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Degeneracy of some matrix graph invariants

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New matrices associated with graphs and induced global and local topological indices of molecular graphs were proposed recently by Diudea, Minailiuc and Balaban. These matrices in canonical form are matrix graph invariants. A combined degeneracy of such invariants is considered. For every case of degeneracy corresponding graphs are presented.

1. Introduction

Matrices associated with graphs are widely used for designing and computing local and global topological indices of molecular graphs [1–9]. Some of these matrices naturally arise from considering distances between vertices of a graph. For example, the well known topological index, Wien number, can be defined and calculated from the distance matrix or from the layer matrix of a graph [8].

Three new graph matrices **B**, **E** and **S** were proposed recently by Diudea, Minailiuc and Balaban [9]. These matrices were used for designing families of local (BR, ER and SR) and global (BY, EY and SY) topological indices. It was shown that the topological indices are able to express the branching (or complexity) and to induce a particular ordering of molecular graphs. They also correlate well with van der Waals volumes and boiling points in alkane series.

We also consider the layer matrix of a graph (or distance degree sequence), based on distances between vertices of a graph. This matrix is used for characterizing the structure of graphs, establishing the similarity of molecular graphs, calculating topological indices, designing graph algorithms, and in other applications [10–23].

An interesting problem about properties of these matrices is the question of their degeneracy. A coincidence of the matrices for nonisomorphic graphs implies a degeneracy of all derived topological indices. We shall consider some cases of combined degeneracy of the layer matrix $\boldsymbol{\lambda}$ and the matrices **B**, **E** and **S**.

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2. Matrices of a graph

We consider the graph matrices which do not represent a graph uniquely. For example, the distance matrix determines a graph up to isomorphism.

The distance $d(v, u)$ between two vertices u and v in a graph G is the minimal number of edges in G from u to v. The eccentricity $\mathrm{ecc}(v)$ of a vertex v is $\max d(v, u)$ for all u in G, and the diameter $\mathrm{diam}(G)$ of a graph is the maximum eccentricity. The degree of a vertex $v \in V(G)$ is the number of its adjacent vertices and is denoted by $\deg(v)$. We assume throughout this paper that a graph G has p vertices and q edges.

Define the partition of vertices of a graph G with respect to $v_i \in V(G)$ as the set of layers $G(v_i) = \{V_j(v_i) | j = 0, 1, \ldots, \mathrm{ecc}(v)$ and $u \in V_j(v_i) \Leftrightarrow d(v_i, u) = j\}$. Figure 1 shows a polycyclic graph G and the partition of its vertices. The set of partitions $G(v_i)$ for all $v_i \in V(G)$ is a source for generating various matrices of a graph. Now we consider four such matrices.

The layer matrix $\boldsymbol{\lambda}(G) = \|\lambda_{ij}\|$ of a graph G includes the cardinalities of layers in all partitions. Its entries λ_{ij} are the number of vertices situated at distance j from the vertex v_i, i.e. $\lambda_{ij} = |V_j(v_i)|$ for all $i = 1, 2, \ldots, p$ and $j = 1, 2, \ldots, \mathrm{diam}(G)$.

The matrix $\mathbf{B}(G) = \|b_{ij}\|$ of a graph G contains information about degrees of vertices in the layers of partitions. The entry b_{ij} is defined as sum of the vertex degrees for all vertices situated at distance j from the vertex v_i, i.e. $b_{ij} = \{\sum \deg(u) | u \in V_{j-1}(v_i)\}$ for all $i = 1, 2, \ldots, p$ and $j = 1, 2, \ldots, \mathrm{diam}(G) + 1$.

The matrix $\mathbf{E}(G) = \|e_{ij}\|$ of a graph G contains the cardinalities of edge sets around layers. The component e_{ij} is equal to sum of the number of edges incident only with the vertices of layer $V_{j-1}(v_i)$ and the number of edges from $V_{j-1}(v_i)$ to $V_j(v_i)$ for all $i = 1, 2, \ldots, p$ and $j = 1, 2, \ldots, \mathrm{diam}(G) + 1$.

The matrix $\mathbf{S}(G) = \|s_{ij}\|$ is introduced for increasing the discriminating power of the matrices $\mathbf{B}$ and $\mathbf{E}$. The matrix entry is defined by the equality $s_{ij} = b_{ij} + e_{ij}$ for all $i = 1, 2, \ldots, p$ and $j = 1, 2, \ldots, \mathrm{diam}(G) + 1$.

Figure 2 shows the matrices for a tree G_1, for a bipartite graph G_2 and for a graph G_3 with old cycles. Note that all entries of the last column in the matrix $\mathbf{E}$ are always equal to zero for a bipartite graph.

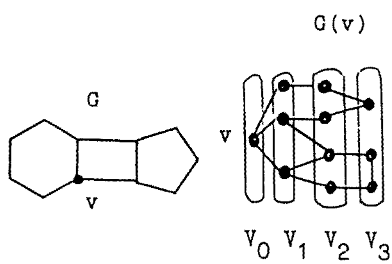
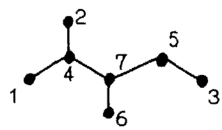


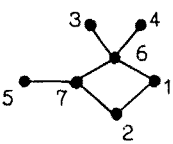
Fig. 1. Partition of graph vertices with respect to the vertex v.

G_1



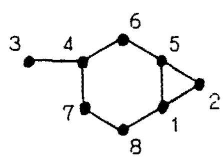
$$\lambda=\begin{bmatrix}1&2&2&1\\1&2&2&1\\1&1&2&2\\3&2&1&0\\2&2&2&0\\1&2&3&0\\3&3&0&0\end{bmatrix}\quad B=\begin{bmatrix}1&3&4&3&1\\1&3&4&3&1\\1&2&3&4&2\\3&5&3&1&0\\2&4&4&2&0\\1&3&5&3&0\\3&6&3&0&0\end{bmatrix}\quad E=\begin{bmatrix}1&2&2&1&0\\1&2&2&1&0\\1&1&2&2&0\\3&2&1&0&0\\2&2&2&0&0\\1&2&3&0&0\\3&3&0&0&0\end{bmatrix}\quad S=\begin{bmatrix}2&5&6&4&1\\2&5&6&4&1\\2&3&5&6&2\\6&7&4&1&0\\4&6&6&2&0\\2&5&8&3&0\\6&9&3&0&0\end{bmatrix}$$

G_2



$$\lambda=\begin{bmatrix}2&3&1\\2&2&2\\1&3&2\\1&3&2\\1&2&3\\4&2&0\\3&3&0\end{bmatrix}\quad B=\begin{bmatrix}2&6&5&1\\2&5&5&2\\1&4&6&3\\1&4&6&3\\1&3&6&4\\4&7&3&0\\3&7&4&0\end{bmatrix}\quad E=\begin{bmatrix}2&4&1&0\\2&3&2&0\\1&3&3&0\\1&3&3&0\\1&2&4&0\\4&3&0&0\\3&4&0&0\end{bmatrix}\quad S=\begin{bmatrix}4&10&6&1\\4&8&7&2\\2&7&9&3\\2&7&9&3\\2&5&10&4\\8&10&3&0\\6&11&4&0\end{bmatrix}$$

G_3



$$\lambda=\begin{bmatrix}3&2&1&1\\2&2&2&1\\1&2&2&2\\3&2&2&0\\3&2&2&0\\2&4&1&0\\2&3&2&0\\2&3&2&0\end{bmatrix}\quad B=\begin{bmatrix}3&7&4&3&1\\2&6&4&5&1\\1&3&4&5&5\\3&7&5&3&0\\3&5&5&5&0\\2&6&8&2&0\\2&5&8&3&0\\2&5&6&5&0\end{bmatrix}\quad E=\begin{bmatrix}3&3&2&1&0\\2&3&2&2&0\\1&2&2&3&1\\3&3&3&0&0\\3&2&3&1&0\\2&4&3&0&0\\2&3&4&0&0\\2&3&3&1&0\end{bmatrix}\quad S=\begin{bmatrix}6&10&6&4&1\\4&9&6&7&1\\2&5&6&8&6\\6&10&8&3&0\\6&7&8&6&0\\4&10&11&2&0\\4&8&12&3&0\\4&8&9&6&0\end{bmatrix}$$

Fig. 2. Matrix invariants of graphs.

3. Relationships between the matrix entries

One immediate observation is that sums of the first column of considered matrices are the degree sequence of a graph. The number of non-zero elements in a row of a matrix is called the length of the row. The sequence of lengths for all rows in the layer matrix forms the eccentric sequence of a graph [24].

Table 1 presents obvious results of summation for the matrix entries.

In order to compare the matrices we define its canonical form. By ordering the rows of a matrix with respect to the decrease of their length, and then lexicographi-

Table 1
Sums of the matrix entries.

λ	$\mathbf{B}$	$\mathbf{E}$	$\mathbf{S}$
$\sum_i \lambda_{i1} = 2q$	$\sum_i b_{i1} = 2q$	$\sum_i e_{i1} = 2q$	$\sum_i s_{i1} = 4q$
$\sum_j \lambda_{ij} = p - 1$	$\sum_j b_{ij} = 2q$	$\sum_j e_{ij} = q$	$\sum_j s_{ij} = 3q$
$\sum_{ij} \lambda_{ij} = p(p-1)$	$\sum_{ij} b_{ij} = 2pq$	$\sum_{ij} e_{ij} = pq$	$\sum_{ij} s_{ij} = 3pq$

cally arranging the rows with the same length, one can obtain a canonical form of the matrix. It is clear that the matrices, presented in canonical form, are graph invariants. All matrices of graphs of fig. 2 have canonical form. We shall assume that the matrices are always canonical.

Denote by m_{ij} the number of edges in which one of the incident vertices belongs to the layer $V_{j-2}(v_i)$ and an other vertex belongs to $V_{j-1}(v_i)$. Let c_{ij} be the number of edges incident with the vertices of $V_{j-1}(v_i)$ only. For the sake of brevity we shall drop the bounds for entry indices.

PROPOSITION 1

For an arbitrary graph the following inequalities hold

$$s_{ij} \geqslant b_{ij}, \quad s_{ij} \geqslant e_{ij}, \quad b_{ij} \geqslant \lambda_{ij}, \quad b_{ij} \geqslant e_{ij}, \quad e_{ij} \geqslant \lambda_{ij}\,.$$

Proof

The inequalities $s_{ij} \geqslant b_{ij}, s_{ij} \geqslant e_{ij}$ and $b_{ij} \geqslant \lambda_{ij}$ are obvious. An entry of the matrix **B** may be presented as $b_{ij} = m_{ij} + 2c_{ij} + m_{i,j+1}$, where $m_{ij} > 0$ for $j \geqslant 2$. For an entry of the matrix **E** we have $e_{ij} = c_{ij} + m_{i,j+1}$. Therefore, $b_{ij} \geqslant e_{ij}$. □

PROPOSITION 2

For an arbitrary graph the following equality holds:

$$b_{ij} - e_{i,j-1} - e_{ij} = c_{ij} - c_{i,j-1}\,.$$

Proof

Since $e_{ij} = c_{ij} + m_{i,j+1}$ and $e_{i,j-1} = c_{i,j-1} + m_{i,j}$, then $b_{ij} = m_{ij} + 2c_{ij} + m_{i,j+1} = m_{ij} + c_{ij} + e_{ij} = e_{i,j-1} - c_{i,j-1} + c_{ij} + e_{ij}$. □

The relations between matrix entries may be simplified for classes of graphs.

COROLLARY 1

For an arbitrary bipartite graph we have
(a) the first columns of the matrices **B** and **E** are the same;
(b) entries of the last column of the matrix **E** are always equal to zero;
(c) the last column of the matrix **B** and the last but one column of **E** are the same;
(d) $b_{ij} = e_{i,j-1} + e_{ij}$ for $2 \leqslant j \leqslant \mathrm{diam}(G)$.

Proof

Since a bipartite graph has no odd cycles, then $c_{ij} = 0$ for all i and j. This obviously implies the cases (b)–(d). □

All entries of the matrices **B** and **S** are defined completely by the entries of the matrix **E**. This property shows that local and global topological indices based on the matrices **B** and **S** may be calculated by means of the matrix **E**.

COROLLARY 2

For an arbitrary tree we have
(a) the first columns of the matrices **B** and **λ** are the same:
(b) the last columns of the matrices **B** and **λ** are the same;
(c) $e_{ij} = \lambda_{ij}$ and $b_{ij} = \lambda_{i,j-1} + \lambda_{ij}$ for $2 \leqslant j \leqslant \mathrm{diam}(G)$.

Proof

The last layer of any partition consists of vertices with degree 1. Every vertex of the layer $V_j(v_i)$, $j \geqslant 1$, is incident with only vertex of the layer $V_{j-1}(v_i)$ in a tree. Hence, $e_{ij} = \lambda_{ij}$. Since a tree is a bipartite graph, then $b_{ij} = \lambda_{i,j-1} + \lambda_{ij}$ for all $2 \leqslant j \leqslant \mathrm{diam}(G)$. □

The last proposition shows that topological indices of trees may be computed by means of the layer matrix.

The next result provides a relationship between the first and the second columns of the matrices.

PROPOSITION 3

(a) For an arbitrary graph the equality holds

$$\sum_i b_{i1}^2 = \sum_i b_{i2};$$

(b) if a graph has no triangles (simple cycles C_3), then

$$\sum_i e_{i1}^2 - 2q = \sum_i e_{i2};$$

(c) if a graph has no cycles C_3 and C_4, then

$$\sum_i \lambda_{i1}^2 - 2q = \sum_i \lambda_{i2};$$

(d) if a graph has no triangles, then

$$\tfrac{1}{2}\sum_i s_{i1}^2 - 2q = \sum_i s_{i2}.$$

Proof

(a) It is clear, that every vertex v of a graph lies in the layers $V_1(u)$ for all vertices u incident with v, i.e. the vertex v is situated in the first layer of all partitions exactly $\deg(v)$ times. Therefore, $\sum_i b_{i2} = \sum_v \deg^2(v)$.

(b) Consider a vertex v of $V_1(u)$ for an arbitrary vertex u. Only edge connects the vertex v with the vertex u. Since a graph has no triangles, then $\deg(v) - 1$ edges connect v with vertices of the layer $V_2(u)$. Hence, $\sum_i e_{i2} = \sum_v \deg(v)(\deg(v) - 1) = \sum_v \deg^2(v) - 2q$.

(c) The proof is analogous as in the case (b). It should be noted that every edge between v and vertices of $V_2(u)$ connects v with a new vertex of the layer.

(d) Since $b_{i1} = e_{i1} = s_{i1}/2$, then $\sum_i s_{i2} = \sum_i b_{i2} + \sum_i e_{i2} = \sum_i b_{i1}^2 + \sum_v e_{i1}^2 - 2q = \frac{1}{2}\sum_i s_{i1}^2 - 2q$. □

Equalities of proposition 3 may be used as additional necessary conditions to check whether a given integer matrix is graphical.

4. Degeneracy of the matrix graph invariants

We consider the problem of degeneracy of the matrix graph invariants. A degeneracy of the matrices $\boldsymbol{\lambda}$, **B**, **E** and **S** implies a degeneracy of all derived topological indices.

A degeneracy of the layer matrix or the matrix **E** is a sufficient condition for a degeneracy of all other matrices for trees.

PROPOSITION 4

Let G and H be trees. If the equality $\boldsymbol{\lambda}(G) = \boldsymbol{\lambda}(H)$ (or $\mathbf{E}(G) = \mathbf{E}(H)$) holds, then $\mathbf{B}(G) = \mathbf{B}(H), \mathbf{E}(G) = \mathbf{E}(H)$ (or $\boldsymbol{\lambda}(G) = \boldsymbol{\lambda}(H)$) and $\mathbf{S}(G) = \mathbf{S}(H)$.

Proof

The proof immediately follows from the relations between entries of the matrices stated by corollary 2. □

A degeneracy of the matrices **B** and **S** depends from a degeneracy of the matrix **E** for bipartite graphs.

PROPOSITION 5

Let G and H be bipartite graphs. If the equality $\mathbf{E}(G) = \mathbf{E}(H)$ holds, then $\mathbf{B}(G) = \mathbf{B}(H)$ and $\mathbf{S}(G) = \mathbf{S}(H)$.

Proof

The proof follows from the relations between entries of the matrices established by corollary 1. □

The previous propositions are not valid for arbitrary graphs. We consider cases of combined degeneracy of the matrices $\boldsymbol{\lambda}, \mathbf{B}$ and **E** only, since these matrices are constructed independently.

PROPOSITION 6

There are pairs of graphs G and H, which have one of the following properties:
(1) $\boldsymbol{\lambda}(G) \neq \boldsymbol{\lambda}(H), \mathbf{B}(G) = \mathbf{B}(H), \mathbf{E}(G) = \mathbf{E}(H)$ and $\mathbf{S}(G) = \mathbf{S}(H)$;
(2) $\boldsymbol{\lambda}(G) \neq \boldsymbol{\lambda}(H), \mathbf{B}(G) \neq \mathbf{B}(H), \mathbf{E}(G) = \mathbf{E}(H)$ and $\mathbf{S}(G) \neq \mathbf{S}(H)$;
(3) $\boldsymbol{\lambda}(G) \neq \boldsymbol{\lambda}(H), \mathbf{B}(G) = \mathbf{B}(H), \mathbf{E}(G) \neq \mathbf{E}(H)$ and $\mathbf{S}(G) \neq \mathbf{S}(H)$;
(4) $\boldsymbol{\lambda}(G) = \boldsymbol{\lambda}(H), \mathbf{B}(G) \neq \mathbf{B}(H), \mathbf{E}(G) \neq \mathbf{E}(H)$ and $\mathbf{S}(G) \neq \mathbf{S}(H)$;
(5) $\boldsymbol{\lambda}(G) = \boldsymbol{\lambda}(H), \mathbf{B}(G) = \mathbf{B}(H), \mathbf{E}(G) = \mathbf{E}(H)$ and $\mathbf{S}(G) = \mathbf{S}(H)$;
(6) $\boldsymbol{\lambda}(G) = \boldsymbol{\lambda}(H), \mathbf{B}(G) \neq \mathbf{B}(H), \mathbf{E}(G) = \mathbf{E}(H)$ and $\mathbf{S}(G) \neq \mathbf{S}(H)$;
(7) $\boldsymbol{\lambda}(G) = \boldsymbol{\lambda}(H), \mathbf{B}(G) = \mathbf{B}(H), \mathbf{E}(G) \neq \mathbf{E}(H)$ and $\mathbf{S}(G) \neq \mathbf{S}(H)$.

Figure 3 presents examples of graphs for every case of proposition 6. Note that these graphs are not minimal with given properties. For example, the central cycle C_4 of some graphs of fig. 3 can be substituted by an edge.

An interesting example of graphs of polycyclic catacondensed benzenoid hydrocarbons is shown in fig. 4. All matrix invariants of the graphs degenerate as in

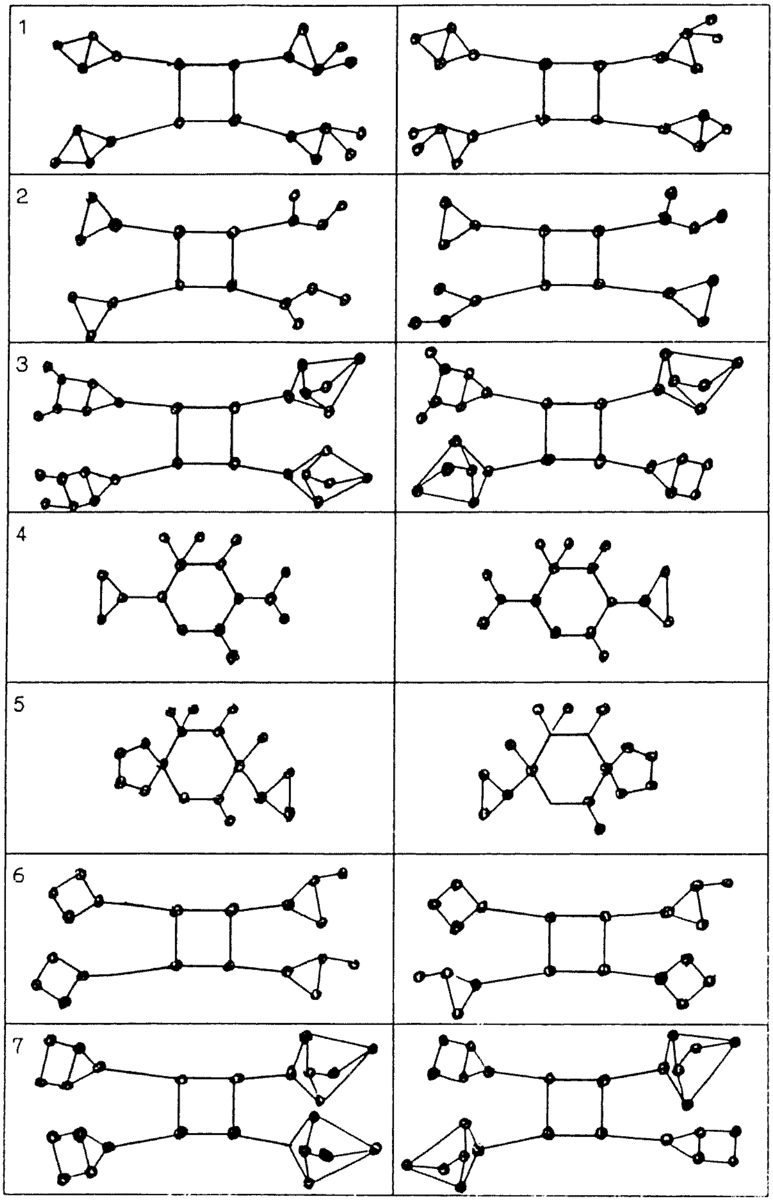


Fig. 3. Pairs of graphs with the same matrix invariants.

case (5). It seems that these graphs have the minimal number of vertices among all graphs of this class.

Next, we shall construct a set of graphs in which the matrix invariants are the same for all graphs. Consider graphs G_1, G_2 and G_3 of fig. 5. These graphs include

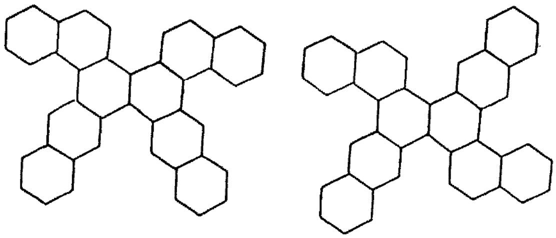


Fig. 4. Cata-condensed benzenoid graphs with the same matrix invariants.

four copies of the connected graph H which consists of a hexagonal ring and four pendant vertices. The neighbor graphs of fig. 5 are distinguished only by the way of attachment of copy of H. We have $\lambda(G_i) = \lambda(G_j)$, $\mathbf{B}(G_i) = \mathbf{B}(G_j)$, $\mathbf{E}(G_i) = \mathbf{E}(G_j)$ and $\mathbf{S}(G_i) = \mathbf{S}(G_j)$ for all $i,j = 1,2,3$.

5. Conclusions

We have presented simple properties of four matrices based on partitions of graph vertices. Also we considered various cases of matrix graph invariants degeneracy, which implies a degeneracy of derived topological indices. A program for computing these matrices from the vertex partitions of a graph was developed. Graphs are input by means of the original screen editor of molecular graphs. The

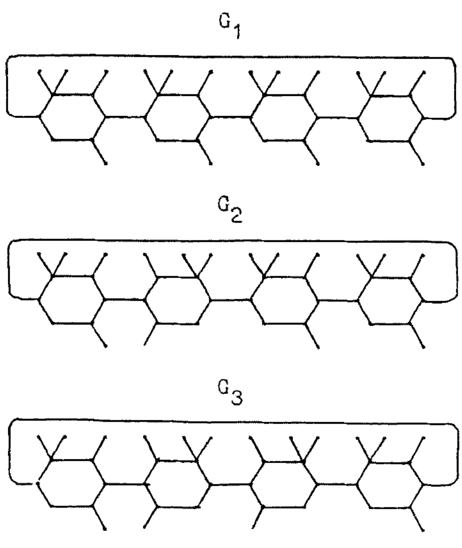


Fig. 5. Graphs with the same matrix invariants.

program is written in Turbo Pascal for an IBM PC XT/AT compatible computer and available on request.

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