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ORIGINAL PAPER

On the path-Zagreb matrix

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Abstract The definition of the path-Zagreb matrix for (chemical) trees PZ and its generalization to any (molecular) graph is presented. Additionally, the upper bound of $\log_2\left(PZ\,(G_n)_{ij}\right)$, where G_n is a graph with n vertices is given.

Keywords Zagreb matrices · Path-Zagreb matrix · Trees · General graphs

1 Introduction and definitions

Several Zagreb matrices (such as the *vertex*-Zagreb matrix, the *edge*-Zagreb matrix and their modified forms) and derived molecular descriptors are discussed extensively in the literature [1–10]. Janežič et al. [11] mentioned the *path-Zagreb matrix*, but did not discussed. The idea about path matrixes has been for the first time elaborated in [12] for trees. Here we first give the defnition of the path-Zagreb matrix for any (molecular) graph. Before we proceed, let us first remind the definition of a path [13]: A path is a walk in which all the vertices are distinct.

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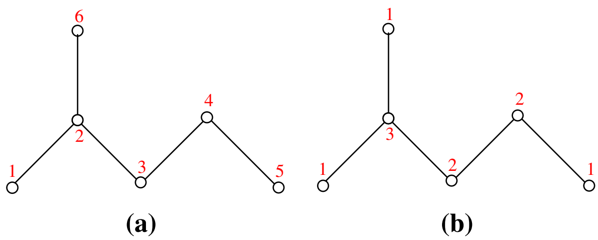


Fig. 1 The vertex-labels (**a**) and the vertex-degrees (**b**) of branched tree T_1 representing the carbon skeleton of 2-methylpentane

Let T be an arbitrary tree. Then the path-Zagreb matrix, denoted by *PZ*, is defined by:

$$PZ\,(T)_{ij} = \prod_{\substack{v \text{ is vertex on the} \\ \text{path from } i \text{ to } j}} d_T\,(v).$$

where d_T is the degree of a vertex v. Below we give, as an example, the path-Zagreb matrix of a branched tree representing the carbon skeleton of 2-methylpentane. In Fig. 1 we give the labeled tree T_1 and the corresponding vertex-degrees.

$$PZ(T_1) = \begin{bmatrix} 0 & 3 & 6 & 12 & 12 & 3 \\ 3 & 0 & 6 & 12 & 12 & 3 \\ 6 & 6 & 0 & 4 & 4 & 6 \\ 12 & 12 & 4 & 0 & 2 & 12 \\ 12 & 12 & 4 & 2 & 0 & 12 \\ 3 & 3 & 6 & 12 & 12 & 0 \end{bmatrix}$$

It is easily seen that the above definition of path-Zagreb matrix for trees cannot be (without modifications) generalized to all graphs. Namely, here we use the special property of trees that every two vertices in a tree are connected by the unique path. However, generally speaking, two vertices in a connected graph, other than a tree, can be linked by more than one path. In this report, we propose the following generalizations of the path-Zagreb matrix.

Let G be any graph. Then the corresponding path-matrix $PZ\,(G)$ is defined by

$$PZ\,(G)_{ij} = \begin{cases} 0 & \text{there is no path from } i \text{ to } j \\ \min\limits_{\substack{v_1 v_2 \ldots v_k \text{ is path} \\ \text{connecting } i \text{ and } j}} \left\{ \prod_{i=1}^{k} d_G\,(i) \right\} & \text{there is at least one path from } i \text{ to } j. \end{cases}$$

For larger graphs, the path-Zagreb matrices are not easy to compute by hand, therefore, the computation needs to be done by computer. This leads to the problem of the efficient storage of the entries of the matrix $PZ\,(G)$. Hence, it is of interest to establish the upper bound for the value of $PZ\,(G_n)_{ij}$ where G_n is any graph with n vertices. Moreover, since computers digitalize the information into *bits*, we may (equivalently) reformulate the problem to search for the upper bound of $\log_2\left(PZ\left(G_n\right)_{ij}\right)$. Hence, our main goal is to prove that $\overline{\lim\limits_{n\to\infty}}\frac{\log_2\left(PZ(G_n)_{ij}\right)}{n}=\frac{6}{5}$, where $\overline{\lim}$ denotes limes superior, i.e., the value of the largest accumulation point.

2 Proofs

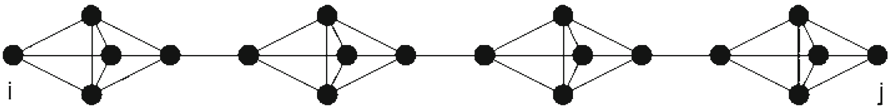
First, let us prove that:

$$\overline{\lim_{n\to\infty}}\frac{\log_2\left(PZ\left(G_n\right)_{ij}\right)}{n}\geq\frac{6}{5}.$$

It is sufficient to construct a sequence of graphs G'_{5k} with $5k$ vertices and their vertices i and j such that

$$\lim_{k\to\infty}\frac{\log_2\left(PZ\left(G'_{5k}\right)_{ij}\right)}{5k}=\frac{6}{5}.$$

Let us define the series of graphs G'_{5k} , shown below.



Since $PZ\left(G'_{5k}\right)_{ij}=\frac{9}{16}\cdot 4^{3k}$, it follows that:

$$\lim_{k\to\infty}\frac{\log_2\left(PZ\left(G'_{5k}\right)_{ij}\right)}{5k}=\lim_{k\to\infty}\frac{\log_2\left(\frac{9}{16}\cdot 4^{3k}\right)}{5k}=\lim_{k\to\infty}\frac{\log_2\left(\frac{9}{16}\right)+3k\cdot\log_2 4}{5k}=\frac{6}{5}.$$

It remains to prove that:

$$\overline{\lim_{n\to\infty}}\frac{\log_2\left(PZ\left(G_n\right)_{ij}\right)}{n}\leq\frac{6}{5}.$$

To accomplish this, it is sufficient to prove that $PZ\left(G_n\right)_{ij}\leq 4^{3n/5}$ for each graph G_n with n vertices and each two vertices i and j. Suppose to the contrary that there is a graph H'_n with n vertices and its vertices i and j such that $PZ\left(G_n\right)_{ij}>4^{3n/5}$. Let $(i=)\,v_0v_1v_2\cdots v_q\,(=j)$ be the shortest path that connects i and j. Let $F_1,\ldots,F_k$ be any graphs (with at least one vertex) with disjoint set of vertices. Denote by $F_1+F_2+\cdots+F_k$ the graph such that

$$V\left(F_1+\cdots+F_k\right)=V\left(F_1\right)\cup V\left(F_2\right)\cup\ldots\cup V\left(F_k\right)$$
$$E\left(F_1+\cdots+F_k\right)=E\left(F_1\right)\cup\ldots\cup E\left(F_k\right)\cup\{v_iv_{i+1}:v_i\in F_i,v_{i+1}\in F_{i+1},i=1,\ldots,k-1\}.$$

Denote by $x(i)$ the number of vertices on the distance i from in H_n and by q' the vertex on the maximal distance from q_i. Note that

$$H'_n \subseteq \overbrace{K_{x(0)} + K_{x(1)} + \cdots + K_{x(q)} + K_{x(q+1)} + K_{x(q+2)} + \cdots K_{x(q')}}^{=H''_n}$$

$$\subseteq \overbrace{K_{x(0)} + K_{x(1)} + \cdots + K_{x(q)+x(q+1)+x(q+2)+\cdots+x(q')}}^{H_n},$$

And that $v_i \in K(x_i)$. It follows that $d_{H'_n}(v_i) \leq d_{H''_n}(v_i) \leq d_{H_n}(v_i)$. Hence,

$$3^{3n/4} \leq PZ\left(H'_n\right)_{ij} \leq \prod_{k=0}^{q} d_{H'_n}(v_k) \leq \prod_{k=0}^{q} d_{H''_n}(v_k) \leq \prod_{k=0}^{q} d_{H_n}(v_k) = PZ(H_n)_{ij}.$$

It follows that

$$[x(0)+x(1)-1]\cdot[x(0)+x(1)+x(2)-1]\cdot[x(1)+x(2)+x(3)-1]\ldots$$
$$[x(q-3)+x(q-2)+x(q-1)-1]\cdot[x(q-2)+x(q-1)+x(q)-1]\cdot$$
$$[x(q-1)+x(q)-1] > 3^{3n/4},$$

where $x(0)+x(1)+\cdots+x(q)=n$.

Denote

$$\begin{aligned} y(0) &= x(0)+x(1)-1; \\ y(1) &= x(0)+x(1)+x(2)-1; \\ &\vdots \\ y(q-1) &= x(q-2)+x(q-1)+x(q)-1; \\ y(q) &= x(q-1)+x(q)-1. \end{aligned}$$

Note that $y(i)$ is a natural number for each $i = 0, \ldots, q$ and that

$$y(0)+y(1)+\cdots+y(q) = 3n - x(0) - x(1) - q - 1 \leq 3n - q - 3.$$

Hence, it is sufficient to prove the following theorem:

Theorem 1 *Let $z_0, \ldots z_q$ be integers such that $z_0 + \cdots + z_q = 3n - q - 3$. Then, $z_0 \cdot z_1 \cdots z_q \leq 4^{3n/5}$.*

Proof It can be easily proved that this product is maximized when all numbers $z_0, z_1, \ldots, z_q$ correspond to one or two successive integers. Moreover, $z_0 \cdot z_1 \cdots z_q \leq \left(\frac{3n-q-3}{q+1}\right)^{q+1}$.

Let us observe the function $f : [1, n-1] \to R$ defined by

$$f(q) = \left(\frac{3n-q-3}{q+1}\right)^{q+1}.$$

The first derivative of this function is equal to

$$f'(q) = \left(\frac{3n-3-q}{1+q}\right)^{1+q} \cdot \left(-1 - \frac{1+q}{-3+3n-q} - \ln\left(\frac{1+q}{3n-3-q}\right)\right).$$

Obviously, $\left(\frac{3n-3-q}{1+q}\right)^{1+q} > 0$. Let us observe the function $h : R^+ \to R$ defined by:

$$h(x) = -1 - x - \ln x.$$

Since, $h'(x) = -1 - \frac{1}{x}$, it follows that this function is a strictly decreasing function. Note that $h(0.27) > 0$, hence $h(x) > 0$ for each $x \in (0, 0.27]$. Also, note that $h\left(\frac{1}{3}\right) < 0$, hence $h(x) < 0$ for each $x \in \left[\frac{1}{3}, +\infty\right)$.

It follows that f is an increasing function for each q such that $\frac{1+q}{3n-3-q} \leq 0.27$ or, equivalently, for each $q \leq \frac{81}{127}n - \frac{181}{127}$. Since, $\frac{3}{5}n - \frac{7}{5} \leq \frac{81}{127}n - \frac{181}{127}$ and

$$f\left(\frac{3}{5}n - \frac{7}{5}\right) = \left(\frac{3n - \frac{3}{5}n + \frac{7}{5} - 3}{\frac{3}{5}n - \frac{7}{5} + 1}\right)^{\frac{3}{5}n - \frac{7}{5} + 1} \leq \left(\frac{\frac{12}{5}n - \frac{8}{5}}{\frac{3}{5}n - \frac{2}{5}}\right)^{3n/5} = 4^{3n/5},$$

it follows that $f(q) \leq 4^{3n/5}$ for each $q \leq \frac{3}{5}n - \frac{7}{5}$. Also, f is a decreasing function for each q such that $\frac{1+q}{3n-3-q} \geq \frac{1}{3}$ or, equivalently, for each $q \geq \frac{3}{4}n - \frac{3}{2}$. Since,

$$f\left(\frac{3}{4}n - \frac{3}{2}\right) = 3^{\frac{3}{4}n - \frac{3}{2} + 1} \leq 3^{3n/4} \leq 4^{3n/5},$$

it follows that $f(q) \leq 4^{3n/5}$ for each $q \geq \frac{3}{4}n - \frac{3}{2}$. It remains to prove the claim for $q \in \left(\frac{3}{5}n - \frac{7}{5}, \frac{3}{4}n - \frac{3}{2}\right)$. In that case, $\frac{3n-3-q}{q+1} \in (3, 4)$. As, we commented above, it is sufficient to observe the cases when numbers $z_0, z_1, \ldots, z_q$ correspond to one or two consecutive integers. Hence, $z_0, z_1, \ldots, z_q \in \{3, 4\}$.

Denote by a the number of factors equal to 3 and by b the number of factors equal to 4. From $a + b = q + 1$ and $3a + 4b = 3n - q - 3$, it follows that $b = 3n - 4q - 6$ and $a = q + 1 - (3n - 4q - 6)$. Hence,

$$z_0 \cdot z_1 \cdots z_q = 3^{q+1-(3n-4q-6)} \cdot 4^{3n-4q-6} = 3^{q+1} \cdot \left(\frac{4}{3}\right)^{3n-4q-6}$$
$$= 3 \cdot \left(\frac{4}{3}\right)^{3n-6} \cdot \left(\frac{3^5}{4^4}\right)^q.$$

Since, $3^5/4^4 < 1$, the last expression is maximized for the minimal value of q which is attained when $\frac{3n-3-q}{q+1} = 4$, i.e., when $q = \frac{3}{5}n - \frac{7}{5}$, but in this case:

$$z_0 \cdot z_1 \cdots z_q = 3^{q+1-(3n-4q-6)} \cdot 4^{3n-4q-6} = 4^{3n-4\left(\frac{3}{5}n-\frac{7}{5}\right)-6} = 4^{\frac{3}{5}n-\frac{2}{5}} \leq 4^{3n/5}.$$

This proves the theorem. □

3 Concluding remarks

In the present report, we defined the path-Zagreb matrix PZ and we gave the upper bound of $\log_2\left(PZ\left(G_n\right)_{ij}\right)$, where G_n is a graph with n vertices. The problem encountered on going from trees T to general graphs G (that is, graphs containing cycles) is related to paths connecting two vertices, in trees and in general graphs, respectively: paths connecting two vertices in T are unique whilst in the case of G it may be more than one path connecting two vertices.

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