# THE REDUCTION OF A GRAPH TO CANONICAL FORM AND THE ALGEBRA WHICH APPEARS THEREIN 

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#### Abstract

We consider an algorithm for the reduction of a given finite multigraph $\Gamma$ to canonical form. Therein the new invariant of a graph appears - the algebra $\mathcal{A}(\Gamma)$. The study of properties of the algebra $\mathcal{A}(\Gamma)$ turns out to be helpful in solving a number of graph-theoretic problems. We pose and discuss some conjectures on the relation between properties of the algebra $\mathcal{A}(\Gamma)$ and the automorphism group $\operatorname{Aut}(\Gamma)$ of a graph $\Gamma$. We give an example of undirected graph $\Gamma$ whose algebra $\mathcal{A}(\Gamma)$ coincides with the group algebra of some noncommutative group.

English abstract from the original article. An algorithm is considered, reducing the specified finite multigraph $\Gamma$ to canonical form. In the course of this reduction, a new invariant of the graph is generated - algebra $\mathcal{A}(\Gamma)$. Study of the properties of the algebra $\mathcal{A}(\Gamma)$ proves helpful in solving a number of graph-theoretic problems. Some propositions concerning the relationships between the properties of the algebra $\mathcal{A}(\Gamma)$ and the graph's automorphism group $\operatorname{Aut}(\Gamma)$ are discussed. An example of non-oriented graph $\Gamma$ is constructed whose algebra $\mathcal{A}(\Gamma)$ coincides with the group algebra of a non-commutative group.

English title from the original article. A reduction of a graph to canonical form and an algebra arising during this reduction.


1. Consider a finite graph $\Gamma$ and its adjacency matrix $A(\Gamma)=\left\{a_{i j}\right\}$, where $a_{i j}$ is the number of edges from $i$ th vertex to $j$ th one; $i, j=1,2, \ldots, n$. If $\Gamma$ is an undirected graph then set $a_{i j}=a_{j i}$. A canonical form of a graph is defined to be its adjacency matrix with respect to a canonical labeling of its vertices, that is a partial ordering of the vertex set such that if vertices $a$ and $b$ are incomparable then there is an automorphism of a graph moving $a$ to $b$ and preserving the adjacency relation.

In Sections 6 and 7, we describe the reduction of a graph to canonical form which consists of a step-by-step reordering of rows and columns of the matrix $A(\Gamma)$ and, roughly speaking, adds up to the following.

Consider for simplicity an undirected graph without multiple edges. Associate with every vertex of the graph the characteristic vector which has one component equal to the number of neighbors of this vertex. Then divide vertices into classes such that vertices with equal characteristic vectors belong to the same class and order classes according to the natural order on the set of characteristic vectors. Further, associate with every vertex the characteristic vector $v_{i}=\left(l, v_{i 1}, v_{i 2}, \ldots\right)$, where $v_{i k}$ is the number of neighbors of vertex $i$ from class $k$ and $l$ is the number of the class which contains vertex $i$. Now again divide vertices into classes according to new characteristic vectors ordered lexicographically, etc. Note that if vertices $a$ and $b$ belong to different classes and the condition $a<b$ holds at some step then this condition also holds at the next steps. This implies that the described process stops after at most $n$ steps and after the stop either all vertices belong to different classes (i.e. a canonical labeling was constructed) or further division does not proceed.

If $\Gamma$ is a directed multigraph then take the ordered $i$ th row of $A(\Gamma)$ as a characteristic vector $v_{i}$ assuming that the diagonal element precedes other elements. Instead of different elements $a_{i j}$ introduce different independent variables $x_{1}, x_{2}, \ldots$ ordered according to the order on $a_{i j}$. Denote the matrix obtained in such way by $X(\Gamma)$. As before, divide vertices into classes assuming that a class consists of vertices with the same characteristic vector. Note that the $k$ th component of vector $v_{i}$ is equal to the sum of all elements of the $i$ th row of $X(\Gamma)$ corresponding to vertices of the $k$ th class from the previous step. The matrix $X(\Gamma)$ is divided into blocks in every of which we can introduce new independent variables, etc. (for exact definitions of these operations see Section 6, operations $\alpha_{1}, \beta_{1}$ ).

Note that the above procedure is similar to methods from $[1,2]$.
For further division of the set of vertices into classes consider an element $u_{i j}$ of the matrix $U=X X^{\prime}$, where $X^{\prime}$ is the matrix obtained from $X$ by replacing variables $x_{1}, x_{2}, \ldots$ by variables $x_{1}^{\prime}, x_{2}^{\prime}, \ldots$. All variables $x_{1}, x_{2}, \ldots, x_{1}^{\prime}, x_{2}^{\prime}, \ldots$ are independent. The element $u_{i j}$ is a quadratic polynomial of $x_{1}, x_{2}, \ldots, x_{1}^{\prime}, x_{2}^{\prime}, \ldots$ Now if we denote different polynomials by new different independent variables then we can apply all above operations to the obtained matrix and so on until this process stops (see Section 6 , operations $\alpha_{2}, \beta_{2}, \beta_{3}$ ).
2. An introduction of independent variables and the matrix $U=X X^{\prime}$ from the above procedure has the following geometrical sense. On the first step of our procedure edges of $\Gamma$ and edges of its complement $\bar{\Gamma}$ will be associated with different variables, i.e. edges of $\Gamma$ and edges of $\bar{\Gamma}$ will be colored in different colors. Further each introduction of new variables defines a new coloring of edges and: (1) edges which have different colors on some step will have different colors on next steps; (2) vertices are divided into classes according to the number of outgoing edges of each color.

It is known that an element $a_{i j} \in A^{2}$, where $A=A(\Gamma)$ and $\Gamma$ is an undirected graph without multiple edges, is equal to the number of paths of length 2 from vertex $i$ to vertex $j$. Similarly, a coefficient at $x_{k} x_{l}^{\prime}$ in polynomial $u_{i j} \in U=X X^{\prime}$ is equal to the number of paths from vertex $i$ to vertex $j$ the first and the second parts of which consist of edges of colors $k$ and $l$ respectively.
3. The next part of the reduction of a graph to canonical form uses an application of the above operations to the matrix obtained from $X(\Gamma)$ by deleting of some row and column. If we define the reduction to canonical form for matricies of order $k \leq n-1$ then it is possible to divide vertices into classes in the following way: a vertex is assumed to be senior if after deleting of this vertex we obtain the lexicographically largest canonical form of the remaining graph (see operations $\alpha_{3}, \alpha_{4}, \beta_{4}, \mathrm{~W}$, Section 7). Clearly, such process will stop at some step. We prove that if two vertices $a$ and $b$ belong to the same class at the last step then $a$ and $b$ are equivalent, i.e. there exists an automorphism of $\Gamma$ which maps $a$ to $b$ and preserves the adjacency relation.

Again, consider the matrix $X=X(\Gamma)$ such that there are equal polynomials in the matrix $U=X X^{\prime}$ in the positions of equal variables in the matrix $X$. The matrix $X(\Gamma)$ is a common point of some matrix algebra $\mathcal{A}(\Gamma)$, i.e. given a ring $K$ (for example, the ring of integers $\mathbb{Z}$ or the ring of rationals $\mathbb{Q}$ ) matrices obtained from $X$ by the replacing of its variables by elements of $K$ form the algebra $\mathcal{A}_{K}(\Gamma)=\mathcal{A}(\Gamma) \otimes K$. Clearly, the algebra $\mathcal{A}(\Gamma)$ is an invariant
of a graph. We discuss on the relationships between the algebra $\mathcal{A}(\Gamma)$ and properties of $\Gamma$ in Sections 8-10.
4. Notation. The automorphism group of a graph $\Gamma$ is denoted by Aut( $\Gamma$ ).

The matrix consisting of independent variables is denoted by $X=\left(x_{i j}\right)$.
Independent variables from the main diagonal of $X$ are denoted by $y_{1}, y_{2}, \ldots$; other independent variables from $X$ are denoted by $x_{1}, x_{2}, \ldots$.
$i$ th row and $i$ th column of a given matrix $A$ are denoted by $f_{i}^{I}(A)$ and $f_{i}^{I I}(A)$ respectively.
The matrix obtained from $X$ by replacing of variables $x_{i}, y_{i}$ by variables $x_{i}^{\prime}, y_{i}^{\prime}$ is denoted by $X^{\prime}=\left(x_{i j}^{\prime}\right)$; here variables $x_{i}, y_{i}, x_{i}^{\prime}, y_{i}^{\prime}$ are independent.

The matrix obtained from $X$ by deleting of $i$ th row and $i$ th column is denoted by $X_{i}$.
Given an ordered set $V$ and a vector $v \in V^{n}$ the vector obtained from $v$ by ordering of its components is denoted by $\bar{v}$.
5. Consider a finite directed multigraph $\Gamma$. We can associate $\Gamma$ in a natural way with the matrix $A(\Gamma)$. Further construct the matrix $X(\Gamma)$ whose elements are independent variables $x_{1}, x_{2}, \ldots, y_{1}, y_{2}, \ldots$ and

$$
\begin{gathered}
x_{k(i j)}=x_{k\left(i^{\prime} j^{\prime}\right)} \Leftrightarrow a_{i j}=a_{i^{\prime} j^{\prime}}, i \neq j, i^{\prime} \neq j^{\prime}, \\
y_{q(i)}=y_{q(j)} \Leftrightarrow a_{i i}=a_{j j} .
\end{gathered}
$$

Define an ordering on the set of variables in the following way:

$$
\begin{aligned}
& y_{i}>x_{k} ; \\
& y_{q(i)}>y_{q(j)} \Leftrightarrow a_{i i}>a_{j j} ; \\
& x_{k(i j)}>x_{k\left(i^{\prime} j^{\prime}\right)} \Leftrightarrow a_{i j}>a_{i^{\prime} j^{\prime}} .
\end{aligned}
$$

Enumerate variables according to this ordering. Define also an ordering on the set of bilinear forms of $x_{i}, x_{i}^{\prime}, y_{i}, y_{i}^{\prime}$ in the following way:

$$
x_{i} x_{j}^{\prime}>x_{k} x_{l}^{\prime} \Leftrightarrow(i j)>(k l) \text { etc. }
$$

6. Basic operations. The operation $\alpha_{0}(X)$ is a permutation of rows and columns of a matrix $X$ such that $i \leq j \Leftrightarrow y_{k(i)} \leq y_{k(j)}$ for all diagonal elements of $\alpha_{0}(X)$. The operation $\alpha_{1}(X)$ is an introduction of new variables. Put in the positions $(i i)$ and $(j j)$ in the matrix $\alpha_{1}(X)$ the elements $y_{l(i)}$ and $x_{l(i j)}$ respectively so that

$$
\begin{gathered}
l(i)<l(j) \Leftrightarrow\left(\widetilde{f}_{i}^{I}(X), \widetilde{f}_{i}^{I I}(X)\right)<\left(\widetilde{f}_{j}^{I}(X), \widetilde{f}_{j}^{I I}(X)\right), \\
l(i, j)<l\left(i^{\prime}, j^{\prime}\right) \Leftrightarrow F(i, j)<F\left(i^{\prime}, j^{\prime}\right),
\end{gathered}
$$

where

$$
\begin{gathered}
F(i, j)=\left(x_{i j, j i}, \widetilde{f}_{i}^{I}(X), \widetilde{f}_{i}^{I I}(X), \widetilde{f}_{j}^{I I}(X)\right) \\
\alpha_{2}(X)=\alpha_{1}\left(X X^{\prime}\right) \\
\beta_{1}(X)=\alpha_{1}^{s}(X)
\end{gathered}
$$

where

$$
\alpha_{1}^{s-1}(X) \neq \alpha_{1}^{s}(X)=\alpha_{1}^{s+1}(X)
$$

$$
\beta_{2}(X)=\left(\alpha_{2} \beta_{1}\right)^{s}(X)
$$

where

$$
\begin{gathered}
\left(\alpha_{2} \beta_{1}\right)^{s-1}(X) \neq\left(\alpha_{2} \beta_{1}\right)^{s}(X)=\left(\alpha_{2} \beta_{1}\right)^{s+1}(X) \\
\beta_{3}(X)=\alpha_{0} \beta_{2}(X)
\end{gathered}
$$

7. Reduction to canonical form. Suppose that the operation $\mathrm{J}(X)$ is defined for matrices $X$ of order $k \leq n-1$ and $\mathrm{J}(X)$ possess the following properties: (1) $\mathrm{J}(X)$ is a composition of reordering of rows and columns and introduction of new variables; (2) all diagonal elements of the matrix $X^{\prime}=\mathrm{H}(X)$ are pairwise distinct. Suppose also that for every permutation $\sigma$ the equality

$$
\mathrm{G}\left(\sigma X \sigma^{-1}\right)=\mathrm{Ы}(X) X^{\prime}
$$

holds. If $k=1$ then put $\mathrm{H}(X)=X$.
Denote by $\beta(X)$ the matrix obtained from $X^{\prime}=\mathrm{y}(X)$ by the replacing of its variables by variables of the matrix $X$ from which they (variables of $X^{\prime}$ ) arise. Clearly,

$$
\begin{equation*}
\beta(X)=\beta(Y) \Leftrightarrow \text { there exists } \sigma: X=\sigma Y \sigma^{-1} \tag{1}
\end{equation*}
$$

Define the lexicographical ordering on the set of matrices of the same order assuming as before that

$$
x_{i}<x_{j} \Leftrightarrow i<j, y_{i}<y_{j} \Leftrightarrow i<j .
$$

The operation $\alpha_{3}(X)$ is an introduction of new variables. Put in the positions (ii) and (ij) in the matrix $\alpha_{3}(X)$ the elements $y_{l(i)}$ and $x_{l(i, j)}$ respectively so that

$$
\begin{gathered}
l(i)<l(j) \Leftrightarrow\left(x_{i i}, \beta\left(X_{i}\right)\right)<\left(x_{j j}, \beta\left(X_{j}\right)\right), \\
l(i j)<l\left(i^{\prime} j^{\prime}\right) \Leftrightarrow\left(x_{i j}, \beta\left(X_{i}\right), \beta\left(X_{j}\right)\right)<\left(x_{i^{\prime} j^{\prime}}, \beta\left(X_{i^{\prime}}\right), \beta\left(X_{j^{\prime}}\right)\right) \\
\beta_{4}(X)=\left(\alpha_{3} \beta_{3}\right)^{s}(X)
\end{gathered}
$$

where

$$
\begin{equation*}
\left(\alpha_{3} \beta_{3}\right)^{s-1}(X) \neq\left(\alpha_{3} \beta_{3}\right)^{s}(X)=\left(\alpha_{3} \beta_{3}\right)^{s+1}(X) \tag{2}
\end{equation*}
$$

Lemma. If $b_{i j}=b_{j i}$ for some elements of the matrix $B=\beta_{4}(X)$ then there exists $a$ permutation $\sigma$ such that $\sigma(i)=j$ and $\sigma B \sigma^{-1}=B$, i. e. $\sigma \in \operatorname{Aut}(B)$.
Proof. $1^{\circ}$. Since $b_{i j}=b_{j i}$, the equality $\beta\left(B_{i}\right)=\beta\left(B_{j}\right)$ holds by (2) and due to (1) there exists an isomorphism $\sigma^{\prime}: B_{i} \rightarrow B_{j}$, i.e. a map $\sigma^{\prime}:(1,2, \ldots, i, \ldots, n) \rightarrow(1,2, \ldots, j, \ldots, n)$ such that $\sigma^{\prime} B_{i} \sigma^{\prime-1}=B_{j}$.
$2^{\circ}$. Put $\sigma(i)=j, \sigma(k)=\sigma^{\prime}(k), k \neq i$. The matrix obtained from $X$ by replacing of variables of $i$ th row and $i$ th column by zeros is denoted by $\widetilde{X}_{i}$. Clearly, $\sigma \widetilde{B}_{i} \sigma^{-1}=\widetilde{B}_{j}$. Prove that $\sigma B \sigma^{-1}=B$.

Let

$$
\begin{gathered}
\sum_{i} b_{i j}=\sum_{s} m_{j s} x_{s}+y_{q(j)}, \\
\widetilde{B}_{i}=\left(c_{k l}\right), \sum_{k} c_{k l}=\sum_{s} n_{l s} x_{s}+y_{q(l)},
\end{gathered}
$$

$$
\widetilde{B}_{j}=\left(d_{k l}\right), \sum_{k} d_{k l}=\sum_{s} n_{l s}^{\prime} x_{s}+y_{q(l)}
$$

The image of $b_{i j} \in B$ under the map $\sigma$ is $b_{j \sigma(l)} \in B$. Obviously,

$$
\begin{gathered}
b_{i l}=\sum_{s}\left(m_{l s}-n_{l s}\right) x_{s}+\delta_{i l} y_{q(i)} \\
b_{j \sigma(l)}=\sum_{s}\left(m_{\sigma(l) s}-n_{\sigma(l) s}^{\prime}\right) x_{s}+\delta_{j \sigma(l)} y_{q(j)}
\end{gathered}
$$

The condition of the lemma implies that $y_{q(i)}=y_{q(j)}$ and $\delta_{i l}=\delta_{j \sigma(l)}$. Since $\sigma \widetilde{B}_{i} \sigma^{-1}=\widetilde{B}_{j}$, we conclude that $y_{q(l)}=y_{q(\sigma(l))}$. So $m_{l s}=m_{\sigma(l) s}$ for all $s$ because otherwise an application of $\alpha_{1}$ to $B$ yields a change of $B$ that contradicts to the definition of $\beta_{4}(X)$. Finally, $n_{l s}=n_{\sigma(l) s}^{\prime}$ for all $s$ because $\sigma \widetilde{B}_{i} \sigma^{-1}=\widetilde{B}_{j}$. Thus, $b_{i l}=b_{j \sigma(l)}$ for every $l$ and the lemma is proved.

Let $\operatorname{sp} X=\sum_{i} n_{i} y_{i}$ and $n_{i}=l$, where $i \leq l \leq n$. If $l=n$ put $\mathrm{J}(X)=X$. If $l<n$ and $n_{l+1} \geq 2$ then define the operation $\alpha_{4}(X)$ which is a deleting of a row and a column. Namely, put

$$
\begin{gathered}
x_{i i}=y_{i}, i \leq l+1 \\
x_{i i}=y_{q(i)+1}, i>l+1
\end{gathered}
$$

Due to Lemma, the operation $\alpha_{4}(X)$ is invariant, i.e. if $\sigma$ is a permutation then $\sigma X \sigma^{-1}=X$ implies that $\sigma \alpha_{4}(X) \sigma^{-1}=\alpha_{4}(X)$.

Finally, put $\mathrm{J}(X)=\left(\alpha_{4} \beta_{4}\right)^{n-l}(X)$. Since operations $\alpha_{i}, \beta_{i}$ are invariant, the operation $\mathrm{J}(X)$ is also invariant.
Definition. Canonical form of a graph $\Gamma$ is defined to be the matrix obtained from $\beta(X(\Gamma))$ by substitution in it the elements of $A(\Gamma)$ from which the corresponding variables of $X(\Gamma)$ arise.

Remark. Clearly, canonical form of a graph $\Gamma$ depends on a way of ordering used in the process of the reduction.
8. Algebra generated by a graph $\Gamma$. Let $\Gamma$ be a graph. Then $Y=\beta_{3}(X(\Gamma))$ is a common point (in the sense of the algebraic geometry) of some associative matrix algebra $\mathcal{A}(\Gamma)$. The algebra $\mathcal{A}(\Gamma)$ consists of matrices obtained by replacing of variables in $Y$ by arbitrary numbers. From the definition of the operation $\alpha_{1}$ it follows that the algebra $\mathcal{A}(\Gamma)$ is invariant under transpose, i.e. it is semisimple. The algebra $\mathcal{A}(\Gamma)$ is invariant of $\Gamma$ and it can be used for studying of $\Gamma$. For example, the group $\operatorname{Aut}(\Gamma)$ coincides with the group of permutation matrices $\sigma$ such that

$$
\begin{equation*}
\sigma Y \sigma^{-1}=Y \tag{3}
\end{equation*}
$$

This fact can be used for solving of the following problem: given a graph $\Gamma$ find the group Aut $(\Gamma)$. Also it can be used for solving of the inverse problem. For graphs with the number of verticies $n \leq 6$ these problems were solved by Kagno [3]. It seems that these problems (at least the direct one) can be solved for graphs with greater number of vertices by using the suggested algebraic approach.
9. Conjectures. (1). If $\operatorname{sp} Y=n y_{0}$ then there exists a group $G$ such that $\mathcal{A}(\Gamma) \subset Z_{R}(G)$, where $Z_{R}(G)$ is the matrix algebra spanned by operators $R_{g}$ of the right multiplication by elements $g \in G$ in the standard basis of the group ring, and the elements $e_{i}$ of the standard basis of $\mathcal{A}(\Gamma)\left(x_{j}=\delta_{i j}\right)$ are equal to sums of some elements of the standard basis $R_{g_{i}}$.

If this conjecture is true then $G \subset \operatorname{Aut}(\Gamma)$ and $G$ acts transitively on the set of vertices of $\Gamma$.
(2). The orbits of $\operatorname{Aut}(\Gamma)$ coincide with the sets of vertices for which diagonal elements in $Y=\beta_{3}(X)$ are the same. If $\operatorname{sp} Y=n y_{0}$ then this statement follows from Conjecture (1).

If Conjecture (2) is true then the process of the reduction of a graph to canonical form becomes much easier. Indeed, in this case we can apply the operation $\alpha_{4}$ to the matrix $\beta_{3}(X)$ and put $\mathrm{J}(X)=\left(\alpha_{4} \beta_{3}\right)^{n}(X)$.

An indirect confirmation of the above conjectures is the next proposition

Proposition. If a group $G \subset \operatorname{Aut}(\Gamma)$ acts regularly on the set of vertices of a graph $\Gamma$ then $\mathcal{A}(\Gamma) \subset Z_{R}(G)$ and the above conjectures hold.

Proof. Since $G$ acts regularly, it is possible to identify elements of $G$ with vertices of $\Gamma$ and the action of $G$ with left multiplication respectively. In view of (3) and $G \subset \operatorname{Aut}(\Gamma)$, the algebra $\mathcal{A}(\Gamma)$ lies inside the centralizer $\mathcal{B}$ of the algebra spanned by operators of the left multiplication. Note that $\mathcal{B} \supset Z_{R}(G)$ because operators of the left multiplication commute with operators of the right multiplication. Prove that $\mathcal{B}=Z_{R}(G)$. Let $B \in \mathcal{B}$. Subtract from $B$ a linear combination of elements of $Z_{R}(G)$ such that the first row of the obtained matrix $B^{\prime}$ consists of zeros. Since $B^{\prime}$ commutes with $G$, every row of $B^{\prime}$ consists of zeros. So $B^{\prime}=0$ and hence $B \in Z_{R}(G)$. Similarly, there exist elements $g_{1}, g_{2}, \ldots, g_{s}$ such that the first row of the matrix $e_{i}-\sum_{j} R g_{j}$ consists of zeros. As before, this implies that $e_{i}=\sum_{j} R g_{j}$.
10. Finally, we give an example of an undirected graph $\Gamma$ without multiple edges whose algebra $\mathcal{A}(\Gamma)$ coincides with the group algebra of some non-abelian group. Let $X$ be a vector space of the group algebra of the symmetric group $S_{4}$ of four variables. The matrix of multiplication by $\omega \in \mathbb{Z}\left[S_{4}\right]$ with respect to the standard basis of $X$ is denoted by $A_{\omega}$. Note that if $\omega=\sum a_{i} \sigma_{i}$ then $A_{\omega}=\sum a_{i} A_{\sigma_{i}}$ and $A_{\omega}^{t}=\sum a_{i} A_{\sigma_{i}^{-1}}$.

Let $\sigma=(1234), \tau=(123), \rho=(14), \omega=\sigma+\sigma^{-1}+\tau+\tau^{-1}+\rho$ and $\Gamma$ be a graph with the matrix $A(\Gamma)=A_{\omega}$. Clearly, $A(\Gamma)$ is symmetric and its elememts are equal to 0 or 1 . So $\Gamma$ is undirected graph without multiple edges.

Put $\widetilde{\omega}=x_{1} \omega+x_{2} \widehat{\omega}+y \cdot 1$, where $\widehat{\omega}=I-\omega$ and $I=\sum_{\varphi \in S_{4}} \varphi$. Direct computation shows that

$$
\begin{array}{r}
\widetilde{\omega} \widetilde{\omega}^{\prime}=x_{1} x_{1}^{\prime} \omega^{2}+x_{2} x_{2}^{\prime}\left(14 I+\omega^{2}\right)+y y^{\prime} \cdot 1+\left(x_{1} y^{\prime}+x_{1}^{\prime} y\right) \omega+ \\
+\left(x_{2} y^{\prime}+x_{2}^{\prime} y\right)(I-\omega)+\left(x_{1} x_{2}^{\prime}+x_{1}^{\prime} x_{2}\right)\left(5 I+\omega^{2}\right)= \\
=I\left(14 x_{2} x_{2}^{\prime}+x_{2} y^{\prime}+x_{2}^{\prime} y+5 x_{1} x_{2}^{\prime}+5 x_{1}^{\prime} x_{2}\right)+\alpha\left(2 x_{1} x_{1}^{\prime}+\right. \\
\left.+2 x_{2} x_{2}^{\prime}+x_{1} y^{\prime}+x_{1}^{\prime} y-x_{2} y^{\prime}-x_{2}^{\prime} y+2 x_{1} x_{2}^{\prime}+2 x_{1}^{\prime} x_{2}\right)+ \\
\beta\left(x_{1} x_{1}^{\prime}+x_{2} x_{2}^{\prime}+x_{1} y^{\prime}+x_{1}^{\prime} y-x_{2} y^{\prime}-x_{2}^{\prime} y+x_{1} x_{2}^{\prime}+x_{1}^{\prime} x_{2}\right)+ \\
+\eta\left(x_{1} x_{1}^{\prime}+x_{2} x_{2}^{\prime}+x_{1} x_{2}^{\prime}+x_{1}^{\prime} x_{2}\right)+ \\
1\left(y y^{\prime}+5 x_{2} x_{2}^{\prime}+5 x_{1} x_{1}^{\prime}+5 x_{1} x_{2}^{\prime}+5 x_{1}^{\prime} x_{2}\right),
\end{array}
$$

where

$$
\begin{gathered}
\alpha=\tau+\tau^{\prime}+\rho \\
\beta=\omega-\alpha=\sigma+\sigma^{-1} \\
\eta=(1342)+(1243)+(234)+(243) .
\end{gathered}
$$

Negative coefficients appear because we collect all summands with $I$ into a separate one. Further,

$$
\varphi=\alpha_{2}(\widetilde{\omega})=x_{1} I+x_{2} \alpha+x_{3} \beta+x_{4}(\varepsilon+\gamma+\theta)+x_{5} \eta+y \cdot 1,
$$

where

$$
\gamma=\sigma^{2}, \varepsilon=(1423)+(1342), \theta=(34) .
$$

Applying the operation $\alpha_{2}$ again we obtain

$$
\psi=\alpha_{2}(\varphi)=x_{1} I+y \cdot 1+x_{2} \rho+x_{3} \theta+x_{4} \gamma+\ldots
$$

At last, prove that $\rho, \theta$, and $\gamma$ generate the group $S_{4}$. This will imply that $\mathcal{A}(\Gamma)=\mathbb{Z}\left[S_{4}\right]$.

$$
\begin{gathered}
\rho=(14), \gamma \rho=(13)(24)(14)=(1342)=\lambda, \\
\lambda^{2}=(14)(23) \\
\lambda^{2} \rho=(23)
\end{gathered}
$$

It is well-known fact that permutations (14), (23), and (34) generate $S_{4}$.
11. Let us study in more details the structure of the algebra $\mathcal{A}(\Gamma)$ in case when $\operatorname{sp} Y=$ $n y_{0}$. We will use only the following apriori description of considered algebras.

Definition. (1) A cell is defined to be a matrix algebra $\mathcal{A}$ invariant under transpose and such that its common point $X=\left(x_{i j}\right)$ satisfies the conditions:

$$
\begin{equation*}
\sum_{i} x_{i j}=\sum_{i} x_{j i}=\sum_{k} n_{k} x_{k} \tag{k}
\end{equation*}
$$

where $x_{k}$ are distinct independent variables (A fixing of a matrix representation means a fixing of a basis $\xi_{1}, \xi_{2}, \ldots, \xi_{n}$ of the corresponding vector space).
(2) A subcell is defined to be a subalgebra of the cell $\mathcal{A}$ that is a cell in the same matrix representation.
(3) A normal subcell is defined to be is a subcell $\mathcal{R}$ preserving a subspace spanned by some proper subset $\xi_{i_{1}}, \xi_{i_{2}}, \ldots, \xi_{i_{s}}$ of vectors of a fixed basis (this means that some permutation of basis vectors reduce matrices from $\mathcal{R}$ to the block form).
(4) A cell is said to be imprimitive if it has a proper non-trivial normal subcell, and it is said to be primitive otherwise.
12. Basic properties of a cell with identity. The matrix from $\mathcal{A}$ obtained from $X$ by replacing of $x_{j}$ by $\delta_{i j}$ is denoted by $e_{i}$. Set $e_{i} e_{j}=\sum_{k} a_{i j}^{k} e_{k}, \widehat{e}=\sum_{i} e_{i}$, and $e_{i^{\prime}}=e_{i}^{\prime}$ (the last definition is correct because $\mathcal{A}$ is invariant under transpose). We assume that $x_{0}$ is a variable from the diagonal and hence $e_{0}$ is the identity matrix. Matrices $e_{i}$ form a basis of $\mathcal{A}$ that we call the standard basis.

P1. $a_{i j}^{k}$ is a non-negative integer because $\mathcal{A}$ is an algebra and (k) holds.
P2. $\sum_{s} a_{i j}^{s} a_{s l}^{k}=\sum_{s} a_{i s}^{k} a_{j l}^{s}$ because $\mathcal{A}$ is associative.
P3. $\left(\sum b_{i} e_{i}\right) \widehat{e}=\widehat{e}\left(\sum b_{i} e_{i}\right)=\left(\sum b_{i} n_{i}\right) \widehat{e}$.
P4. $\sum_{i} a_{k i}^{j}=\sum_{i} a_{i k}^{j}=n_{k}, \sum_{k} n_{k}=n$ because $\widehat{e} e_{k}=e_{k} \widehat{e}=n_{k} \widehat{e}$.
P5. $\sum_{s} a_{i j}^{s} n_{s}=n_{i} n_{j}$ because $\left(e_{i} e\right)_{j} \widehat{e}=\left(\sum_{s} a_{i j}^{s} n_{s}\right) \widehat{e}=n_{i} n_{j} \widehat{e}$.
P6. $a_{i j}^{0}=\delta_{i^{\prime} j} n_{i}$ because P4 holds and $e_{0}=\mathrm{id}, a_{i i^{\prime}}^{0}=n_{i}$ by the definition of $e_{i^{\prime}} ; a_{0 i}^{s}=\delta_{i s}$.
P7. $a_{i j}^{s}=a_{j^{\prime} i^{\prime}}^{s^{\prime}}$ because $\sum a_{i j}^{s} e_{s}^{\prime}=\left(e_{i} e_{j}\right)^{\prime}=e_{j}^{\prime} e_{i}^{\prime}=e_{j^{\prime}} e_{i^{\prime}}=\sum a_{j^{\prime} i^{\prime}}^{s^{\prime}} e_{s^{\prime}}$.
P8. $n_{i} a_{j k}^{i^{\prime}}=n_{j} a_{k i}^{j^{\prime}}=n_{k} a_{i j}^{k^{\prime}}$. This property follows from P2 for $k=0$ and P6: $\sum_{s} a_{i j}^{s} a_{s l}^{0}=$ $\sum_{s} a_{i j}^{s} \delta_{s l^{\prime}} n_{l}=n_{l} a_{i j}^{l^{\prime}}=\sum_{s} a_{i s}^{0} a_{j l}^{s}=\sum_{s} n_{i} \delta_{i^{\prime} s} a_{j l}^{s}=n_{i} a_{j l}^{i^{\prime}}$.

P9. $a_{k j}^{i}$ is divisible by $M=\left[\frac{n_{j}}{\left(n_{i}, n_{j}\right)}, \frac{n_{k}}{\left(n_{i}, n_{k}\right)}\right]$, where $(a, b)$ and $[a, b]$ are the greatest common divisor and the least common multiple of $a$ and $b$ respectively; $M \leq n_{k}$ and $M \leq n_{j}$ whenever $a_{k j}^{i} \neq 0$.

Indeed, $\frac{n_{i}}{n_{j}} a_{k j}^{i^{\prime}}=a_{i k}^{j^{\prime}}$ by P8. If $a_{i k}^{j^{\prime}}=0$ then P9 is obvious; otherwise $a_{i k}^{j^{\prime}}$ is a positive integer and hence $a_{k j}^{i}$ is divisible by $\frac{n_{j}}{\left(n_{i}, n_{j}\right)}$. Similarly, $a_{k j}^{i}$ is divisible by $\frac{n_{k}}{\left(n_{i}, n_{k}\right)}$. Therefore the first statement of P9 holds. The second statement of P9 follows from the first one and P4 because $M \leq a_{k j}^{i} \leq \min \left\{n_{k}, n_{j}\right\}$.

Proposition P10. The algebra $\mathcal{A}$ is decomposable over $\mathbb{Q}$ into the direct sum of the algebras $\{\widehat{\lambda e}\}$ and $\mathcal{A}^{0}=\left\{\sum a_{i} e_{i}: \sum n_{i} a_{i}=0\right\}$.

Proof. The algebra $\{\lambda \widehat{e}\}$ is an ideal by P3. Let $\varphi: \mathcal{A} \rightarrow \mathbb{Q}$ such that $\varphi\left(\sum a_{i} e_{i}\right)=\sum n_{i} a_{i}$. Then $\varphi$ is a homomorphism. So $\mathcal{A}^{0}$ is an ideal. Since $\mathcal{A}^{0}$ and $\{\lambda \widehat{e}\}$ are subalgebras in $\mathcal{A}^{0}$, we obtain that $\mathcal{A}=\mathcal{A}^{0}+\{\widehat{\lambda e}\}$.

Definition. A directed graph $\Gamma$ is called weakly (respectively, strongly) connected if for every two vertices $a$ and $b$ there exists a directed path either from a to $b$ or from $b$ to $a$ (respectively, both paths).

Sometimes we will identify $e_{i}$ or $\sum_{i \in I} e_{i}$ with a graph having the corresponding adjacency matrix. Given verticies $a$ and $b$ of a graph $\Gamma$ we write $a \rightarrow b$ if there exists a directed path from $a$ to $b$ in $\Gamma$ and $a \nrightarrow b$ otherwise.

Proposition P11. If a graph $\Gamma=\sum_{i \in I} e_{i}$ is weakly connected then it is strongly connected.
Proof. Let $a$ be a vertex of $\Gamma$. Put $A_{a}=\{b: b \neq a, b \rightarrow a \rightarrow b\}, B_{a}=\{b: b \neq a, b \rightarrow a \rightarrow$ $b\}$, and $C_{a}=\{b: b \neq a, a \rightarrow b \nrightarrow a\}$. Obviously, the sets $A_{a}, B_{a}, C_{a}$ are pairwise disjoint.

Assume that $A_{a} \neq \varnothing$ and $b \in A_{a}$. There are paths from $a$ only to vertices from $B_{a} \cup C_{a}$; there are paths from $b$ to vertices from $B_{a} \cup C_{a} \cup\{a\}$ and, possibly, to some other vertices. Therefore the sets $\{c: c \neq a, a \rightarrow c\}$ and $\{c: c \neq b, b \rightarrow c\}$ have different cardinalities which contradicts P2 and P4. Therefore $A_{a}=\varnothing$. By the same argument $C_{a}=\varnothing$. Thus $\Gamma$ is strongly connected and the proposition is proved.
13. Imprimitive cells and quotient cells. Let $\mathcal{A}$ be a cell with identity, $\mathcal{B}$ a normal subcell of $\mathcal{A}, f_{1}, f_{2}, \ldots, f_{k}$ the standard basis of $\mathcal{B}$, and $\bar{e}=\sum_{i=1}^{k} f_{i}$. By the definition of a subcell, $\bar{e}=\sum_{i \in I} e_{i}$. Clearly, $i \in I \Leftrightarrow e_{i} \bar{e}=\bar{e} e_{i}=n_{i} \bar{e}$. This yields that the set $\left\{e_{i}: i \in I\right\}$ generates a normal subcell.

From the normality of $\mathcal{B}$ it follows that the graph $\bar{e}$ is non-connected. We may assume that $\bar{e}$ is reduced to a block form according to connected components and there are no zeros in diagonal blocks.

P12. Degrees of diagonal blocks of a normal subcell are equal because these degrees are equal to $m=\sum_{i} \overline{e_{i j}}=\sum_{i \in I} n_{i}$, where $\left(\overline{e_{i j}}\right)=\bar{e}$.

The reduction of $\bar{e}$ to a block form defines a partition of the matrix $X$ (common point of $\mathcal{A}$ ) into $m \times m$ blocks $X_{i j}$. Blocks $X_{i j}$ and $X_{k l}$ are said to be similar if for every $a \in[m(i-1)+1, m i]$ there exists $b \in[m(k-1)+1, m k]$ such that

$$
\begin{equation*}
\sum_{s=m(j-1)+1}^{m j} x_{a s}=\sum_{s=m(i-1)+1}^{m i} x_{b s} \tag{S}
\end{equation*}
$$

and the same conditions hold for columns. If $X_{i j}$ and $X_{k l}$ are similar then we write $X_{i j} \sim X_{k l}$.
P13. $X_{l l} \sim X_{k k}$ for all $l, k$ because $\mathcal{B}$ is a cell and $X_{i j} \nsim X_{k k}$ whenever $i \neq j$ because blocks are defined by connected components and variables from diagonal blocks do not appear outside these blocks.

P14. If $X_{i j} \nsim X_{k k}$ then every variable from $X_{i j}$ does not appear in $X_{l s}$ and conversely, if there are ones in the block $X_{i j}$ of the matrix $e_{q}$ then there are only zeros in the block $X_{l s}$ of this matrix.

Let us prove P14. Consider a row $S_{1}$ of $X_{i j}$ and an arbitrary row $S_{2}$ of $X_{l s}$. Since $X_{i j} \nsim X_{l s}$, there exists $r$ such that the variable $x_{r}$ appears $p_{1} \neq 0$ times in $S_{1}$ and $p_{2} \neq p_{1}$ times in $S_{2}$. All elements of the rows $S_{1}$ and $S_{2}$ of $e_{r} \bar{e}$ are equal to $p_{1}$ and $p_{2}$ respectively. From the definition of a cell it follows that in this case $S_{1}$ and $S_{2}$ do not have common variables and we are done.

P15. If sets of variables of two rows of the same block $X_{i j}$ do not coincide then these sets are disjoint. The proof of P15 is similar to the proof of P14.

Definition. Let $n=m k$. The quotient cell $\mathcal{A} / \mathcal{B}$ is defined to be the set of $k \times k$-matrices with a common point $Z$ defined by the following condition:

$$
z_{i j}=z_{l s} \Leftrightarrow X_{i j} \sim X_{l s}
$$

Theorem P16. The quotient cell $\mathcal{A} / \mathcal{B}$ is a cell.
Proof. Consider the algebra $\mathcal{A}_{C}$ with the common point $X_{C}$ obtained from $X$ by the following replacement: two elements of $X$ are replaced by the same variable if and only if they are from similar blocks. It follows that $X_{C}=Z \otimes M$, where $M$ is an $m \times m$-matrix consisting of ones. Due to P14, $X_{C} X_{C}^{\prime} \in \mathcal{A}_{C}$. This implies that $Z$ is a common point of a matrix algebra. Obviously, this algebra is a cell.

Theorem P17. A cell $\mathcal{A}$ is imprimitive if and only if contains an ideal $\mathcal{L}$ which is a subcell. If $\mathcal{B}$ is a normal subcell of $\mathcal{A}$ and $\mathcal{L}=\mathcal{A} / \mathcal{B}$ then $\mathcal{A}$ contains an ideal isomorphic to $\mathcal{L}$ as an algebra.

Proof. Let $\mathcal{A}$ be imprimitive cell with identity, $\mathcal{B}$ its normal subcell, and $\mathcal{A}_{C}$ the algebra defined in the proof of Theorem P16. In view of P14, the algebra $\mathcal{A}_{C}$ is an ideal of $\mathcal{A}$. Conversely, let $\mathcal{L}$ be an ideal of $\mathcal{A}$ that is a subcell. Let $f_{i}=\sum_{j \in G_{i}} e_{j}$ be the standard basis of $\mathcal{L}$. Prove that there exists $i$ with $0 \in J_{i}$. Indeed, if $s \in J_{k}$ then there exists an $m$ such that $e_{s}^{m} f_{k}$ has a non-trivial projection onto $e_{0}$ because every connected component of $e_{s}$ contains a directed cycle (see P11). Since $\mathcal{L}$ is an ideal, $e_{s}^{m} f_{k}=\sum d_{i} f_{i}$, i.e. $e_{0}$ is contained in some $f_{i}$. Moreover, $e_{0}$ is contained in exactly one $f_{i}$ because $\mathcal{L}$ is a subcell. Denote this $f_{i}$ by $f_{0}$. Consider $f_{0}^{\prime} f_{0}$. If $q=\sum_{i \in J_{0}} n_{i}$ then $f_{0}^{\prime} f_{0}=q f_{0}+g$. Since $\mathcal{L}$ is a subcell and the number of elements equal to 1 in rows of matrices $f_{0}$ and $f_{0}^{\prime}$ is equal to $q$, we obtain that $g=0$, i.e. the graph $f_{0}$ is non-connected and its connected components define a desired normal subcell. Thus P17 is proved.
14. Primitive cells. Let $\mathcal{A}$ be a primitive cell with identity. Then the graphs $e_{i}$ and hence their sums are strongly connected (see P11 and Section 13). Put $e_{J}=\sum_{i \in J} e_{i}$, $n_{J}=\sum_{i \in J} n_{i}$, and let $n_{J}<n-1$.

P18. Rows of $e_{I}$ are pairwise distinct.
Indeed, we may assume that the first $q$ rows in $e_{I}$ are pairwise equal and different from other rows. All elements of the upper left minor $M$ of order $q$ in $f=e_{J} e_{J}^{\prime}$ are equal to $n_{J}$ whereas all elements of the first $q$ rows outside $M$ are less than $n_{J}$. In view of the definition of a cell, this implies that if $e_{i}$ has elements equal to 1 inside $M$ then all elements outside $M$ which belong to the first $q$ rows of $e_{i}$ are equal to 0 , i.e. $e_{i}$ is non-connected.

P19. If $a_{i j}^{k}=n_{j}$ then $n_{i}>n_{j}$.
Indeed, $n_{j}=a_{i j}^{k} \leq n_{i}$ by P4. Let $u(f)$ be the first row of $f$. We may assume that $u\left(e_{k}\right)=(0111 \ldots 100 \ldots 0), u\left(e_{i}\right)=(00 \ldots 01 \ldots 1)$. Then $u\left(e_{i} e_{j}\right)=\left(* n_{j} n_{j} \ldots n_{j} * * \ldots *\right)$ ( $n_{j}$ appears $n_{k}$ times). If $n_{i}=n_{j}$ then the 2nd, 3rd, $\ldots,\left(n_{k}+1\right)$ th columns of $e_{j}$ are pairwise equal which contradicts P18.

Let $q_{1}<q_{2}<\ldots<q_{m}, J_{k}=\left\{i: n_{i}=q_{k}\right\}, i \in \bigcup_{k} J_{k}$ for every $i$.
P20. For every $i$ and $j$ there exists $s \neq j$ such that $a_{i s}^{j} \neq 0$.
P21. For every $l$ and every $i \notin J_{l}$ there exists $j \notin J_{l}$ such that $a_{i j}^{k} \neq 0$ for every $k \in J_{l}$.
Indeed, since $e_{i}$ is connected, $e_{i}^{n}$ has a projection onto $e_{s}$ for every $s$, in particular, onto $e_{j}$. So there exists $s$ such that $a_{i s}^{j} \neq 0$. Let $r=\min \left\{t: e_{i}^{t}\right.$ has a projection onto $\left.\bigcup_{s \in G_{l}} e_{s}\right\}$. Since $e_{i}^{r-1}=\sum_{i \notin J_{l}} b_{i} e_{i}$, there exists $j \notin J_{l}$ such that $a_{i j}^{k} \neq 0$ for every $k \in J_{l}$ and P21 is proved.

P22. For every $i$ the following inequality holds: $\left(q_{i}, q_{m}\right) \geq \frac{q_{m}}{q_{m-1}}>1$.
In view of P 21 , for every $i$ there exist $j$ and $k$ such that $n_{j} \leq q_{m-1}, n_{k}=q_{m}$, and $a_{i j}^{k} \neq 0$. Due to P9, we have $n_{j} \geq \frac{q_{m}}{\left(n_{i}, q_{m}\right)}$ and hence P22 holds.

P23. If $q_{m}=p^{k}$, where $p$ is a prime, then $p^{k-\left[\log _{p} q_{m-1}\right]}$ divides $q_{i}$ for every $i$.
P24. If $q_{m}$ is a prime then $m=1$, i.e. all $n_{i}$ are equal.
P23 and P24 are easy corollaries of P22.
P25. $q_{k+1} \leq q_{k} q_{1} ; q_{m} \leq q_{1}^{\operatorname{dim} \mathcal{A}-2}$.
Indeed, let $e_{g_{1}}^{t}=\sum_{i} b_{i t} e_{i}$ and $q(t)=\max \left\{n_{i}: b_{i s} \neq 0, s \leq t\right\}$. Obviously, $q(t+1) \leq q(t) q_{1}$ and $q\left(t_{0}\right)=q_{m}$, where $t_{0}=\operatorname{dim} \mathcal{A}-\left|J_{1} \cup 0\right|$. This yields P 25 .

P26. If $q_{1}=1$ then $\mathcal{A}=\mathbb{Z}\left[\mathbb{Z}_{p}\right]$, where $p$ is a prime.
Indeed, if $n_{i}=1$ then $e_{i}$ is a permutation matrix. The set $\left\{\sum_{i \in J} a_{i} e_{i}\right\}$ forms a normal subcell and it is isomorphic to the group algebra of the group $G=\left\{e_{i}: i \in J_{1}\right\}$. This cell is primitive only if $G=\mathbb{Z}_{p}$.

P27. If $q_{1}=2$ then $\mathcal{A}=\mathbb{Z}\left[\sigma+\sigma^{-1}\right]$, where $\sigma^{p}=1$ for some prime $p$.
Indeed, if $n_{i}=2$ then by Hall's theorem there exist permutation matrices $\sigma$ and $\tau$ such that $e_{i}=\sigma+\tau$. Further, $e_{i}^{\prime}=\sigma^{-1}+\tau^{-1}$ and $e_{i} e_{i}^{\prime}=2+\sigma \tau^{-1}+\tau \sigma^{-1}=2+\varphi+\varphi^{-1}=2+e_{k}$. So $e_{k}=e_{k}^{\prime}$ and $n_{k}=2$, i.e. $e_{k}$ is an undirected cycle. Now the argument similar to the argument from P26 yields P27.
15. Constructing of examples. Let $G$ be a finite group, $H \leq \operatorname{Aut}(G), \mathbb{Z}[G]$ the group algebra of $G$ with the standard basis consisting of elements of $G$. Let $\mathcal{A}=\{a \in$ $\mathbb{Z}[G]: h(a)=a$ for every $h \in H\}$. Then $\mathcal{A}$ is a cell with the standard basis $\sum_{h \in H} h(g), g \in G$. The cell $\mathcal{A}$ is primitive, for example, in the following cases: $G$ is a simple group and $H$ is the group of its inner automorphisms; $G=\left(\mathbb{Z}_{p}\right)^{n}$ and $H$ is an irreducible subgroup of GL $\left(n, \mathbb{Z}_{p}\right)$.

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## References

1. H. Bouman, Computer program for the LINCO System, J. Chem. Docum., 5, No. 1 (1965), 14-23.
2. H.L. Morgan, The generation of a unique machine description for chemical structures, J. Chem. Docum., 5, No. 2 (1965), 107-112.
3. J.N. Kagno, Linear graphs of degree $\leq 6$ and their groups, Amer. J. Math., 68, No. 3 (1946), 505-520.
4. D. G. Higman, Intersection matricies for finite permutation groups, J. Algebra, 6, No. 1 (1967), 22-42.
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