, k_{t-1}$ is equal to the old color $k$ and which ones are new colors. The effort for each iteration is kept low if $T_M$ contains only a small number of triangles. Therefore it is favourable to identify $k$ with that color $k_p$ where $R_{k_p}$ contains the largest number of arcs. It is not hard to check the correctness of this method (for details see [Bab95]). The worst case complexity is determined as follows.

Let $\tau_h$ denote the cardinality of $T_M$ in the $h$th iteration. Then obviously $|R_M| \leq \tau_h$. Therefore, multisets of at most $\tau_h$ arcs $(u, v)$ have to be computed. These multisets are stored as lists $S(u, v)$ and are obtained as follows. Order the $\tau_h$ triangles from $T_M$ lexicographically according to the colors $(i, j)$ of the nonbasis arcs (a pair $(i, j)$ appears before $(i', j')$ if and only if $i < i'$ or $i = i'$ and $j < j'$). Note that the colors are in the range $\{0, 1, \ldots, n^2 - 1\}$ (since the graph has $n^2$ arcs, not more than $n^2$ colors can occur). It is well known that lexicographical ordering of $\tau_h$ pairs of integers from $\{0, 1, \ldots, n^2 - 1\}$ can be done in time $O(\tau_h + n)$ using the sorting routine bucket sort. Now, the lists $S(u, v)$ are obtained by passing through the ordered list of triangles and assigning the actual triangle to its basis arc $(u, v)$, i.e. the colors of the nonbasis arcs are inserted at the end of $S(u, v)$. Obviously, this requires time $O(\tau_h)$. Note that the pairs of colors in the lists $S(u, v)$ appear now in lexicographical order.

To identify the different multisets we have to order the lists $S(u, v)$, $(u, v) \in R_M$, lexicographically. Since the total length of all lists is $\tau_h$ and the entries are pairs of numbers from $\{0, 1, \ldots, n^2 - 1\}$, this again can be done with bucket sort in time $O(\tau_h + n)$. Now the arc sets $R_k$ are split in the obvious way by passing through the ordered list of multisets $S(u, v)$. This, as well as finding the subsets $R_{k_p}$ of largest cardinality, requires time $O(\tau_h)$. So far we have seen that the complexity for the $h$th iteration of this method is $O(\tau_h + n)$. It remains to compute the total complexity for all iterations (trivially, the number of iterations is restricted by the maximal number $n^2$ of colors).

Since $R_{k_p}$ has been chosen to be that subset of $R_k$ with largest cardinality, each of the other subsets (which contain the arcs with new colors) has at most half the size of $R_k$. Therefore, each time a certain triangle is inspected, at least one arc set which shares an arc with this triangle is at most half as large than before. As a consequence, each of the $n^3$ triangles is examined not more than $3\log n^2 = 6\log n$ times. This shows that $\sum_h \tau_h \leq 6n^3\log n$. Finally we obtain a worst case time complexity of $O(n^3\log n)$.

8.3. These ideas have been realized in a computer program by L. Babel, S. Baumann and M. Lüdecke. The program is termed STABCOL, due to the fact that the coloring of the complete directed graph is modified in each iteration until the process is stable, i.e. until a STABile COLORing is obtained. It is coded in programming language C and was also tested on the same SUN-Sparcstation. Just as for the program STABIIL, the input is a file containing the number of colors, the vertex number and the adjacency matrix of a graph $\Gamma$, the output contains the
number of colors, the number of cells and the adjacency matrix of the cellular algebra which is generated by \( \Gamma \).

Contrary to STABIL, the program STABCOL does not work with vectors of predefined lengths but uses more sophisticated data structures. The set \( T_M \) of triangles and the multisets \( S(u,v) \) are stored in lists which are linked by pointers and which are of variable length. In this way, waste of memory space is avoided. Furthermore, memory space which is no longer needed is set free immediately.

The complexity analysis of STABIL shows that most of its time is spent in order to compare a new sequence of numbers with old sequences. Since this is done in the obvious way by passing through the entire vector of sequences, it requires time proportional to the length of the vector. This somewhat tremendous procedure is avoided in STABCOL by means of very special sorting techniques. These techniques and the more complicated data structures make the implementation much more ambitious. However, we do not have enough space to go into details here. The interested reader may consult the program description [BabBLT97].

8.4. At first glance, a comparison of the theoretical complexities indicates that the implementation of [Bab95] should be preferred. However, it turns out that this implementation, although theoretically very fast, is rather slow in practice and applicable only for relatively small graphs, whereas our implementation, although inferior with respect to the worst case bound, is practically very fast and is able to handle very large graphs (the practical behaviour of both program implementations is documented in the next section).

Here we are confronted with a situation which seems to be strange but which rather frequently occurs on the construction of algorithms. There are two algorithms or two implementations of an algorithm solving the same problem, one of them theoretically fast (i.e. with a good worst case complexity) but practically slow, the other one practically fast in spite of a relatively bad worst case complexity.

There are two main reasons for this paradox. First, and perhaps most important is that the sign “O” in the evaluation means in fact the existence of some constant as a multiplier with the monom depending on \( n \). The actual value of this constant depends on many factors, in particular on the “complexity” of the data structures. In our case the multiplier for the implementation of STABIL is essentially smaller than the one for STABCOL. Thus the advantages of the theoretically faster algorithm cannot be felt on comparably small graphs. Second, one algorithm has been constructed from a purely theoretical point of view with the aim to obtain a worst case complexity as good as possible. No practical considerations are taken into account such as simplicity of data structures, easy way of implementing, small space requirements, etc. In particular, the running time of the algorithm in the mean (the mean taken over a large representative selection of practically relevant examples) is not considered. This average behaviour, however, is much more important for practitioners than the worst case behaviour, which often occurs only for pathological examples. The second algorithm is constructed from that practical point of view. It aims to solve the “real world” problems very fast, without paying attention to its theoretical complexity.
8.5. It is worthwhile to stress that the worst case time bound $O(n^7)$ (see 8.1) is a very rough upper bound.

In fact we see a number of opportunities to diminish this bound essentially. One of them was mentioned in Remark (ii) in Subsection 8.1.

Also (as a result of restricting the length of vector MEMORY to $O(n^2)$) the complexity of one elementary step in the current version of the program is actually reduced from $O(n^3)$ to $O(n^2)$. In spite of the fact that the total number of steps may slightly grow, here we have one more standby to reduce the upper bound.

A more careful analysis of the applied technique of hashing together with a more clever organization of storage (via the use, e.g., of balanced binary trees) may essentially decrease the number of comparisons when we operate with the vector MEMORY.

However we do not use these and other possible options in the current preliminary version of our report. In contrast to [BabBLT97], our report is oriented on those practical users of STABIL, for whom the theoretical question of the evaluation of the efficiency does not play a crucial role.

Nevertheless, we intend to return to the consideration of this question in the future.
# Testing the Program

The presented implementation STABIL has been tested on a large number of structures. All computations were done on a SUN-Sparcstation 10 with 128MB RAM. On this machine, the program is able to handle graphs with up to 2000 vertices. To demonstrate the capability of the program we considered acyclic compounds and compounds containing multiple bonds or heteroatoms as depicted in Figure 8. These structures also appeared as illustrations in papers by other authors (see e.g. [RanBW80], [RueR90b]). The results are summarized in Table I. Besides the running time of the program, the number of cells in the standard partition and the number of colors in the stable coloring (i.e. the number of equivalence classes of atoms and ordered pairs of atoms) are stated. In order to make evident the practical efficiency of our program, we also state the running time of the program implementation STABCOL. Note that STABCOL requires space proportional to $n^3$, therefore it can handle graphs with not more than 150 vertices.

### Table I. Results for the structures in Figure 8

<table>
<thead>
<tr>
<th>structure (graph)</th>
<th>n of cells</th>
<th>number of colors</th>
<th>CPU time</th>
<th>STABIL</th>
<th>seconds</th>
<th>STABCOL</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
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<td>2</td>
<td>16</td>
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<td>0.05</td>
<td></td>
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<tr>
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<td>3</td>
<td>18</td>
<td>0.03</td>
<td>0.01</td>
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The program has also been tested on first members of three infinite families of graphs where the automorphism groups and the numbers of orbits on the vertices and ordered pairs of vertices are known. We give a description of these families. The results are shown in Tables II–IV.

**Benzene stacks.** We denote by $P_k$ the graph from this family consisting of $n = 6k$ vertices. The vertices of $P_k$ form $k$ stages (strata), each stage (stratum) is a cycle of 6 vertices. Besides the edges in these cycles there are edges between stages. The graphs $P_k$, $k = 2, 3, 4$, are depicted in Figure 9. A formal description of the graphs $P_k$ is the following.

Let $L = \{a, b, c, d, e, f\}$, $K = \{1, 2, \ldots, k\}$, $x_i = (x, i)$ for $x \in L$, $i \in K$.

Then $P_k = (\Omega(P_k), E(P_k))$, where $\Omega(P_k) = L \times K$, $E(P_k) = \bigcup_{i=1}^{k} R_i \cup \bigcup_{j=1}^{k-1} Q_j$, and

$R_i = \{\{a_i, b_i\}, \{b_i, c_i\}, \{c_i, d_i\}, \{d_i, e_i\}, \{e_i, f_i\}, \{f_i, a_i\}\},$

$Q_j = \begin{cases} 
\{\{a_j, a_{j+1}\}, \{c_j, c_{j+1}\}, \{e_j, e_{j+1}\}\} & : j = 2l - 1 \\
\{\{b_j, b_{j+1}\}, \{d_j, d_{j+1}\}, \{f_j, f_{j+1}\}\} & : j = 2l.
\end{cases}$

It is known from [KilLP89] and from [KilLPZ92] that the automorphism group of $P_k$ is isomorphic to $S_3 \times S_2$. $Aut(P_k)$ has $k$ orbits on the set $\Omega(P_k)$ and $4k^2$ orbits on the set $\Omega(P_k) \times \Omega(P_k)$.

**Table II.** Results for benzene stacks

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Möbius ladders. We denote by $M_k = (\Omega(M_k), E(M_k))$ the graph with the set of $n = 2k$ vertices $\Omega(M_k) = \{a_1, \ldots, a_k, a_{k+1}, \ldots, a_{2k}\}$ and the set of edges $E(M_k) = \{\{a_i, a_j\} \mid j - i = x \pmod{2k}, x \in \{1, k, 2k - 1\}\}$. For example, the graph $M_5$ is depicted in Figure 10, which may serve as an explanation of the name.

The symmetry of the graphs $M_k$ has been investigated in [KliKZ90], [Sim86], [WalSH88], [FarKM94] and [KliRRT95]. It was proved in [KliKZ90] that, for $k > 3$, the automorphism group of $M_k$ is isomorphic to the dihedral group $D_{2k}$. This group has one orbit on the set $\Omega(M_k)$ and $k + 1$ orbits on the set $\Omega(M_k) \times \Omega(M_k)$. 

Figure 9
### Table III. Results for Möbius ladders

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![Figure 10](image_url)
Dynkin graphs. Let $D_n$ denote the tree with $n$ vertices as depicted in Figure 11. For $n > 4$ the automorphism group of $D_n$ is isomorphic to $Z_2$. It has $n - 1$ orbits on the set of vertices and $n^2 - 2n + 2$ orbits on the set of ordered pairs of vertices.

Table IV. Results for Dynkin graphs

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Figure 11
The program STABIL has a rather long history. The first attempt of an implementation was done by E.V. Krukovskaya in PASCAL, see [KliK90]. A draft version of the present program was written in C by I.V. Chuvaeva and D.V. Pasechnik at the N. D. Zelinskii Institute of Organic Chemistry (Moscow) in 1990–1992, see [ChuKP92]. Finally this version was improved at the Technical University Munich in 1995. The improved version had statical memory and, by this reason, was available only to graphs with up to 200 vertices. This version was carefully tested and the results of this testing are presented above. In 1996 new improvements were done according to the suggestions of Ch. Pech (Dresden): dynamical memory management was created. Now the current version, in principle, can handle graphs with an arbitrary number of vertices. If for a given graph \( \Gamma \) the number of vertices is sufficiently small (that is if there will be enough memory for saving all data structures) then we will get \( W(\Gamma) \) as output. Otherwise, the program will inform the user that the task cannot be fulfilled completely.

This last version of the program was used for other purely theoretical purposes. Our experience shows that graphs with up to 500 vertices can be successfully managed, however in some cases we were able to handle even larger graphs.

The codes of both programs STABIL and STABCOL and a read.me file which describes how to use the programs are now available by ftp from the address “ftp://math.statistik.tu-muenchen.de/pub/DiskMath”.

The practical users of the programs are kindly invited to make a reference to this report whenever results are published which were obtained via the use of STABIL or STABCOL.

The programs STABIL and STABCOL cannot be involved to other programs or computer packages without a special permission which might be obtained from the authors of STABIL and STABCOL.
10 Discussion

The presented algorithm provides a very powerful and efficient tool to determine equivalence of atoms and pairs of atoms in molecules. The equivalence classes are obtained by examining in a systematic way all configurations of three vertices in the underlying graph. The partitions of the vertices and edges are the finest which can be deduced using configurations of this size.

As already mentioned before, the standard partition of a graph not necessarily coincides with its automorphism partition. Indeed, there exist graphs where the former partition is coarser than the latter. Methods which settle this shortcoming to a certain extent are based on the following idea. Classify vertices and edges by examining configurations which consist not only of three but of a larger number of vertices. This proceeding is generally called deep stabilization or stabilization of depth $t$.

Roughly speaking, the situation is the following. Let $\Gamma$ be a graph with $n$ vertices (possibly a directed multigraph) and $t$ a fixed integer, $2 \leq t \leq n$. All possible $n^t$ subgraphs of $\Gamma$ which are induced by the ordered $t$-tuples of vertices are examined. We have to find all $\nu$ isomorphism types of these subgraphs. To each pair $(u,v)$ of vertices a vector of length $\mu$ is associated, each component of the vector being equal to the number of subgraphs of the corresponding isomorphism type which contain the pair $(u,v)$. Any iteration of the stabilization procedure of depth $t$ assigns two pairs $(u,v)$ and $(u',v')$ the same color if and only if the vectors corresponding to these pairs are equal. It is clear that the computation of the total degree partition is nothing else than stabilization of depth $2$, Weisfeiler-Leman stabilization has depth $3$. For depth at least $4$ we obtain stronger algorithms, however at the price of a considerably higher complexity. One of the first attempts of a program implementation of stabilization of depth $t \geq 4$ for purely chemical goals and on a rather “naive” level was done in [Rue91].

It will be demonstrated in the next paper [FurKT] of this series that, in contrast to first expectations, stabilization of depth $t$ with some $t \geq 4$ is also not sufficient to rigorously settle the automorphism partitioning problem. It turns out (see [Fur87], [Cai92]) that for any fixed value of $t$ there exist graphs with the property that the standard partition of depth $t$ does not coincide with the automorphism partition.

In future work we intend to develop an implementation of the WL-stabilization which eventually is even faster than the implementation STABIL presented in this paper. A very promising approach is to perform in an alternative way stabilization steps of depth $2$ and $3$. Given a colored complete directed graph $\Delta = (\Omega, R)$, we start with stabilization of depth $2$, i.e. we compute the total degree partition of $\Delta$ (let $\Delta_k$ be the graph consisting of the arcs of color $k$; then the total degree partition of $\Delta$ is the coarsest partition of $V$ such that any two vertices belonging to the same cell of the partition have the same valencies with respect to any other cell in any graph $\Delta_k$). The arcs of a given color are recolored according to the colors of their end vertices such that arcs between different colored pairs of vertices are assigned different colors. In the next step the coloring of the arcs and vertices is refined analogously as in algorithm STABIL by considering all triangles of the graph. However, in order to decrease the effort, this is not
done iteratively, but only once. After that we again compute the total degree partition, perform one stabilization step of depth 3, etc. The algorithm stops if the coloring of \( \Delta \) is stable.

As it was mentioned before, we can only be sure to get the automorphism partition of a graph \( \Gamma \) by means of WL-stabilization if it is known in advance that the algebra \( W(\Gamma) \) is Schurian.

In general, we can only suggest to proceed in the following way:
find the automorphism group \( G = \text{Aut}(\Gamma) \) of the graph \( \Gamma \);
describe the set of 2-orbits (or only 1-orbits) of the action of \( G \) on the vertex set of \( \Gamma \).

This problem, in principle, may be solved using e.g. the computer package COCO (I.A. Faradžev, M.H. Klin), the UNIX implementation by A.E. Brouwer.

The preliminary versions of COCO are described in [FarK91] and [FarKM94]. With the use of COCO one may handle graphs with a few thousands of vertices. The current version of COCO (which is available from the Technical University Eindhoven) is oriented for purely mathematical goals, namely for the investigation of graphs having a sufficiently large prescribed subgroup of the automorphism group. In such a case the input graph is described by a set of arcs as a union of suitable 2-orbits of a prescribed permutation group. For purely chemical purposes such a mode of input is certainly inconvenient. Hopefully, in the future a more suitable interface for chemists will be created.

This technical report is considered by the authors as a preliminary version of a future regular publication. We will be very grateful to everybody who supplies us with remarks, comments, criticism or improvements.

Unless more convenient M. Klin should be regarded as the corresponding author.

Acknowledgments

We want to express our deep gratitudes to the following colleagues:

G.M. Adel’son-Velskii for helpful discussions concerning the complexity of the WL-stabilization;

S. Baumann and M. Lüdecke for their help in preparing the manuscript and testing the program;

I.A. Faradžev for very important consultations related to dealing with hashing problems (during the creation of the first draft of the program);

Ch. Pech for all suggested improvements, in particular for assistance in implementing a dynamical memory management;
Ch. and G. Rücker for the fruitful discussions and remarks which reflect real requests of chemists to the use of algebraic combinatorics;

G. Tinhofer for permanent interest and support of this project;

N.S. Zefirov for creating a lucky opportunity for mathematicians to work with chemists and to realize their practical interests.

References


