Communications in Combinatorics and Optimization
Vol. 2 No. 2, 2017 pp.99-117
DOI: 10.22049/cco.2017.25949.1059

CCO
Commun. Comb. Optim.

On leap Zagreb indices of graphs

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Received: 30 May 2017; Accepted: 8 July 2017
Published Online: 9 July 2017

Communicated by ***Zehui Shao***

Abstract: The first and second Zagreb indices of a graph are equal, respectively, to the sum of squares of the vertex degrees, and the sum of the products of the degrees of pairs of adjacent vertices. We now consider analogous graph invariants, based on the second degrees of vertices (number of their second neighbors), called leap Zagreb indices. A number of their basic properties is established.

Keywords: Degree (of vertex), Second degree, Zagreb indices, Leap Zagreb indices

AMS Subject classification: 05C07

1. Introduction

In this paper, we are concerned with simple graphs, i.e., finite graphs having no loops, multiple and directed edges. Let $G = (V, E)$ be such a graph with vertex set $V(G)$ and edge set $E(G)$. As usual, we denote by $n = |V|$ and $m = |E|$ the number of vertices and edges of G. The distance $d(u, v)$ between any two vertices u and v of a graph G is equal to the length of (number of edges in) a shortest path connecting them. For a vertex $v \in V(G)$ and a positive integer k, the open k-neighborhood of v in the graph G, denoted by $N_k(v/G)$, is defined as $N_k(v/G) = \{u \in V(G) : d(u, v) = k\}$.
The k-distance degree of a vertex v in G, denoted by $d_k(v/G)$ (or simply $d_k(v)$ if no misunderstanding is possible), is the number of k-neighbors of the vertex v in G, i.e., $d_k(v/G) = |N_k(v/G)|$. It is clear that $d_1(v/G) = d(v/G)$ for every $v \in V(G)$.

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The complement $\overline{G}$ of a graph G is a graph with vertex set $V(G)$ in which two vertices are adjacent if and only if they are not adjacent in G. $\overline{K_n}$ is the empty (totally disconnected) graph, in which no two vertices are adjacent (i.e., its edge set is empty).

If a graph G consists of disconnected components H_1 and H_2, then we write $G = H_1 \cup H_2$. If G consists of $p \geq 2$ disjoint copies of a graph H, then we write $G = p\,H$.

For a vertex v of G, the eccentricity $e(v) = \max\{d(v,u) : u \in V(G)\}$. The diameter of G is $diam(G) = \max\{e(v) : v \in V(G)\}$ and the radius of G is $r = r(G) = \min\{e(v) : v \in V(G)\}$.

Let $H \subseteq V(G)$ be any subset of vertices of G. Then the induced subgraph $G[H]$ of G is the graph whose vertex set is H and whose edge set consists of all edges in $E(G)$ that have both endpoints in H. A graph G is said to be F-free if no induced subgraph of G is isomorphic to F.

For any terminology or notation not mention here, we refer to [15].

In the current mathematical and mathematico–chemical literature a large number of vertex–degree–based graph invariants are being studied [8, 10]. Among them, the so-called first M_1 and second M_2 Zagreb indices are the far most extensively investigated ones. These have been introduced more than forty years ago [13, 14] and are defined as:

$$M_1 = M_1(G) = \sum_{v \in V(G)} d_1(v/G)^2$$

and

$$M_2 = M_2(G) = \sum_{uv \in E(G)} d_1(u/G)\, d_1(v/G).$$

For properties of the two Zagreb indices see [3, 5, 11, 20] and the papers cited therein. In recent years, some novel variants of Zagreb indices have been put forward, such as Zagreb coindices [1, 6, 12], reformulated Zagreb indices [17, 19], Zagreb hyperindex [2, 21], multiplicative Zagreb indices [9, 25], multiplicative sum Zagreb index [7, 23], and multiplicative Zagreb coindices [24], etc. The Zagreb coindices are defined as:

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} \big[d_1(u/G) + d_1(v/G)\big]$$

and

$$\overline{M_2}(G) = \sum_{uv \notin E(G)} d_1(u/G)\, d_1(v/G).$$

In [12] the following identities were established:

Theorem 1. [12] *Let G be a graph with n vertices and m edges. Then*

$$\begin{aligned}
\overline{M_1}(G) &= \overline{M_1}(\overline{G}) = 2m(n-1) - M_1(G) \\
\overline{M_2}(G) &= 2m^2 - \frac{1}{2}M_1(G) - M_2(G) \\
\overline{M_2}(\overline{G}) &= M_2(G) - (n-1)M_1(G) + m(n-1)^2 .
\end{aligned}$$

The aim of the present work is to extend the concept of Zagreb indices to analogous graph invariants based on the second vertex degrees. We propose to name these graph invariants *leap Zagreb indices*.
The following fundamental results which will be used in many of our subsequent considerations are found in the earlier papers [22] and [26].

Lemma 1. [22, 26] *Let G be a connected graph with n vertices and m edges. Then*

$$d_2(v/G) \leq \left(\sum_{u \in N_1(v/G)} d_1(u/G) \right) - d_1(v/G)\,. \tag{1}$$

Equality holds if and only if G is a $\{C_3, C_4\}$–free graph.

Lemma 2. [26] *Let G be a connected graph with n vertices. Then for any vertex $v \in V(G)$*

$$d_2(v/G) \leq n + 1 - d_1(v/G) - e(v/G).$$

Observation 1. Let G be a connected graph with n vertices. Then for any vertex $v \in V(G)$

$$d_2(v/G) \leq d_1(v/\overline{G}) = n - 1 - d_1(v/G)\,.$$

Equality holds if and only if G has diameter at most two.

From Lemma 1, it follows,

Corollary 1. *Let G be a $\{C_3, C_4\}$-free k-regular graph with n vertices. Then $d_2(v/G) = k(k-1)$.*

2. Leap Zagreb indices of a graph

Definition 1. For a graph G, the first, second, and third leap Zagreb indices are:

$$\begin{aligned} LM_1 = LM_1(G) &= \sum_{v \in V(G)} d_2(v/G)^2 \\ LM_2 = LM_2(G) &= \sum_{uv \in E(G)} d_2(u/G)\, d_2(v/G) \\ LM_3 = LM_3(G) &= \sum_{v \in V(G)} d(v/G)\, d_2(v/G)\,. \end{aligned}$$

From the above definitions, we immediately get

$$\begin{aligned}
LM_1 &= \sum_{v\in V(G)} \sum_{u\in N_2(v/G)} d_2(u/G) \\
LM_2 &= \frac{1}{2} \sum_{v\in V(G)} d_2(v/G) \sum_{u\in N(v/G)} d_2(u/G) \\
LM_3 &= \sum_{v\in V(G)} \sum_{u\in N(v/G)} d_2(u/G) \\
&= \sum_{v\in V(G)} \sum_{u\in N_2(v/G)} d_1(u/G) \\
&= \sum_{uv\in E(G)} \Big[d_2(u/G) + d_2(v/G) \Big] \,.
\end{aligned}$$

Another straightforward consequence of Definition 1 is:

Theorem 2. *Let G_1 and G_2 be two vertex–disjoint graphs. Then for $i = 1, 2, 3$,*

$$LM_i(G_1 \cup G_2) = LM_i(G_1) + LM_i(G_2)\,.$$

Corollary 2. *Let $G_1, G_2, \ldots, G_p$ be pairwise vertex–disjoint graphs, $p \geq 2$. Then for $G = G_1 \cup G_2 \cup \cdots \cup G_p$ and $j = 1, 2, 3$,*

$$LM_j(G) = \sum_{i=1}^{p} LM_j(G_i)\,.$$

3. Leap Zagreb indices of some graph families

For the complete graph K_n and the empty graph $\overline{K_n}$, $n \geq 1$,

$$LM_i(K_n) = LM_i(\overline{K_n}) = 0 \qquad \text{for } i = 1, 2, 3.$$

For the path P_n, $n \geq 3$,

$$LM_1(P_n) = \begin{cases} 2 & \text{if } n = 3 \\ 4(n-3) & \text{otherwise} \end{cases}$$

$$LM_2(P_n) = \begin{cases} 0 & \text{if } n = 3 \\ 3 & \text{if } n = 4 \\ 2(2n-7) & \text{otherwise} \end{cases}$$

$$LM_3(P_n) = 2(2n-5)\,.$$

For the cycle C_n, $n \geq 3$, and for $i = 0, 1, 2$,

$$LM_i(C_n) = \begin{cases} 0 & \text{if } n = 3,\ i = 1,2,3 \\ 4 & \text{if } n = 4,\ i = 1,2 \\ 8 & \text{if } n = 4,\ i = 3 \\ 4n & \text{otherwise.} \end{cases} \tag{2}$$

For the star $K_{1,n}$, $n \geq 1$,

$$\begin{aligned} LM_1(K_{1,n}) &= n(n-1)^2 \\ LM_2(K_{1,n}) &= 0 \\ LM_3(K_{1,n}) &= n(n-1)\,. \end{aligned}$$

For the complete bipartite graph $K_{r,s}$, $s \geq r \geq 1$,

$$\begin{aligned} LM_1(K_{r,s}) &= r(r-1)^2 + s(s-1)^2 \\ LM_2(K_{r,s}) &= rs(r-1)(s-1) \\ LM_3(K_{r,s}) &= rs(r+s-2)\,. \end{aligned}$$

For the wheel graph $W_{1,n} = K_1 + C_n$, $n \geq 3$,

$$\begin{aligned} LM_1(W_{1,n}) &= LM_2(W_{1,n}) = n(n-3)^2 \\ LM_3(W_{1,n}) &= 3n(n-3)\,. \end{aligned}$$

For a $\{C_3, C_4\}$-free k-regular graph of order n,

$$\begin{aligned} LM_1(G) &= nk^2(k-1)^2 \\ LM_2(G) &= \frac{nk^3}{2}(k-1)^2 \\ LM_3(G) &= nk^2(k-1)\,. \end{aligned}$$

4. Some properties of leap Zagreb indices

Theorem 3. *Let G be a connected graph with n vertices and m edges. Then*

$$LM_1(G) \leq M_1(G) + n(n-1)^2 - 4m(n-1) \tag{3}$$
$$LM_2(G) \leq M_2(G) - (n-1)M_1(G) + m(n-1)^2 \tag{4}$$
$$LM_3(G) \leq 2m(n-1) - M_1(G)\,. \tag{5}$$

Equalities hold if and only if the diameter of G is at most two.

Proof. We prove only the inequality (3). The proofs of the inequalities (4) and (5) are analogous.
By Observation 1,

$$\begin{aligned} LM_1(G) &\leq \sum_{v\in V(G)} [n-1-d_1(v/G)]^2 \\ &= \sum_{v\in V(G)} \left[(n-1)^2 - 2(n-1)d_1(v/G) + d_1(v/G)^2\right] \\ &= n(n-1)^2 - 4m(n-1) + M_1(G)\,. \end{aligned}$$

Suppose now that G has diameter at most two. Then we have to distinguish between the following cases:

Case 1. If $diam(G) \leq 1$, then $G = K_n$, $n \geq 1$ and hence $d_2(v/G) = d(v/\overline{G}) = 0$, for every $v \in V(G)$. Thus, $LM_1(G) = M_1(\overline{G}) = M_1(K_n) + n(n-1)^2 - 4m(n-1) = 0$.

Case 2. If $diam(G) = 2$, then by Observation 1, $d_2(v/G) = d_1(v/\overline{G}) = n-1-d_1(v/G)$, for every $v \in V(G)$. Hence,

$$\begin{aligned} LM_1(G) &= \sum_{v\in V(G)} d_2(v/G)^2 = \sum_{v\in V(G)} d_1(v/\overline{G})^2 = \sum_{v\in V(G)} (n-1-d_1(v/G))^2 \\ &= \sum_{v\in V(G)} \left[(n-1)^2 - 2(n-1)d(v/G) + d(v/G)^2\right] \\ &= n(n-1)^2 - 4m(n-1) + M_1(G)\,. \end{aligned}$$

Suppose on contrary, that G has diameter $diam(G) \geq 3$. Then there is at least one vertex v such that $e(v/G) \geq diam(G) \geq 3$. Thus, $d_2(v/G) < d_1(v/\overline{G})$, for every vertex v with $e(v/G) \geq 3$. Therefore,

$$LM_1(G) < \sum_{v\in V(G)} \left[n-1-d_1(v/G)\right]^2 = n(n-1)^2 - 4m(n-1) + M_1(G)\,.$$

□

In what follows, we establish the relationships between the leap Zagreb indices of a graph G and the Zagreb indices and co-indices of the complement of G.

Theorem 4. *Let G be a connected graph with n vertices and m edges. Then*

$$LM_1(G) \leq M_1(\overline{G}) \tag{6}$$
$$LM_1(G) \leq n(n-1)^2 - 2m(n-1) - \overline{M_1}(G) \tag{7}$$
$$LM_2(G) \leq \overline{M_2}(\overline{G}) \tag{8}$$
$$LM_3(G) \leq \overline{M_1}(\overline{G}) = \overline{M_1}(G)\,. \tag{9}$$

Equalities hold if and only if the diameter of G is at most two.

Proof. By Observation 1,

$$LM_1(G) = \sum_{v \in V(G)} d_2(v/G)^2 \leq \sum_{v \in V(G)} d_1(v/\overline{G})^2 = \sum_{v \in V(\overline{G})} d_1(v/\overline{G})^2 = M_1(\overline{G})\,.$$

This implies

$$\begin{aligned}
LM_1(G) &\leq M_1(\overline{G}) \\
&= \sum_{uv \in E(\overline{G})} \Big[d_1(u/\overline{G}) + d_1(v/\overline{G}) \Big] \\
&= \sum_{uv \in E(\overline{G})} \Big[n-1-d_1(u/G) + n-1-d(v/G) \Big] \\
&= \sum_{uv \in E(\overline{G})} \Big[2(n-1) - (d_1(u/G) + d_1(v/G)) \Big] \\
&= 2(n-1)\left(\frac{n(n-1)}{2} - m\right) - \sum_{uv \notin E(G)} \Big[d_1(u/G) + d_1(v/G) \Big] \\
&= n(n-1)^2 - 2m(n-1) - \overline{M_1}(G)
\end{aligned}$$

$$\begin{aligned}
LM_2(G) &= \sum_{uv \in E(G)} d_2(u/G) d_2(v/G) \\
&\leq \sum_{uv \in E(G)} d_1(u/\overline{G}) d_1(v/\overline{G}) \\
&= \sum_{uv \notin E(\overline{G})} d_1(u/\overline{G}) d_1(v/\overline{G}) = \overline{M_2}(\overline{G})
\end{aligned}$$

$$\begin{aligned}
LM_3(G) &= \sum_{uv \in E(G)} \Big[d_2(u/G) + d_2(v/G) \Big] \\
&\leq \sum_{uv \in E(G)} \Big[d_1(u/\overline{G}) + d_1(v/\overline{G}) \Big] \\
&= \sum_{uv \notin E(\overline{G})} \Big[d_1(u/\overline{G}) + d_1(v/\overline{G}) \Big] \\
&= \overline{M_1}(\overline{G}) \\
&= \overline{M_1}(G)\,.
\end{aligned}$$

Suppose that equality holds in (6). Then by Observation 1, equality $d_2(v/G) = d_1(v/\overline{G})$ holds for every vertex $v \in V(G)$, if and only if the diameter of G is at most two. By similar arguments, equalities hold in (7), (8), and (9), if and only if G has diameter at most two.

Conversely, if G has diameter at most two, then it is immediate to check that (6)–(9) are equalities. □

Let G be a connected graph with n vertices and let v be any vertex of G. Then the inequality

$$d_2(v/\overline{G}) \leq d_1(v/G)\,.$$

is easily verified. By Observation 1, equality holds for every vertex $v \in V(G)$, if and only if either $\overline{G}$ has diameter at most two, or G has diameter at least four, or G is a regular graph with diameter at least two, or $G = K_1$. Hence we have the following result.

Proposition 1. *Let G be a connected graph with n vertices and m edges. Then*

$$\begin{aligned} LM_1(\overline{G}) &\leq M_1(G) \\ LM_2(\overline{G}) &\leq \overline{M_2}(G) \\ LM_3(\overline{G}) &\leq \overline{M_1}(G) = \overline{M_1}(\overline{G})\,. \end{aligned}$$

Equalities hold, if and only if either G has diameter at least four, or G is a regular graph with diameter at least two, or $G = K_1$.

In [12], it was shown that for a a simple graph G with n vertices and m edges, $M_1(G) = M_1(\overline{G})$ holds if and only if $m = \frac{n(n-1)}{4}$. Bearing this in mind we arrive at:

Corollary 3. *Let G be a graph with n vertices and m edges. If $m = \frac{n(n-1)}{4}$ and $diam(G) = 2$, then*

$$LM_1(G) = M_1(G)\,.$$

Remark 1.
1) If a graph G is self-complementary with $diam(G) = 2$, then $m = \frac{n(n-1)}{4}$ must hold and the result in Corollary 3 is obeyed in a trivial manner.
2) In the general case, the converse of Corollary 3 is not true. For example, $LM_1(C_n) = M_1(C_n)$ for any cycle C_n with $n \geq 5$ vertices.
3) $LM_1(G) = M_1(G^2)$, where G^2 is the square (second power) of the graph G, which has the same vertices as G and two vertices u and v are adjacent in G^2 if and only if $d_G(u,v) = 2$. On the other hand, in the general case, for $i = 2,3$, $LM_i(G)$ differs from $M_i(G^2)$.

Theorem 5. *Let G be a $\{C_3, C_4\}$–free graph with n vertices and m edges. Then*

$$\frac{\big[M_1(G) - 2m\big]^2}{n} \leq LM_1(G) \leq \big[M_1(G) - 2m)\big]^2\,.$$

The lower bound attains on the $\{C_3, C_4\}$–free regular graphs whereas the upper bound attains on the graphs $G = sK_1 \cup tK_2$, for $s + 2t = n$.

Proof. Since for any positive integers a_i , $i = 1, 2, \ldots, n$,

$$\sum_{i=1}^{n} a_i^2 \leq \left(\sum_{i=1}^{n} a_i \right)^2$$

it follows that

$$\sum_{v \in V(G)} d_2(v/G)^2 \leq \left(\sum_{v \in V(G)} d(v/G) \right)^2$$

and hence by Lemma 1,

$$LM_1(G) \leq \Big(M_1(G) - 2m \Big)^2 .$$

Now, consider the Cauchy–Schwarz inequality

$$\left(\sum_{i=1}^{n} a_i \; b_i \right)^2 \leq \left(\sum_{i=1}^{n} a_i^2 \right) \left(\sum_{i=1}^{n} b_i^2 \right) .$$

By choosing $a_i = 1$ and $b_i = d_2(v_i/G)$ and by Lemma 1, we obtain

$$\left(\sum_{i=1}^{n} d_2(v_i/G) \right)^2 \leq \left(\sum_{i=1}^{n} 1 \right) \left(\sum_{i=1}^{n} d_2(v/G)^2 \right) .$$

This means that

$$\Big(M_1(G) - 2m \Big)^2 \leq n LM_1(G) .$$

□

From Theorem 5, by using the fact that for any connected graph G with $n \geq 2$ vertices and m edges, $M_1(G) \geq \frac{4m^2}{n}$ (see [3, 16]), the following result follows.

Corollary 4. *Let G be a $\{C_3, C_4\}$–free graph with n vertices and m edges. Then*

$$LM_1(G) \geq \frac{4m^2(2m-n)^2}{n^3} .$$

The bound attains on the $\{C_3, C_4\}$–free regular graphs.

Recall [4], that the Moore graphs with diameter two are the pentagon, Petresen graph, Hoffman singleton graph, and possibly a 57-regular with $57^2 + 1$ vertices. Yamaguchi [26] established the following interesting result:

Theorem 6. [26] *Let G be a connected $\{C_3, C_4\}$–free graph with n vertices, m edges and radius r. Then*

$$M_1(G) \leq n(n+1-r) \tag{10}$$
$$M_2(G) \leq m(n+1-r)\,. \tag{11}$$

Equalities in (10) and (11) hold if and only if G is a Moore graph of diameter two, or $G = C_6$.

Theorem 7. *Let G be a connected graph with n vertices, m edges and radius r. Then*

$$LM_1(G) \leq (n+1-r)\big[n^2 + (2-r)n - 4m\big]\,. \tag{12}$$

Equality holds if and only if G is a Moore graph of diameter two, or $G = C_6$.

Proof. From Lemma 2 and Theorem 6, we have

$$\begin{aligned}
LM_1(G) &= \sum_{v\in V(G)} d_2(v/G)^2 \\
&\leq \sum_{v\in V(G)} \Big[n+1-e(v/G)-d_1(v/G)\Big]^2 \\
&\leq \sum_{v\in V(G)} \Big[n+1-r-d_1(v/G)\Big]^2 \\
&= \sum_{v\in V(G)} \Big[(n+1-r)^2 - 2(n+1-r)d_1(v/G) + d_1(v/G)^2\Big] \\
&= n(n+1-r)^2 - 4m(n+1-r) + M_1(G) \\
&\leq n(n+1-r)^2 - 4m(n+1-r) + n(n+1-r) \\
&= (n+1-r)\big[n^2 + (2-r)n - 4m\big]\,.
\end{aligned}$$

Suppose that equality holds in (12). Yamaguchi [26] proved that equalities in

$$\sum_{v\in V(G)} d_2(v/G) \leq \sum_{v\in V(G)} \Big[n+1-e(v/G)-d_1(v/G)\Big] \leq n+1-r-d_1(v/G)$$

and

$$M_1(G) \leq n(n+1-r)$$

hold if and only if G is a Moore graph with diameter two or $G = C_6$. Hence, by similar arguments as in the proof of Theorem 6, G is a Moore graph of diameter two, or $G = C_6$.
Conversely, if G is a Moore graph of diameter two, or $G = C_6$, then it is immediate to check that (12) is an equality. □

Theorem 8. *Let G be a connected graph with n vertices, m edges, and radius r. Then*

$$LM_2(G) \leq \frac{m}{n}(n+1-r)\big[n^2+(2-r)n-4m\big]\,. \tag{13}$$

Equality holds if and only if G is a Moore graph of diameter two, or $G = C_6$.

Proof. From Lemma 2, Theorem 6, and by using the well-known result [3, 16] $M_1(G) \geq \frac{4m^2}{n}$, we get:

$$\begin{aligned}
LM_2(G) &= \sum_{uv\in E(G)} d_2(u/G)d_2(v/G)\\
&\leq \sum_{uv\in E(G)} \Big(n+1-e(u/G)-d_1(u/G)\Big)\Big(n+1-e(v/G)-d_1(v/G)\Big)\\
&\leq \sum_{uv\in E(G)} \Big(n+1-r-d_1(u/G)\Big)\Big(n+1-r-d_1(v/G)\Big)\\
&= \sum_{uv\in E(G)} \Big[(n{+}1{-}r)^2-(n{+}1{-}r)(d_1(u/G)+d_1(v/G))+d_1(u/G)d_1(v/G)\Big]\\
&= m(n+1-r)^2-(n+1-r)M_1(G)+M_2(G)\\
&\leq m(n+1-r)^2-(n+1-r)\frac{4m^2}{n}+m(n+1-r)\\
&= \frac{m}{n}(n+1-r)\big[n^2+(2-r)n-4m\big]\,.
\end{aligned}$$

By similar arguments as in the proof of Theorems 6 and 7, we obtain the equality conditions for (13). □

Theorem 9. *Let G be a connected graph with n vertices, m edges, and radius r. Then*

$$LM_3(G) \leq \frac{2m}{n}\big[n^2+(1-r)n-2m\big]\,. \tag{14}$$

Equality holds if and only if G is a Moore graph of diameter two, or $G = C_6$.

Proof. From Lemma 2 and Theorem 6, we have

$$\begin{aligned}
LM_3(G) &= \sum_{v\in V(G)} d_1(v/G)d_2(v/G)\\
&\leq \sum_{v\in V(G)} \Big[d_1(v/G)(n+1-e(v/G)-d_1(v/G))\Big]\\
&\leq \sum_{v\in V(G)} \Big[d_1(v/G)(n+1-r-d_1(v/G))\Big]
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{v\in V(G)} \Big[(n+1-r)d_1(v/G) - d_1(v/G)^2\Big] \\
&= 2m(n+1-r) - M_1(G) \\
&\le 2m(n+1-r) - \frac{4m^2}{n} \\
&= \frac{2m}{n}\big[n^2 + (1-r)n - 2m\big]\,.
\end{aligned}
$$

The equality conditions are terated analogously as in the proofs of Theorems 6 and 7. □

Corollary 5. *Let G be a connected graph with n vertices, m edges, and radius r. Then*

$$LM_1(G) - M_1(G) \le (n+1-r)\big[n^2 - (r-1)n - 4m\big] \tag{15}$$

$$LM_2(G) - M_2(G) \le \frac{m}{n}(n+1-r)\big[n^2 - (r-1)n - 4m\big] \tag{16}$$

$$LM_3(G) + M_1(G) \le 2m(n+1-r)\,. \tag{17}$$

The bounds in (15), (16), and (17) are sharp, the cycles C_n , $n = 4,5,6$, are attending it.

Theorem 10. *Let G be a connected graph. Then*

$$LM_3(G) \le 2M_2(G) - M_1(G)\,. \tag{18}$$

Equality holds if and only if G is $\{C_3, C_4\}$–free.

Proof. Since inequality (1) holds for every vertex $v \in V(G)$, and

$$M_2(G) = \frac{1}{2}\sum_{v\in V(G)} d_1(v/G) \sum_{u\in N_1(v/G)} d_1(u/G)$$

it follows that,

$$
\begin{aligned}
LM_3(G) &= \sum_{v\in V(G)} d_1(v/G)\, d_2(v/G) \\
&\le \sum_{v\in V(G)} d_1(v/G) \left[\sum_{u\in N_1(v/G)} d_1(u/G)) - d_1(v/G)\right] \\
&= \sum_{v\in V(G)} d_1(v/G) \sum_{u\in N_1(v/G)} d_1(u/G) - \sum_{v\in V(G)} d_1(v/G)^2\,.
\end{aligned}
$$

Therefore, $LM_3(G) = 2M_2(G) - M_1(G)$.
Suppose that equality holds in (18). Then inequality (1) holds for every vertex $v \in V(G)$ if and only if G is $\{C_3, C_4\}$-free [22, 26]. □

From Theorem 3, and bearing in mind that $M_1(G) \geq \frac{4m^2}{n}$ [3, 16], it follows:

Corollary 6. *Let G be a connected graph with n vertices, m edges, and radius r. Then*

$$LM_3(G) \leq \frac{2m}{n}(n^2 - n - 2m)\,.$$

The bound attains on C_4, C_5, and Petersen graph.

Theorem 11. *Let G be a connected graph with n vertices and m edges. Then*

$$LM_3(G) \leq \sqrt{M_1(G)\,LM_1(G)}\,. \tag{19}$$

Equality holds if one of the following conditions is satisfied:
(a) G is regular with diameter $diam(G) \leq 2$.
(b) G is regular and $\{C_3, C_4\}$–free.

Proof. By the Cauchy–Schwarz inequality,

$$\begin{aligned} LM_3(G) &= \sum_{v\in V(G)} d_1(v/G)\,d_2(v/G) \leq \sqrt{\sum_{v\in V(G)} d_1(v/G)^2 \sum_{v\in V(G)} d_2(v/G)^2} \\ &= \sqrt{M_1(G)\,LM_1(G)}\,. \end{aligned}$$

Suppose that G is a k-regular graph with diameter $diam(G) \leq 2$. Then we have the following cases:

Case 1. If $diam(G) < 2$, then G is the complete graph and hence $d_2(v/G) = 0$, for every vertex $v \in V(G)$. Thus the equality in (19) holds.

Case 2. If $diam(G) = 2$, then $d_2(v/G) = n - 1 - d_1(v/G) = n - 1 - k$, for every vertex $v \in V(G)$ and hence $LM_1(G) = nk(n-1-k)$, $M_1(G) = nk^2$, and $LM_1(G) = n(n-1-k)^2$. Therefore the equality in (19) holds.
Now, suppose that G is a k-regular $\{C_3, C_4\}$–free graph. Then by Corollary 1, $d_2(v/G) = k(k-1)$, for every vertex $v \in V(G)$ and by an easy check we conclude that $LM_3(G) = \sqrt{M_1(G)\,LM_1(G)}$. □

In the general case, the converse of Theorem 11 is not true. For example, for a graph G shown in Fig. 1, the equality holds in (19), because $d_2(v/G) = d_1(v/G)$ for every vertex $v \in V(G)$, but the conditions (a) and (b) do not hold.

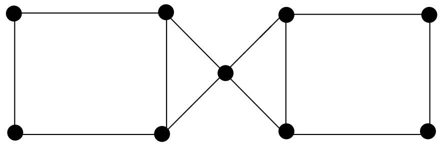

Fig. 1. A graph for which $LM_3 = \sqrt{M_1\, LM_1}$

Theorem 12. *Let G be a $\{C_3, C_4\}$–free graph with n vertices and m edges, such that $d_1(v_1/G) \geq d_1(v_2/G) \geq \cdots \geq d_1(v_n/G)$ and $d_2(v_1/G) \geq d_2(v_2/G) \geq \cdots \geq d_2(v_n/G)$. Then,*

$$LM_3(G) \geq \left(\frac{2m}{n}\right)^2 (2m-n)\,. \tag{20}$$

The bound attains on $\{C_3, C_4\}$–free regular graphs.

Proof. The Chebyshev's sum inequality states that if $a_1 \geq a_2 \geq \cdots \geq a_n$ and $b_1 \geq b_2 \geq \cdots \geq b_n$, then

$$n\sum_{i=1}^{n} a_i\, b_i \geq \left(\sum_{i=1}^{n} a_i\right)\left(\sum_{i=1}^{n} b_i\right). \tag{21}$$

By Lemma 1, if G is $\{C_3, C_4\}$–free, then

$$\sum_{v\in V(G)} d_2(v/G) = M_1(G) - 2m\,. \tag{22}$$

Applying (21), (22), and bearing in mind $M_1(G) \geq \frac{4m^2}{n}$, we obtain

$$\begin{aligned} nLM_3(G) &\geq \sum_{v\in V(G)} d_1(v/G) \sum_{v\in V(G)} d_2(v/G) \\ &= 2m(M_1(G)-2m) \geq 2m\left(\frac{4m^2}{n} - 2m\right) = \frac{4m^2}{n}(2m-n)\,. \end{aligned}$$

Hence, inequality (20) follows. □

5. Nordhaus–Gaddum–type relations for leap Zagreb indices

The following result is an immediate consequence of Theorem 4 and Proposition 1.

Proposition 2. *Let G be a graph with n vertices and m edges. Then*

$$\begin{aligned} LM_1(G) + LM_1(\overline{G}) &\le M_1(G) + M_1(\overline{G}) \\ LM_2(G) + LM_2(\overline{G}) &\le \overline{M_2}(G) + \overline{M_2}(\overline{G}) \\ LM_3(G) + LM_3(\overline{G}) &\le \overline{M_1}(G) + \overline{M_1}(\overline{G}) \,. \end{aligned}$$

From Theorem 7 and Proposition 1, it follows:

Theorem 13. *Let G be a connected graph with n vertices, m edges, and radius r. Then*

$$0 \le LM_1(G) + LM_1(\overline{G}) \le (n+1-r)\big[n^2 + (3-r)n - 4m\big]\,.$$

The lower bound attains on the complete graph K_n whereas the upper bound attains on the Moore graphs with diameter two.

The following result is an immediate consequence of Theorems 1, 4, and Proposition 1.

Proposition 3. *Let G be a connected graph of order n and size m. Then*

$$0 \le LM_2(G) + LM_2(\overline{G}) \le m(n-1)\left(n - 1 - \frac{2m}{n}\right).$$

The lower bound attains on the complete graph K_n, for every n, and the upper bound attains on the Petersen graph and C_5.

Proposition 4. *Let G be a connected graph of order n and size m. Then*

$$0 \le LM_3(G) + LM_3(\overline{G}) \le 4nm(n-1)\,.$$

The lower bound attains on the complete graph K_n, for every n, and the upper bound attains on the Petersen graph, C_5, and P_4.

From Eq. (2), we know that for every $n \ge 5$,

$$LM_1(C_n) = LM_2(C_n) = LM_3(C_n) = M_1(C_n) = M_2(C_n) = 4n\,.$$

Theorem 14. *For every positive integer p, there exists a graph G with $\Delta(G) = 2p$, such that $LM_1(G) = LM_3(G) = M_1(G)$ and $LM_2(G) = M_2(G)$.*

Proof. The result is true for $p = 1$, since $G = C_n$, for $n \geq 5$, has the desired properties. For $p \geq 2$, we have the following cases.

Case 1. If p is even, then we construct a graph G from a vertex v_0, four copies of a complete graph with $\frac{p}{2}$ vertices and two copies of an empty graph with p vertices. Let $K_{p/2}^{(i)}$, $i = 1, 2, 3, 4$, denote the i-th copy of a complete graph and $\overline{K_p}^{(j)}$, $j = 1, 2$, the j-th copy of the empty graph. Next, we join a vertex v_0 to every vertex $v \in V(K_{p/2}^{(i)})$, for every $i \in \{1, 2, 3, 4\}$. Then we join every vertex $u \in V(\overline{K_p}^{(1)})$ to every vertex $v \in V(K_{p/2}^{(i)})$, $i = 1, 2$ and we join every vertex $u \in V(\overline{K_p}^{(2)})$ to every vertex $v \in V(K_{p/2}^{(i)})$, $i = 3, 4$. By this we arrive at a graph G with $\Delta = d(v_0) = 2p$ and $d_1(v/G) = d_2(v/G)$, for every vertex v in G.

Case 2. If p is odd, then we construct a graph G from a vertex v_0, two graphs H_1 and H_2 and two copies of an empty graph with p vertices, where H_1 is a $(\frac{p-3}{2})$-regular graph and H_2 is a $(\frac{p-1}{2})$-regular graph. Let $\overline{K_p}^{(j)}$, $j = 1, 2$, denote the j-th copy of the empty graph. We join a vertex v_0 to every vertex $v \in V(H_1) \cup V(H_2)$. Then we join every vertex $v \in V(H_1)$ to every vertex $u \in V(\overline{K_p}^{(1)})$ and we join every vertex $v \in V(H_2)$ to every vertex $u \in V(\overline{K_p}^{(2)})$. This construction results in a graph G with $\Delta = d(v_0) = 2p$ and $d_1(v/G) = d_2(v/G)$, for every vertex v in G. □

6. Leap Zagreb indices of graph joins

Definition 2. Let G_1 and G_2 be two graphs with disjoint vertex sets $V(G_1)$ and $V(G_2)$ and edge sets $E(G_1)$ and $E(G_2)$, respectively. Then the join of G_1 and G_2, denoted by $G_1 + G_2$, is the graph with vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2) \cup \{uv | u \in V(G_1) \,\&\, v \in V(G_2)\}$.

Evidently, $G_1 + G_2$ is connected, $n = n_1 + n_2$, $m = n_1\, n_2 + m_1 + m_2$, where $n_i = |V(G_i)|$ and $m_i = |E(G_i)|$, $i = 1, 2$, and

$$diam(G_1 + G_2) = \begin{cases} 1 & \text{if } G_1 \text{ and } G_2 \text{ are both complete graphs} \\ 2 & \text{otherwise.} \end{cases}$$

Khalifeh at el. in [18] obtained expressions for the first and second Zagreb indices of the join $G_1 + G_2 + \cdots + G_p$. Here we need the following especial cases of their result.

Lemma 3. [18] *Let G_1 and G_2 be connected graphs with $n_i = |V(G_i)|$, $m_i = |E(G_i)|$, $i = 1, 2$. Then*

$$M_1(G_1 + G_2) = M_1(G_1) + M_1(G_2) + n_1^2 n_2 + n_1 n_2^2 + 4n_1 m_2 + 4n_2 m_1 \qquad (23)$$

$$\begin{aligned} M_2(G_1 + G_2) = {} & M_2(G_1) + M_2(G_2) + n_2 M_1(G_1) + n_1 M_1(G_2) + \\ & n_1^2 m_2 + n_2^2 m_1 + n_1^2 n_2^2 + 2n_1 n_2 (m_1 + m_2) + 4m_1 m_2. \end{aligned} \qquad (24)$$

Theorem 15. *Let G_1 and G_2 be connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively. Then*

$$\begin{aligned} LM_1(G_1+G_2) &= \Big[M_1(G_1)+n_1(n_1-1)^2-4m_1(n_1-1)\Big]+ \\ & \Big[M_1(G_2)+n_2(n_2-1)^2-4m_2(n_2-1)\Big]. \end{aligned}$$

Proof. Since, G_1+G_2 has order $n=n_1+n_2$, size $m=n_1n_2+m_1+m+2$ and diameter at most two, by Theorem 3 and using Eq. (23) in Lemma 3, we obtain

$$\begin{aligned} LM_1(G_1+G_2) &= M_1(G_1+G_2)+n(n-1)^2-4m(n-1) \\ &= \Big[M_1(G_1)+M_1(G_2)+n_1n_2^2+n_1^2n_2+4n_1m_2+4n_2m_1\Big]+ \\ & \Big[(n_1+n_2)[(n_1+n_2)-1]^2\Big]-\Big[4(n_1n_2+m_1+m_2)(n_1+n_2-1)\Big] \\ &= \Big[M_1(G_1)+n_1(n_1-1)^2-4m_1(n_1-1)\Big]+ \\ & \Big[M_1(G_2)+n_2(n_2-1)^2-4m_2(n_2-1)\Big]. \end{aligned}$$

□

The following result is also an immediate consequences of Theorem 15.

Theorem 16. *Let $G_1, G_2, \ldots, G_p$, $p \geq 2$, be graphs and let $G = G_1+G_2+\cdots+G_p$. For i=1,2,...,p, let G_i has n_i vertices and m_i edges. Then*

$$LM_1(G)=\sum_{i=1}^{p}\Big[M_1(G_i)+n_i(n_i-1)^2-4m_i(n_i-1)\Big].$$

Corollary 7. *Let G be same as in Theorem 16. Then*

$$LM_1(G)=\sum_{i=1}^{p}M_1(\overline{G_i}).$$

Theorem 17. *Let G_1 and G_2 be connected graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively. Then*

$$\begin{aligned} LM_2(G_1+G_2) &= M_2(G_1)+M_2(G_2)-(n_1-1)M_1(G_1)-(n_2-1)M_1(G_2)+ \\ & m_1(n_1-1)^2+m_2(n_2-1)^2-2m_1n_2(n_2-1)-2m_2n_1(n_1-1)+ \\ & n_1n_2(n_1-1)(n_2-2)+4m_1m_2 \end{aligned}$$

$$\begin{aligned} LM_3(G_1+G_2) &= n_1n_2(n_1+n_2-2)+2(n_1-n_2)(m_1-m_2)-2(m_1+m_2)- \\ & M_1(G_1)-M_1(G_2). \end{aligned}$$

Proof. The proof is analogous to that of Theorem 15. □

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