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ORIGINAL PAPER

Some properties of the reformulated Zagreb indices

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Abstract Miličević, Nikolić and Trinajstić (Mol Divers 8:393–399, 2004) proposed the reformed Zagreb indices in 2004. Now we give some properties for the reformed Zagreb indices.

Keywords First Zagreb index · Second Zagreb index · Reformed Zagreb indices · Degree of vertex · Degree of edge

1 Introduction

A pair of molecular descriptors, known as the first Zagreb index M_1 and the second Zagreb index M_2 [1], first appeared in the topological formula for the total π- energy of conjugated molecules that has been derived in 1972 [2]. Soon after these indices have been used as branching indices [3]. Later the Zagreb indices found applications in QSPR and QSAR studies [1,4,5].

For a simple graph G with the vertex set $V(G)$ and the edge set $E(G)$, the Zagreb indices are given by:

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$$\mathrm{M}_1 = \mathrm{M}_1(G) = \sum_{u \in V(G)} d(u)^2$$

$$\mathrm{M}_2 = \mathrm{M}_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

where $d(u)$ denotes the degree (number of first neighbors) of vertex u in G. Properties of the Zagreb indices may be found in a number of reports [6–18].

Miličević, Nikolić and Trinajstić [19] in 2004 reformulated the Zagreb indices in terms of edge-degrees instead of vertex-degrees:

$$\mathrm{EM}_1 = \mathrm{EM}_1(G) = \sum_{e \in E(G)} d(e)^2$$

$$\mathrm{EM}_2 = \mathrm{EM}_2(G) = \sum_{e \sim f} d(e)d(f)$$

where $d(e)$ denotes the degree of the edge e in G, which is defined by $d(e) = d(u) + d(v) - 2$ with $e = uv$, and $e \sim f$ means that the edges e and f are adjacent, *i.e.*, they share a common end-vertex in G. The use of these descriptors in QSPR study was also discussed in their report [19].

For a graph G with at least one edge, its line graph L_G is the graph in which $V(L_G) = E(G)$, where two vertices of L_G are adjacent if and only if they are adjacent as edges of G. Then

$$\mathrm{EM}_1(G) = \mathrm{M}_1(L_G)$$
$$\mathrm{EM}_2(G) = \mathrm{M}_2(L_G).$$

In this report, we establish some basic mathematical properties of the reformulated Zagreb indices.

2 Preliminaries

For real number α and a graph G, let ${}^{\alpha}\mathrm{M}_1 = {}^{\alpha}\mathrm{M}_1(G) = \sum_{u \in V(G)} d(u)^{\alpha}$, where if $\alpha \leq 0$, then the summation goes over non-isolated vertices. Evidently, $\mathrm{M}_1(G) = {}^{2}\mathrm{M}_1(G)$. For a vertex u of the graph G, $\Gamma(u)$ denotes the set of (first) neighbors of u in G.

Let P_n, S_n, C_n and K_n be respectively the path, the star, the cycle and the complete graph with n vertices.

The adjacency matrix $\mathbf{A}(G)$ of the graph G is an $n \times n$ matrix $(\mathbf{A}_{ij})$ such that $\mathbf{A}_{ij} = 1$ if the vertices v_i and v_j are adjacent and 0 otherwise [20]. Let $\rho(G)$ be the largest eigenvalue of G, i.e., the largest eigenvalue of $\mathbf{A}(G)$.

Let G be a connected graph on n vertices and m edges. Then L_G possesses m vertices and $\frac{1}{2}\mathrm{M}_1 - m$ edges. The following lemma is obvious. Note that a line graph does not contain induced subgraph S_4.

Lemma 1 *Let G be a connected graph. Then* $L_G = K_n$ *for* $n \geq 4$ *or* $n = 1, 2$ *if and only if* $G = S_{n+1}$, *while* $L_G = K_3$ *if and only if* $G = S_4$ *or* $G = K_3$.

Lemma 2 [10] *Let G be a graph. Then* $2\mathrm{M}_2 \leq \rho(G)\mathrm{M}_1$.

Lemma 3 *Let G be a connected graph with* $m \geq 1$ *edges. Then* $\rho(L_G) \leq \sqrt{\mathrm{M}_1 - 3m + 1}$ *if and only if* $G = S_{m+1}$ *or* $G = K_3, P_4$ *with* $m = 3$.

Proof Let n be the number of vertices of G. Then $\rho \leq \sqrt{2m - n + 1}$ with equality if and only if $G = K_n$ or S_n [21]. Using this result to L_G and noting that S_m cannot be a line graph for $m \geq 4$, we have $\rho(L_G) \leq \sqrt{2\left(\frac{\mathrm{M}_1}{2} - m\right) - m + 1} = \sqrt{\mathrm{M}_1 - 3m + 1}$ with equality if and only if $L_G = K_m$ or $L_G = S_3$ with $m = 3$, i.e., $G = S_{m+1}$ or $G = K_3, P_4$ with $m = 3$. □

The clique number of a graph G is the number of vertices in a largest complete subgraph of G.

Lemma 4 [22] *Let G be a graph with m edges and clique number k. Then* $\mathrm{M}_2 \leq \frac{2(k-1)}{k} m^2$ *with equality for graph G with no isolated vertices if and only if G is either a complete bipartite graph for* $k = 2$ *or a regular complete k-partite graph for* $k \geq 3$.

For graphs G, H *and nonnegative integer* k, $G \cup kH$ *denotes the vertex-disjoint union of G and k copies of H. In particular,* $G \cup 0H = G$.

3 Results

It is easy to see that the complete graph K_n is the unique n-vertex connected graph with maximum M_1 and M_2, and since P_n is the unique n-vertex tree with minimum M_1 and M_2 [8,9], it is also the unique n-vertex connected graph with minimum M_1 and M_2. Note that the line graph of S_n and P_n are respectively K_{n-1} and P_{n-1}. Thus among all n-vertex trees, S_n and P_n are respectively the unique trees with maximum and minimum of both EM_1 and EM_2.

Proposition 1 *Let G be a graph with m edges. Then*

$$\mathrm{EM}_1 = {}^3\mathrm{M}_1 + 4m + 2\mathrm{M}_2 - 4\mathrm{M}_1.$$

Proof It is easily seen that

$$\begin{aligned}
\mathrm{EM}_1 &= \sum_{uv \in E(G)} [d(u) + d(v) - 2]^2 \\
&= \sum_{uv \in E(G)} \left[d(u)^2 + d(v)^2\right] + 4m + 2 \sum_{uv \in E(G)} d(u)d(v) \\
&\quad -4 \sum_{uv \in E(G)} [d(u) + d(v)] \\
&= \sum_{uv \in E(G)} \left[d(u)^2 + d(v)^2\right] + 4m + 2\mathrm{M}_2 - 4\mathrm{M}_1 \\
&= {}^3\mathrm{M}_1 + 4m + 2\mathrm{M}_2 - 4\mathrm{M}_1,
\end{aligned}$$

where we use

$$\sum_{uv\in E(G)} [d(u)+d(v)] = \sum_{u\in V(G)} \sum_{v\in \Gamma(u)} d(u) = \mathrm{M}_1$$

and

$$\sum_{uv\in E(G)} \left[d(u)^2+d(v)^2\right] = \sum_{u\in V(G)} \sum_{v\in \Gamma(u)} d(u)^2 = {}^3\mathrm{M}_1.$$

□

Proposition 2 *Let G be a graph on n vertices and $m \geq 1$ edges. Then*

$$\mathrm{EM}_1 \leq (n-4)\mathrm{M}_1 + 4\mathrm{M}_2 - 4m^2 + 4m$$

with equality if and only if any two non-adjacent vertices have equal degrees.

Proof It is easily seen that

$$\begin{aligned}
{}^3\mathrm{M}_1 &= \sum_{u\in V(G)} d(u)^3 = \sum_{u\in V(G)} \sum_{v\in\Gamma(u)} d(u)d(v) + \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in\Gamma(u)} [d(u)-d(v)]^2 \\
&= 2\mathrm{M}_2 + \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in\Gamma(u)} [d(u)-d(v)]^2 \\
&\leq 2\mathrm{M}_2 + \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in V(G)} [d(u)-d(v)]^2 \\
&= 2\mathrm{M}_2 + \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in V(G)} \left[d(u)^2+d(v)^2\right] - \sum_{u\in V(G)} \sum_{v\in V(G)} d(u)d(v) \\
&= 2\mathrm{M}_2 + n\mathrm{M}_1 - 4m^2
\end{aligned}$$

with equality if and only if any two non-adjacent vertices have equal degrees. Now the result follows from Proposition 1. □

Proposition 3 *Let G be a graph with $m \geq 1$ edges. Then*

$$\mathrm{EM}_2 \leq \left(\frac{1}{2}\mathrm{M}_1 - m\right)\left(\sqrt{\mathrm{M}_1 - 2m + \frac{1}{4}} - \frac{1}{2}\right)^2 \tag{1}$$

with equality if and only if for the graph G' resulting from G by the deletion of possible isolated vertices, $G' = S_{k+1} \cup (m-k)K_2$ for integer k with $1 \leq k \leq m$ or $G' = K_3 \cup (m-3)K_2$ with $m \geq 3$.

Proof It is known that $M_2 \leq m\left(\sqrt{2m+\frac{1}{4}}-\frac{1}{2}\right)^2$ with equality if and only if G is the union of a complete graph and isolated vertices (see [6]). Apply this result to L_G. Note that the number of edges of L_G is equal to $\frac{1}{2}M_1 - m$. Hence (1) follows and equality holds in (1) if and only if L_G is the union of a complete graph and isolated vertices, say $L_G = K_k \cup (m-k)K_1$, where k is an integer with $1 \leq k \leq m$, which by Lemma 1, is equivalent to $G' = S_{k+1} \cup (m-k)K_2$ with $1 \leq k \leq m$ or $G' = K_3 \cup (m-3)K_2$ with $m \geq 3$. □

Proposition 4 *Let G be a connected graph with $m \geq 1$ edges. Then*

$$EM_2 \leq \frac{1}{2}\sqrt{M_1 - 3m + 1}EM_1 \tag{2}$$

with equality if and only if $G = S_{m+1}$ or $G = K_3$ with $m = 3$.

Proof If $m = 1$, (2) is obviously an equality. Suppose that $m \geq 2$. By Lemma 2, we have $2EM_2 \leq \rho(L_G)EM_1$. By Lemma 3, we have $\rho(L_G) \leq \sqrt{M_1 - 3m + 1}$ with equality if and only if $G = S_{m+1}$ or $G = K_3, P_4$ with $m = 3$. Now (2) follows and equality holds in (2) if and only if $2EM_2 = \rho(L_G)EM_1$ and $G = S_{m+1}$or $G = K_3, P_4$ with $m = 3$. Note that $\rho(L_G) = m - 1$ if $G = S_{m+1}, K_3$, and $\rho(L_G) = \sqrt{2}$ if $G = P_4$. Then $2EM_2 = \rho(L_G)EM_1$ if $G = S_{m+1}, K_3$, and $2EM_2 \neq \rho(L_G)EM_1$ if $G = P_4$. It follows that equality holds in (2) if and only if $G = S_{m+1}$ or $G = K_3$ with $m = 3$. □

Proposition 5 *Let G be a graph with m edges and maximum vertex-degree $\Delta \geq 1$, and G contains no triangle if $\Delta = 2$. Then*

$$EM_2 \leq \frac{(\Delta-1)(M_1-2m)^2}{2\Delta} \tag{3}$$

with equality for graph G with no isolated vertices and edges if and only if $G = P_3$ with $m = 2$, $G = P_4$ with $m = 3$, $G = C_4$ with $m = 4$ for $\Delta = 2$, $G = K_4$ with $m = 6$, $G = S_4$ with $m = 3$ for $\Delta = 3$, and $G = S_{\Delta+1}$ with $m = \Delta$ for $\Delta \geq 4$.

Proof Note that there are two kinds of clique in L_G: (i) the one corresponding to a set of edges in G sharing a common end-vertex, and (ii) the one corresponding to the set of edges of a triangle. Thus, the clique number of L_G is equal to the maximum vertex-degree Δ of G. Recall that the number of edges of L_G is equal to $\frac{1}{2}M_1 - m$. By Lemma 4, (3) follows.

If $\Delta = 2$, then by Lemma 4, equality holds in (3) for graph G with no isolated edges if and only if L_G is a complete bipartite graph, which for graph G with no isolated vertices and edges is equivalent to $G = P_3, P_4$, or C_4.

Suppose that $\Delta \geq 3$, and G has no isolated vertices and edges. By Lemma 4, equality holds in (3) if and only if L_G is a complete Δ-partite graph. Suppose that L_G is a complete Δ-partite graph. Let r be the number of vertices in a partite set of L_G. Since L_G is a regular, then G is a regular graph or a bipartite graph for which vertices in the same partite set have equal degrees. Suppose first that G is a regular graph.

Then $2\Delta - 2 = (\Delta - 1)r$, i.e., $r = 2$. Thus $\frac{1}{2}|V(G)|\Delta = |E(G)| = |V(L_G)| = 2\Delta$, i.e., $|V(G)| = 4$, and then $G = K_4$ with $\Delta = 3$. Now suppose that G is a non-regular bipartite graph for which vertices in the same partite set have equal degrees. Then vertices in one partite set of G have degree Δ. Let Δ' be the degree of vertices in the other partite set of G. Thus $\Delta + \Delta' - 2 = (\Delta - 1)r$, i.e., $\Delta' - 1 = (\Delta - 1)(r - 1)$. Since $\Delta > \Delta'$, we have $r = \Delta' = 1$, and then $G = S_{\Delta+1}$. Conversely, it is easily seen that if $G = K_4$ with $\Delta = 3$ or $G = S_{\Delta+1}$ then L_G is a complete Δ-partite graph. □

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