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On reformulated Zagreb indices

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ABSTRACT

The first and second reformulated Zagreb indices are defined respectively in terms of edge-degrees as $EM_1(G) = \sum_{e \in E} \deg(e)^2$ and $EM_2(G) = \sum_{e \sim f} \deg(e)\deg(f)$, where $\deg(e)$ denotes the degree of the edge e, and $e \sim f$ means that the edges e and f are adjacent. We give upper and lower bounds for the first reformulated Zagreb index, and lower bounds for the second reformulated Zagreb index. Then we determine the extremal n-vertex unicyclic graphs with minimum and maximum first and second Zagreb indices, respectively. Furthermore, we introduce another generalization of Zagreb indices.
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1. Introduction

Let $G = (V, E)$ be a connected simple graph with $n = |V|$ vertices and $m = |E|$ edges. The degree of a vertex v is denoted as $\deg(v)$. Specially, $\Delta = \Delta(G)$ and $\delta = \delta(G)$ are called the maximum and minimum degree of G, respectively.

Zagreb indices were first introduced in [7], and they are among oldest and most used molecular structure-descriptors. The first Zagreb index is defined as the sum of the squares of the degrees of the vertices

$$M_1(G) = \sum_{v \in V} \deg(v)^2.$$

The second Zagreb index is defined as the sum of the product of the degrees of adjacent vertices

$$M_2(G) = \sum_{uv \in E} \deg(v) \cdot \deg(u).$$

The survey of properties of M_1 and M_2 are given in [14,15]. There was a vast research concerning the mathematical properties and bounds for Zagreb indices [1,3–6,9,11,17–19,22,23,20,21] and comparing Zagreb indices [2,8,10,16].

Milićević et al. [12] in 2004 reformulated the Zagreb indices in terms of edge-degrees instead of vertex-degrees:

$$EM_1(G) = \sum_{e \in E} \deg(e)^2$$

$$EM_2(G) = \sum_{e \sim f} \deg(e)\deg(f),$$

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where $\deg(e)$ denotes the degree of the edge e in G, which is defined by $\deg(e) = \deg(u)+\deg(v)-2$ 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. Recently, upper and lower bounds on $EM_1(G)$ and $EM_2(G)$ were presented in [24].

Let L_G be the line graph of G. Then

$$EM_1(G) = M_1(L_G) \quad \text{and} \quad EM_2(G) = M_2(L_G).$$

Recall that the line graphs are claw-free graphs (graphs without an induced star on four vertices).

Let P_n and C_n be the path and the cycle on n vertices. A bidegreed graph is a graph whose vertices have exactly two degrees Δ and δ.

In this paper we establish further mathematical properties of the reformulated Zagreb indices. In Section 2 we present upper and lower bounds for the first reformulated Zagreb index, while in Section 3 we present lower bounds for the second reformulated Zagreb index. In Section 4, we determine the extremal unicyclic graphs with minimum and maximum first and second Zagreb indices, respectively. In Section 5, we generalize the definition of Zagreb indices and present some basic properties.

2. Upper and lower bounds for $EM_1(G)$

Zhou and Trinajstić established in [24] the following relation

$$EM_1(G) = \sum_{v\in V} \deg(v)^3 + 4m + 2M_2(G) - 4M_1(G). \tag{1}$$

We will use the following Diaz-Metcalf inequality [13] to present a new upper bound for $EM_1(G)$.

Lemma 2.1. *Let a_i and b_i, $i = 1, 2, \ldots, n$ be real numbers such that $ma_i \le b_i \le Ma_i$ for $i = 1, 2, \ldots, n$. Then*

$$\sum_{i=1}^{n} b_i^2 + mM \sum_{i=1}^{n} a_i^2 \le (M+m) \sum_{i=1}^{n} a_i b_i$$

with equality if and only if either $b_i = ma_i$ or $b_i = Ma_i$ for every $i = 1, 2, \ldots, n$.

Theorem 2.2. *Let G be a simple graph with n vertices and m edges. Then*

$$EM_1(G) \le (\Delta + \delta - 4)M_1(G) - 2m\delta\Delta + 4m + 2M_2(G)$$

with equality if and only if G is a regular or bidegreed graph.

Proof. By setting $b_i = \deg(v_i)^{3/2}$ and $a_i = \deg(v_i)^{1/2}$ in Lemma 2.1, we have $\delta a_i \le b_i \le \Delta a_i$, and

$$\sum_{i=1}^{n} \deg(v_i)^3 + \delta\Delta \sum_{i=1}^{n} \deg(v_i) \le (\Delta + \delta) \sum_{i=1}^{n} \deg(v_i)^2.$$

After simplification and using (1), it follows that

$$EM_1(G) \le (\Delta + \delta)M_1(G) - 2m\delta\Delta + 4m + 2M_2(G) - 4M_1(G),$$

with equality if and only if either $\deg(v_i) = \delta$ or $\deg(v_i) = \Delta$ for every $i = 1, 2, \ldots, n$. □

We will use Chebyschev's inequality [13] to derive a lower bound for $EM_1(G)$.

Lemma 2.3. *Let $a_1 \ge a_2 \ge \cdots \ge a_n$ and $b_1 \ge b_2 \ge \cdots \ge b_n$ be real numbers. Then*

$$n \cdot \sum_{i=1}^{n} a_i b_i \ge \sum_{i=1}^{n} a_i \cdot \sum_{i=1}^{n} b_i$$

with equality if and only if $a_1 = a_2 = \cdots = a_n$ or $b_1 = b_2 = \cdots = b_n$.

Theorem 2.4. *Let G be a simple graph with n vertices and m edges. Then*

$$EM_1(G) \ge \frac{2m}{n} \cdot M_1(G) + 4m + 2M_2(G) - 4M_1(G),$$

with equality if and only if G is regular.

Proof. By setting $a_i = \deg(v_i)$ and $b_i = \deg(v_i)^2$ for $i = 1, 2, \ldots, n$ in Lemma 2.3, we have

$$n \cdot \sum_{i=1}^{n} \deg(v_i)^3 \ge \sum_{i=1}^{n} \deg(v_i) \cdot \sum_{i=1}^{n} \deg(v_i)^2 = 2m \cdot M_1(G)$$

with equality if and only if G is regular. Then the result follows from Eq. (1). □

3. Lower bounds for $EM_2(G)$

In this section, we give two lower bounds for $EM_2(G)$.

Theorem 3.1. *Let G be a simple graph with n vertices and m edges. Then*

$$EM_2(G) \geq EM_1(G) - \frac{1}{2}M_1(G) + m,$$

with equality if and only if G is a union of isolated vertices and paths P_2 and P_3.

Proof. Since $\deg(e), \deg(f) \geq 1$, by summing the obvious inequalities $\deg(e) \cdot \deg(f) \geq \deg(e) + \deg(f) - 1$ we get

$$\begin{aligned} EM_2(G) &= \sum_{e\sim f} \deg(e)\deg(f) \geq \sum_{e\sim f} (\deg(e) + \deg(f) - 1) \\ &= \sum_{e\in E} \deg(e)^2 - |E(L_G)| = EM_1(G) - \frac{1}{2}M_1(G) + m. \end{aligned}$$

The equality holds if and only if for each two neighboring edges e and f we have $\deg(e) = 1$ or $\deg(f) = 1$. It follows that the graph G cannot contain a vertex of degree at least 3 and cannot contain a path of length greater than 3. Therefore, the equality holds if and only if G is a disjoint union of P_1, P_2 or P_3. □

Ilić and Stevanović in [10] proved the following inequality

Lemma 3.2. *Let G b a graph with n vertices and m edges. Then*

$$M_2(G) \geqslant \frac{4m^3}{n^2}$$

with equality if and only if G is regular.

For a graph G with n vertices and m edges, L_G possesses m vertices and $\sum_{v\in V(G)} \binom{\deg(v)}{2} = \frac{1}{2}(M_1(G) - 2m)$ edges. By Lemma 3.2, we have

Theorem 3.3. *Let G be a simple graph with n vertices and m edges. Then*

$$EM_2(G) \geqslant \frac{(M_1(G) - 2m)^3}{2m^2}$$

with equality if and only if L_G is regular.

4. Unicyclic graphs

A non-complete graph is a graph not isomorphic to a complete graph K_n. Since the addition of new edges in the graph increases some vertex degrees, we have the following lemma.

Lemma 4.1. *Let G be a non-complete connected graph. Then $M_1(G) < M_1(G + e)$ and $M_2(G) < M_2(G + e)$.*

The line graph of n-vertex unicyclic graphs is a connected graph of n vertices. If $\Delta = 2$, we have a cycle C_n and the line graph has exactly n edges, while for $\Delta > 2$ the line graph contains at least one cycle and at least n edges. Deng proved in [4] that among n-vertex unicyclic graphs C_n has minimum Zagreb indices, and therefore by Lemma 4.1, we have the following result.

Theorem 4.2. *Let G be a unicyclic graph with n vertices. Then*

$$EM_i(G) \geq EM_i(C_n), \quad i = 1, 2$$

with equality if and only if $G \cong C_n$.

Let S'_n be the unicyclic graph with n vertices obtained by adding an edge to an n-vertex star, connecting two pendent vertices.

Lemma 4.3. *Among the line graphs of n-vertex unicyclic graphs, the line graph of S'_n has uniquely the maximum number of edges, which is $\binom{n}{2} - n + 3$.*

Proof. Let $C = u_1u_2 \cdots u_k$ be a cycle of an n-vertex unicyclic graph G, and let T_i, $i = 1, 2, \ldots, k$, be a tree attached at u_i, such that T_i does not contain any other cycle vertices. Assume that the order of tree T_i is $a_i \geq 1$ and $a_1 + a_2 + \cdots + a_k = n$. For each edge u_iu_{i+1} of the cycle there are at least $n - a_i - a_{i+1} - 1$ non-adjacent edges ($u_{k+1} \equiv u_1$). Similarly for each edge from T_i, we have additional $(a_1-1)+(a_2-1)+\cdots+(a_{i-1}-1)+(a_{i+1}-1)+\cdots+(a_k-1)=n-k-a_i+1$ non-adjacent edges. Thus

$$\begin{aligned}|E(L_G)| &\le \binom{n}{2}-\sum_{i=1}^{k}(n-a_i-a_{i+1}-1)-\sum_{i=1}^{k}(a_i-1)(n-k-a_i+1)\\ &=\binom{n}{2}-(nk-2\sum_{i=1}^{k}a_i-k)-(n-k+1)\sum_{i=1}^{k}(a_i-1)+\sum_{i=1}^{k}a_i^2-\sum_{i=1}^{k}a_i\\ &=\binom{n}{2}-n^2+\sum_{i=1}^{k}a_i^2-k^2+kn+2k.\end{aligned}$$

The maximum of the expression

$$f(n,k)=\sum_{i=1}^{k}a_i^2-k^2+kn+2k,$$

under restrictions $a_i \ge 1$ and $a_1+a_2+\cdots+a_k=n$ and $k\ge 3$, is achieved if and only if $a_1=n-k+1$, $a_2=a_3=\cdots=a_k=1$. This can be easily proved by the transformation $(a_i,a_j)\mapsto(a_i+1,a_j-1)$ with $a_i\ge a_j>2$, since

$$(a_i+1)^2+(a_j-1)^2-a_i^2-a_j^2=2(a_i-a_j)+2>0.$$

This transformation strictly increases the value of $f(n,k)$ and by applying the transformation several times it follows that $a_1=n-k+1$. Therefore, we have

$$f(n,k)\le(n-k+1)^2+(k-1)-k^2+kn+2k=n^2+2n-k(n-1),$$

and finally

$$\begin{aligned}|E(L_G)| &\le \binom{n}{2}-n^2+n^2+2n-k(n-1)\\ &=\binom{n}{2}+2n-k(n-1)\\ &\le\binom{n}{2}+2n-3(n-1)=\binom{n}{2}-n+3\end{aligned}$$

with equalities if and only if $k=3$ and $G\cong S'_n$. □

Let G be a unicyclic graph with n vertices. Deng proved in [4] that

$$M_i(G)\le M_i(S'_n),\quad i=1,2$$

with equality if and only if $G\cong S'_n$.

By direct calculation, we have the following expressions.

$$EM_1(S'_n)=n^3-5n^2+12n-6,$$

$$\begin{aligned}EM_2(S'_n) &= 4(n-1)+(n-1)(n-1)+2(n-3)(n-1)(n-2)+(n-2)(n-2)\binom{n-3}{2}\\ &=\frac{n^4}{2}-\frac{7n^3}{2}+11n^2-14n+9.\end{aligned}\qquad(2)$$

Now we can prove the main result of this section. Let the weight of the edge $e=uv$ be $\deg(u)+\deg(v)$.

Theorem 4.4. *Let G be a unicyclic graph with n vertices. Then*

$$EM_i(G)\le EM_i(S'_n),\quad i=1,2$$

with equality if and only if $G\cong S'_n$.

Proof. Let $d_1\ge d_2\ge\cdots\ge d_n$ be the vertex degrees of L_G, where d_i is the degree of vertex i of L_G. Since G contains exactly one cycle, there cannot be three vertices in L_G with degree $n-1$.

By Lemma 4.3, $L_{S'_n}$ has the maximum number of edges among the line graphs of n-vertex unicyclic graphs. The degrees of the vertices of $L_{S'_n}$ are $n-1, n-1, n-2, n-2, \ldots, n-2, 2$.

Using transformation $(d_i,d_j)\mapsto(d_i+1,d_j-1)$ with $n-1>d_i\ge d_j>2$, we increase the first reformulated Zagreb index, since

$$(d_i+1)^2+(d_j-1)^2-d_i^2-d_j^2=2(d_i-d_j)+2>0.$$

Therefore, the graph S'_n uniquely maximizes the first reformulated Zagreb index among the n-vertex unicyclic graphs.

By Lemma 4.3, there is exactly one unicyclic graph S'_n, for which the degrees of the vertices of the line graph are $n-1, n-1, n-2, n-2, \ldots, n-2, 2$. It follows that if $d_n = 1$ or $d_n = 2$, then $EM_2(S'_n) \geq EM_2(G)$ with equality if and only if $G \cong S'_n$.

If $d_1 < n-1$, all weights of edges are bounded above by $(n-2)(n-2)$. By Lemma 4.3, we have

$$EM_2(G) \leq (n-2)(n-2)\left(\binom{n}{2} - n + 3\right) = \frac{n^4}{2} - \frac{7n^3}{2} + 11n^2 - 18n + 12,$$

and finally $EM_2(G) < EM_2(S'_n)$ by comparing with (2).

We are left with the last case that $d_1 = n-1$ and $d_n > 2$. This means that there exist at least one edge, say $e = uv$, adjacent to all other edges from $E(G)$. Since G is unicyclic, the edge e belongs to a triangle uvw and the degree of the vertex w is 2. Assume that $\deg(u) = 2 + a$ and $\deg(v) = 2 + b$. It follows that $3 + a + b = n$. Then $EM_2(G)$ equals

$$f(a,b) = (a+b+2)\left(a(a+1) + b(b+1) + a + 2 + b + 2\right) + a(a+2)(a+1) + b(b+2)(b+1)$$
$$+ (a+2)(b+2) + (a+1)(a+1)\binom{a}{2} + (b+1)(b+1)\binom{b}{2}.$$

For $a \geq b > 1$, after some manipulations we have

$$f(a+1, b-1) - f(a,b) = \frac{1}{2}(1+a-b)\left(18 + 4a^2 + 4b^2 + 11b + 15a + 4ab\right)$$
$$= \left(2a^3 + \frac{19a^2}{2} + \frac{33a}{2} + 9\right) - \left(2b^3 + \frac{7b^2}{2} + \frac{7b}{2}\right) > 0.$$

Note that $f(a,b)$ is symmetric with respect to a and b. Then the maximum of $f(a,b)$ is achieved for $a = 0$ or $b = 0$, i.e.,

$$f(a,b) \leq f(0, n-3) = \frac{n^4}{2} - \frac{7n^3}{2} + 11n^2 - 18n + 12$$

with equality if and only if $G \cong S'_n$. This completes the proof. □

5. Generalized Zagreb indices

Here we present another generalization of Zagreb indices. Let A be the adjacency matrix of a graph G. It is well known that the (i,j)-th element of the power matrix A^k, $k \geq 1$, represents the number of walks from the vertex i to the vertex j of length k. Therefore, for each $k \geq 1$, we can define the following indices

$$M_1^{(k)}(G) = \sum_{v \in V} \sum_{u \in V} A^k(u,v) \cdot \deg(v),$$

and

$$M_2^{(k)}(G) = \sum_{v \in V} \sum_{u \in V} A^k(u,v) \cdot \deg(u) \cdot \deg(v),$$

where $A^k(u,v)$ represents the element (u,v) of A^k. For the degrees vector $D = [\deg(v_1), \deg(v_2), \ldots, \deg(v_n)]$ and identity vector $I = [1, 1, \ldots, 1]$, we have

$$M_1^{(k)}(G) = IA^kD^T \quad \text{and} \quad M_2^{(k)}(G) = DA^kD^T.$$

It can be easily seen that for $k = 1$, we have the original Zagreb indices. For $k = 2$, we have

$$M_1^{(2)}(G) = \sum_{v \in V} \sum_{uv \in E(G)} \deg(u) = M_2(G)$$

and

$$M_2^{(2)}(G) = \sum_{v \in V} \sum_{uv, wv \in E(G)} \deg(u) \cdot \deg(w).$$

For the second reformulated Zagreb index, we have

$$EM_2(G) = \sum_{v \in V} \sum_{uv, wv \in E(G)} (\deg(v) + \deg(u) - 2)(\deg(v) + \deg(w) - 2),$$

which is directly connected to the value of $M_2^{(2)}(G)$.

It would be nice to find some arguments (either from the chemical or mathematical point of view) why these quantities should be considered.

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