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Leap Zagreb Indices of Trees and Unicyclic Graphs

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Abstract: By $d(v|G)$ and $d_2(v|G)$ are denoted the number of first and second neighbors of the vertex v of the graph G. The first, second, and third leap Zagreb indices of G are defined as $LM_1(G) = \sum_{v\in V(G)} d_2(v|G)^2$, $LM_2(G) = \sum_{uv\in E(G)} d_2(u|G)\, d_2(v|G)$, and $LM_3(G) = \sum_{v\in V(G)} d(v|G)\, d_2(v|G)$, respectively. In this paper, we generalize the results of Naji et al. [Commun. Combin. Optim. **2** (2017), 99–117], pertaining to trees and unicyclic graphs. In addition, we determine upper and lower bounds on these leap Zagreb indices and characterize the extremal graphs.

Keywords: Leap Zagreb index, Zagreb index, degree (of vertex)

AMS Subject classification: 05C10, 05C35, 05C90

1. Introduction

In this paper, we only consider graphs without multiple edges or loops. The degree of a vertex v in a considered graph is denoted by $d(v)$. A double star $S_{r,s}$ is a tree with exactly two vertices u and v that are not leaves, such that $(d(u), d(v)) = (r+1, s+1)$.

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The triangular unicyclic graph $T_{r,s,t}$ is a unicyclic graph containing a triangle uvw with vertices u, v, and w, such that $(d(u), d(v), d(w)) = (r+2, s+2, t+2)$. If uvw is the triangle of an n-vertex triangular unicyclic graph G, and if $G - uvw \cong P_{n-3}$, then G will be denoted TP_n. By $S_n + e$ is denoted the graph obtained by connecting with a new edge e two leaf vertices of the star S_n. A graph is called a $\{C_3, C_4\}$-free graph if it contains neither C_3 nor C_4.

In the interdisciplinary area where chemistry, physics and mathematics meet, molecular–graph–based structure descriptors, usually referred to as topological indices, are of significant importance [3, 4, 11]. Among the most important such structure descriptors are the classical two Zagreb indices [6, 7],

$$M_1(G) = \sum_{u \in V(G)} d(u|G)^2 \qquad \text{and} \qquad M_2(G) = \sum_{uv \in E(G)} d(u|G)\, d(v|G),$$

where G is a graph whose vertex set is $V(G)$ and whose edge set is $E(G)$. By $d(u|G)$ is denoted the degree (= number of first neighbors) of the vertex $v \in V(G)$ and by uv the edge between the vertices u and v. For details of the theory of Zagreb indices see the recent survey [2] and the references cited therein.

Motivated by the success of Zagreb indices, and following an earlier work [10], Naji et al. [9] introduced the concept of leap Zagreb indices, based on the second degrees of vertices.

The k-degree of the vertex $v \in V(G)$, denoted by $d_k(v|G)$ or $d_k(v)$, is the number of vertices of G whose distance to v is equal to k. Evidently, $d_1(v|G) = d(v|G)$.

The first, second, and third leap Zagreb indices of a graph G, proposed in [9], are defined respectively as

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

In fact, a quantity identical to the third leap Zagreb index $LM_3(G)$ of a graph G appeared in a paper published in the 1970 [7], but did not attract any attention. The same was the case with a paper from 2008 [12]. Quite recently, independently of [9], Ali and Trinajstić re-invented this leap Zagreb index and named it "*modified first Zagreb connection indices*" [1].

In [9], the leap Zagreb indices of some graph families and graph joins were determined, as well as of triangle– and quadrangle–free graphs. In a later work [8], the leap Zagreb indices of graph operations were studied. Leap Zagreb indices are considered in a recent survey [5].

Motivated by these researches, in the present paper we establish sharp upper and lower bounds on the leap Zagreb indices of trees and unicyclic graphs and characterize the extremal graphs.

2. Preliminaries

The following functions and definitions will be used throughout the paper. Let

$$g(n) = \begin{cases} \frac{2(n-3)^2(n+6)}{9}, & n \equiv 0 \pmod 3 \\ \frac{2(n-3)^2(n+6)}{9} - \frac{11}{9}, & n \equiv 1 \pmod 3 \\ \frac{2(n-3)^2(n+6)}{9} - \frac{7}{9}, & n \equiv 2 \pmod 3). \end{cases}$$

It can be seen that

$$g(n) - g(n-1) \geq \frac{2n^2 - 2n - 21}{3}\,. \tag{1}$$

For an edge $e = uv \in E(G)$, we define $LM_2(e|G) = d_2(u|G)\, d_2(v|G)$, and $LM_2(e|G)$ is written as $LM_2(e)$ when no confusion can arise.

Proposition 1. *[9] Let P_n and S_n be the path and star on n vertices. For $n \geq 4$,*
(i) $LM_1(S_n) = (n-1)(n-2)^2$ and $LM_1(P_n) = 4(n-3)$,
(ii) $LM_2(S_n) = 0$ and $LM_2(P_n) = 4n - 14$,
(iii) $LM_3(S_n) = (n-1)(n-2)$ and $LM_3(P_n) = 4n - 10$.

The following results are immediate and their proofs are omitted.

Lemma 1. *Let r, s be positive integers with $r+s+2 = n$. Then $LM_1(S_{r,s}) = r^3+s^3+r^2+s^2$ and $LM_2(S_{r,s}) = rs(1+r+s)$.*
(i) If n is even, then $LM_2(S_{r,s}) \leq (n-1)(\frac{n}{2}-1)^2$. The equality holds if and only if $r = s$.
(ii) If n is odd, then $LM_2(S_{r,s}) \leq \frac{1}{4}(n-3)(n-1)^2$. The equality holds if and only if $|r-s| = 1$.

Proof. By the definitions of LM_1 and LM_2, it is clear that $LM_1(S_{r,s}) = r^3 + s^3 + r^2 + s^2$ and $LM_2(S_{r,s}) = rs(1+r+s)$. Then

$$LM_2(S_{r,s}) = rs(1+r+s) = r(n-2-r)(n-1)\,.$$

Therefore, (i) If n is even, then $LM_2(S_{r,s}) = r(n-2-r)(n-1) \leq \left(\frac{n-2-r+r}{2}\right)^2(n-1) = (n-1)(\frac{n}{2}-1)^2$. The equality holds if and only if $r = n-2-r$, i.e., $r = s = \frac{n-2}{2}$.
(ii) If n is odd, we consider the function $h(r) = r(n-2-r)(n-1)$ and obtain that $h(r) = r(n-2-r)(n-1) \leq \frac{1}{4}(n-3)(n-1)^2$, and the equality holds if and only if $|r-s| = 1$. $\square$

Lemma 2. *Let $n \geq 6$. Then*

$$LM_1(TP_n) = 4n - 10\ ,\ \ LM_1(S_n + e) = (n-3)(n^2 - 2n - 2)\,.$$

Lemma 3. *Let $n \geq 6$ with $r+s+t+3 = n$. Then $LM_2(TP_n) = 4n-13$ and $LM_2(T_{r,s,t}) = (r+s)(r+t) + (r+s)(s+t) + (r+t)(s+t) + r(r+1)(s+t) + s(s+1)(r+t) + t(t+1)(r+s)$.*

Lemma 4. *Let $x \leq y \leq z$ be non-negative integers such that $x + y + z + 3 = n$ and $f(x, y, z) = (x + y)(x + z) + (x + y)(y + z) + (x + z)(y + z) + x(x + 1)(y + z) + y(y + 1)(x + z) + z(z + 1)(x + y)$. Then $f(x, y, z) \leq g(n)$. Moreover,*
(i) if $n \equiv 0 \pmod 3$, then the equality holds if and only if $x = y = z$.
(ii) If $n \equiv 1 \pmod 3$, then the equality holds if and only if $x = y = z - 1$.
(iii) If $n \equiv 2 \pmod 3$, then the equality holds if and only if $x = y - 1 = z - 1$.

Lemma 5. *Let $n \geq 6$ with $r+s+t+3 = n$. Then $LM_3(TP_n) = 4n-8$ and $LM_3(T_{r,s,t}) = (n - 3)(n + 2)$.*

Lemma 6. *Let G be a $\{C_3, C_4\}$-free graph. Then for any $v \in V(G)$,*

$$d_2(v) = \sum_{u \in N(v)} (d(u) - 1)$$

where $N(v)$ is the set of first neighbors of the vertex v.

Recall that Lemma 6 was earlier communicated by Naji et al., [9].

3. Main results

In this section, we obtain bounds on the leap Zagreb indices of trees and unicyclic graphs.

3.1. Extremal trees on leap Zagreb indices

Theorem 1. *Let T be an n-vertex tree with $n \geq 4$. Then*

$$4(n - 3) \leq LM_1(T) \leq (n - 1)(n - 2)^2$$

with the left equality if and only if $T \cong P_n$ and the right equality if and only if $T \cong S_n$.

Proof. Since $n \geq 4$, we have $diam(T) \geq 2$. If $diam(T) = 2$, then $T \cong S_n$. By Proposition 1, we know that the result is true. If $diam(T) = 3$, then $T \cong S_{r,s}$, where r and s are two positive integers such that $r + s + 2 = n$. Then by Lemma 1, $LM_1(T) = r^3 + s^3 + r^2 + s^2$.

Since $r, s \geq 1$, we have $LM_1(T) \geq 2(r^2+s^2) \geq (r+s)^2 = (n-2)^2 \geq 4(n-3)$. If $n = 4$, then $T \cong P_4$ and $LM_1(T) = (n-2)^2 = 4(n-3)$. Thus, the result is true. If $n \geq 5$, then $LM_1(T) = (n-2)^2 > 4(n-3)$.
On the other hand,

$$\begin{aligned} LM_1(T) &= r^2(r+1) + s^2(s+1) \\ &= (n-s-2)^2(n-s-2+1) + s^2(s+1) \\ &= (n-1)(n-2)^2 + s^2(3n-4) - s(3n^2-10n+8)\,. \end{aligned}$$

Since $s < n-2$, we have $s(3n-4)-(3n^2-10n+8) < (n-2)(3n-4)-(3n^2-10n+8) = 0$. Thus, $LM_1(T) < (n-1)(n-2)^2$.
Assume now that $diam(T) \geq 4$ and proceed by induction on n. Let $P = x_1x_2\ldots x_{diam(T)}$ be a longest path of T. Then x_1 is a leaf of T. Let $T' = T - x_1$. Then we have $d_2(v|T') = d_2(v|T) - 1$ if $v \in N(x_2|T')$, and $d_2(v|T') = d_2(v|T)$ otherwise. By Lemma 6, we have

$$d_2(x_1|T) = d(x_2|T) - 1. \tag{2}$$

Thus,

$$\begin{aligned} LM_1(T) &= LM_1(T') - \sum_{v\in N(x_2|T')} d_2(v|T')^2 + \sum_{v\in N(x_2|T)} d_2(v|T)^2 \\ &= LM_1(T') + d_2(x_1|T)^2 + \sum_{v\in N(x_2|T')} (d_2(v|T)^2 - d_2(v|T')^2) \\ &= LM_1(T') + (d(x_2|T)-1)^2 + \sum_{v\in N(x_2|T')} (2d_2(v|T)-1) \text{ (Applying Eq. (2))} \\ &= LM_1(T') + (d(x_2|T)-1)(d(x_2|T)-2) + 2\sum_{v\in N(x_2|T')} d_2(v|T)\,. \end{aligned}$$

By induction, $4(n-4) \leq LM_1(T') \leq (n-2)(n-3)^2$, with the left equality if and only if $T' \cong P_{n-1}$ and the right equality if and only if $T' \cong S_{n-1}$. Moreover, by Lemma 6 we have $d_2(v|T) = d(x_2|T)-1$ for each $v \in N(x_2|T)\setminus\{x_3\}$ and $d(x_2|T) \leq d_2(x_3|T) \leq n-3$ since $diam(T) \geq 4$. Note that $2 \leq d(x_2|T) \leq n-3$. Therefore,

$$\begin{aligned} LM_1(T) &= LM_1(T') + (d(x_2|T)-1)(d(x_2|T)-2) + 2\sum_{v\in N(x_2|T')} d_2(v|T) \\ &\geq 4(n-4) + 2d_2(x_3|T) \geq 4(n-4) + 2d(x_2|T) \geq 4(n-3) \end{aligned}$$

with equality if and only if $LM_1(T') = 4(n-4)$ and $d(x_2|T) = 2$, which yields $T \cong P_n$.

On the other hand,

$$\begin{aligned}LM_1(T) &= LM_1(T') + (d(x_2|T)-1)(d(x_2|T)-2) + 2\sum_{v\in N(x_2|T')} d_2(v|T)\\ &\le LM_1(T') + 3(d(x_2|T)-1)(d(x_2|T)-2) + 2d_2(x_3|T)\\ &\le (n-2)(n-3)^2 + 3(n-4)(n-5) + 2(n-3)\\ &< (n-2)(n-3)^2 + (n-3)(3n-10)\\ &< (n-1)(n-2)^2\,.\end{aligned}$$

□

By Proposition 1, we have

Corollary 1. *Let T be an n-vertex tree with $n \geq 3$. Then $LM_2(T) = 0$ if and only if $diam(T) \leq 2$.*

Proof. If $T \cong S_n$, then by Proposition 1, part (ii), $LM_2(T) = 0$.
Suppose that $LM_2(T) = 0$. Then $diam(T) \leq 2$. Otherwise, T would contain a path $P = x_1x_2x_3x_4$, which would imply $LM_2(T) \geq d_2(x_2|T)d_2(x_3|T) \geq 1$, a contradiction. Therefore, $T \cong S_n$. □

We use $E(x|G)$ to denote the set of edges incident with x in G.

Lemma 7. *For any tree T with $diam(T) \geq 4$, there exists a tree T^* with $|V(T^*)| = |V(T)|$ and $diam(T^*) = diam(T) - 1$, such that $LM_2(T^*) > LM_2(T)$.*

Proof. Choose a longest path $P = x_1x_2\dots x_t$ in T and let $N(x_2|T) = \{x_1, x_3, y_1, \dots, y_r\}$. Then $t \geq 5$ since $diam(T) \geq 4$. We construct a new tree T_1 as follows:

$$\begin{aligned}&V(T_1) = V(T),\\ &E(T_1) = E(T) \cup \{x_4x_1, x_4y_1, \dots, x_4y_r\} \setminus \{x_2x_1, x_2y_1, \dots, x_2y_r\}\,.\end{aligned}$$

It can be checked that $d_2(v|T_1) \geq d_2(v|T)$ for any vertex $v \in V(T_1)$ and $d_2(x_5|T_1) > d_2(x_5|T)$. Thus, $LM_2(T_1) > LM_2(T)$. If $diam(T_1) = diam(T) - 1$, then T_1 is a desired graph and we set $T^* = T_1$. Otherwise, $diam(T_1) = diam(T)$. By repeating the procedure we obtain a tree T_m with $|V(T_m)| = |V(T)|$, $diam(T_m) = diam(T) - 1$ and $LM_2(T_m) > LM_2(T)$. Then T_m is the desired graph and we set $T^* = T_m$. □

Theorem 2. *For any n-vertex tree with $n \geq 5$ vertices and $diam(T) \geq 3$, it holds $LM_2(P_n) \leq LM_2(T) \leq LM_2(S_{r,s})$, where r, s are two positive integers such that $r+s+2 = n$ and $|r-s| \in \{0, 1\}$.*

Proof. The proof is by induction on n. If $n = 5$, then the result is trivial. Therefore, assume that $n \geq 6$. Let $P = x_1 x_2 \dots x_{diam(T)}$ be a longest path of T and $T' = T - (N(x_2|T) \setminus \{x_3\})$. Then $d_2(v|T') = d_2(v|T) - d(x_2|T) + 1$ if $v = x_3$ and $d_2(v|T') = d_2(v|T)$ otherwise. Thus,

$$\begin{aligned}
LM_2(T) &= LM_2(T') - \sum_{uv \in E(x_3|T')} d_2(u|T')\, d_2(v|T') + \sum_{uv \in E(x_2|T) \cup E(x_3|T)} d_2(u|T)\, d_2(v|T) \\
&= LM_2(T') + \sum_{uv \in E(x_3|T)} (d_2(u|T)\, d_2(v|T) - d_2(u|T')\, d_2(v|T')) \\
&+ \sum_{uv \in E(x_2|T) \setminus \{x_2 x_3\}} d_2(u|T)\, d_2(v|T) \\
&= LM_2(T') + \sum_{v \in N(x_2|T) \setminus \{x_3\}} d_2(x_2|T)\, d_2(v|T) \\
&+ \sum_{v \in N(x_3|T)} (d_2(x_3|T)\, d_2(v|T) - d_2(x_3|T')\, d_2(v|T')) \\
&= LM_2(T') + d_2(x_2|T)(d(x_2|T) - 1)^2 + (d(x_2|T) - 1) \sum_{v \in N(x_3|T)} d_2(v|T)\,.
\end{aligned}$$

By induction, we have $4n - 18 = LM_2(P_{n-1}) \leq LM_2(T') \leq LM_2(S_{r',s'})$, with the left equality if and only if $T' \cong P_{n-d(x_2|T)+1}$ and the right equality if and only if $T' \cong S_{r',s'}$, where r', s' are two positive integers such that $r' + s' + 2 = n - d(x_2|T) + 1$ and $|r' - s'| \in \{0, 1\}$. Since $LM_2(T) > 0$, by Theorem 1, $diam(T) \geq 3$. Then $d(x_2|T) \geq 2$ and $d(x_3|T) \geq 2$.
If $d(x_2|T) \geq 3$, then

$$\begin{aligned}
LM_2(T) &\geq LM_2(T') + 4d_2(x_2|T) + 2 \sum_{v \in N(x_3|T)} d_2(v|T) \geq 4n - 18 + 4(d(x_3|T) - 1) \\
&+ 2d(x_3|T)(d(x_3|T) - 1) \geq 4n - 10 > 4n - 14\,.
\end{aligned}$$

If $d(x_3|T) \geq 3$, then

$$\begin{aligned}
LM_2(T) &\geq LM_2(T') + d_2(x_2|T) + \sum_{v \in N(x_3|T)} d_2(v|T) \geq 4n - 18 + (d(x_3|T) - 1) \\
&+ d(x_3|T)(d(x_3|T) - 1) \geq 4n - 10 > 4n - 14\,.
\end{aligned}$$

Assume now that $d(x_2|T) = d(x_3|T) = 2$. Since $n \geq 6$, we have $diam(T) \geq 4$. If $diam(T) = 4$, then $T' \cong S_{1,n-4}$ and by Lemma 1, $LM_2(T') = (n-4)(n-2)$. Thus,

$$\begin{aligned}
LM_2(T) &= LM_2(T') + d_2(x_2|T)(d(x_2|T) - 1)^2 + (d(x_2|T) - 1) \sum_{v \in N(x_3|T)} d_2(v|T) \\
&= (n-4)(n-2) + 1 + 2 > 4n - 14\,.
\end{aligned}$$

If $diam(T) \geq 5$, then $d_2(x_4|T) \geq 2$ and $\sum_{v \in N(x_3|T)} d_2(v|T) \geq 3$. Thus,

$$\begin{aligned} LM_2(T) &= LM_2(T') + d_2(x_2|T)(d(x_2|T)-1)^2 + (d(x_2|T)-1) \sum_{v \in N(x_3|T)} d_2(v|T) \\ &\geq 4n - 18 + 1 + 3 = 4n - 14\,, \end{aligned}$$

with the equality if and only if $T' \cong P_{n-d(x_2|T)+1}$ and $\sum_{v \in N(x_3|T)} d_2(v|T) = 3$. Note that $d(x_2|T) = 2$, from which it follows $T \cong P_n$.
Now we show the right inequality.
If $diam(T) = 3$, then T is a double star. By Lemma 1, we know that the inequality is true. Now we assume that $diam(T) = p \geq 4$. By Lemma 7, there exists a sequence of n-vertex trees $T_1, T_2, \ldots, T_{p-3}$ such that $diam(T_i) = diam(T) - i$ and $LM_2(T_{i-1}) < LM_2(T_i)$, where $i = 1, 2, \ldots, p-3$ and $T_0 = T$. Hence, $LM_2(T) < LM_2(T_{p-3})$. Note that $diam(T_{p-3}) = diam(T) - (p-3) = 3$, that is, T_{p-3} is a double star. By Lemma 1, $LM_2(T_{p-3}) \leq LM_2(S_{r,s})$, where r, s are two positive integers such that $r+s+2 = n$ and $|r-s| \in \{0, 1\}$. Hence, $LM_2(T) < LM_2(S_{r,s})$, which completes the proof. □

Theorem 3. *Let T be an n-vertex tree with $n \geq 5$ vertices. Then $2(2n-5) \leq LM_3(T) \leq (n-1)(n-2)$. The left equality holds if and only if $T \cong P_n$ whereas the right equality holds if and only if T is a star or a double star.*

Proof. The proof is by induction on n and is fully analogous to that of Theorem 2. We omit the details. □

3.2. Extremal unicyclic graphs on leap Zagreb indices

Theorem 4. *Let G be an n-vertex unicyclic graph with $n \geq 6$. Then*

$$4n - 10 \leq LM_1(G) \leq (n-3)(n^2 - 2n - 2)$$

with the left equality if and only if $G \cong TP_n$ and the right equality if and only if $G \cong S_n + e$.

Proof. The proof is by induction on n. If $n = 6$, then the result is trivial. Now we assume that $n \geq 7$. Let $P = x_1 x_2 \ldots x_t$ be a longest path of G from a leaf to the cycle. If $t = 0$, then $G \cong C_n$ and $LM_1(G) = 4n < (n-3)(n^2 - 2n - 2)$. So the result is true.
Assume now that $t \geq 1$ and let $G' = G - x_1$. Then $d_2(v|G) = d_2(v|G') + 1$ if

$v \in N(x_2|G')$ and $d_2(v|G') = d_2(v|G)$ otherwise. Thus,

$$\begin{aligned}
LM_1(G) &= LM_1(G') - \sum_{v\in N(x_2|G')} d_2(v|G')^2 + \sum_{v\in N(x_2|T)} d_2(v|G)^2 \\
&= LM_1(G') + d_2(x_1|G)^2 + \sum_{v\in N(x_2|G')} (d_2(v|G)^2 - d_2(v|G')^2) \\
&= LM_1(G') + (d(x_2|G)-1)^2 + \sum_{v\in N(x_2|G')} (2d_2(v|G)-1) \\
&= LM_1(G') + (d(x_2|G)-1)(d(x_2|G)-2) + 2\sum_{v\in N(x_2|G')} d_2(v|G)\,.
\end{aligned}$$

By induction, we have $4n-14 \leq LM_1(G') \leq (n-4)(n^2-4n+1)$, with the left equality if and only if $G' \cong TP_{n-1}$ and the right equality if and only if $G' \cong S_{n-1}+e$. If $d(x_2|G) \geq 3$ or $d_2(x_3|G) \geq 2$, then $LM_1(G) \geq LM_1(G') + 4 = 4n-10$, with the equality if and only if $G' \cong TP_{n-1}$, and $d(x_2|G) = 3$ and $d_2(x_3|G) \leq 1$ or $d(x_2|G) \leq 2$ and $d_2(x_3|G) = 2$. Since $n \geq 7$, $d_2(x_3|G) \geq 2$. So the equality holds if and only if $G' \cong TP_{n-1}$, $d(x_2|G) = 2$, and $d_2(x_3|G) = 2$, which implies that $G' \cong TP_n$.
If $d(x_2|G) \leq 2$ and $d_2(x_3|G) \leq 1$, then $d(x_2|G) = 2$ and $d_2(x_3|G) = 1$. Thus, $N[x_3|G] = V(G)\setminus\{x_1\}$ and $G' \cong S_{n-1}+e$. It follows hat $LM_1(G) \geq LM_1(G') + 2 = (n-4)(n^2-4n+1)+2 > 4n-10$.
On the other hand, if $d(x_2|G) \leq n-2$, then

$$\begin{aligned}
LM_1(G) &\leq LM_1(G') + (n-3)(n-4) + 2(n-3)^2 \\
&\leq (n-4)(n^2-4n+1) + (n-3)(3n-10) \\
&= (n-3)(n^2-2n-2) - (6n-20) \\
&< (n-3)(n^2-2n-2)\,.
\end{aligned}$$

If $d(x_2|G) \geq n-1$, then $G' \cong S_n + e$ and $LM_1(G) = (n-3)(n^2-2n-2)$. □

Theorem 5. *Let G be an n-vertex unicyclic graph with at least eight vertices. Then*

$$LM_2(TP_n) < LM_2(G) < LM_2(T_{r,s,t})$$

where r, s, and t are positive integers, such that $r \geq s \geq t$, $r+s+t+3 = n$, and $|r-t| \leq 1$.

Proof. We first prove the left inequality. The proof is by induction on n. If $n = 8$, then the result can be verified by computer search. Therefore, we assume that $n \geq 9$. Note that if $G \cong TP_n$, then $LM_2(G) = 4n-13$. Now we show that there exists no unicyclic graph G having minimum $LM_2(G)$, but $G \ncong TP_n$. Otherwise, let G^* be such a graph for which

$$LM_2(G^*) \geq LM_2(TP_n) = 4n-13\,. \tag{3}$$

Note that $LM_2(C_n) = 4n > 4n-13$, implying that G^* is not a cycle. Therefore, there exists a vertex v with degree one in G^*. Let vuw be a path in G^* with $d(w|G^*) \neq 1$.

Case 1. If $d(u|G^*) \geq 3$, then $d_2(v|G^*) \geq 2$.

If $d_2(u|G^*) \geq 2$, then $LM_2(uv|G^*) \geq 4$. Let $H = G^* - v$. Then $LM_2(G^*) \geq LM_2(H) + LM_2(uv|G^*) \geq LM_2(H) + 4$. By induction, $LM_2(H) \geq 4(n-1) - 13$ and so we have $LM_2(G^*) \geq 4n - 13$. Due to $LM_2(G^*)$ being minimum, we can deduce $H \cong TP_{n-1}$. Therefore, G^* is the graph obtained by adding a vertex u and an edge uv, where v is a vertex with degree one in TP_{n-1}. It is clear that $LM_2(G^*)$ is minimum if and only if $G^* \cong TP_n$.

If $d_2(u|G^*) = 1$, then $d_2(v|G^*) \geq 2$. Then $d_2(x|H) = d_2(x|G^*) - 1$ for any $x \in N(u) \setminus \{v\}$. Therefore,

$$\begin{aligned}
LM_2(G^*) \geq & LM_2(H) + LM_2(uv|G^*) + \sum_{e \in E(u|G^*) \setminus \{uv\}} LM_2(e) - \sum_{e \in E(u|H) \setminus \{uv\}} LM_2(e) \\
\geq & 4(n-1) - 13 + 2 + d_2(u)(d(u)-1) \geq 4n - 13\,.
\end{aligned}$$

Since $LM_2(G^*)$ is minimum, we have $H \cong TP_{n-1}$. Therefore, G^* is the graph obtained by adding a vertex u and an edge uv, where v is a vertex with degree one in TP_{n-1}. Clearly, $LM_2(G^*)$ is minimum if and only if $G^* \cong TP_n$.

If $d_2(u) = 0$, then G^* is the graph obtained by adding an edge to the star. Clearly, $LM_2(G^*) > 4n - 13$, a contradiction with Eq. (3).

Case 2. If $d(u) = 2$, then $d_2(u) = d(w) - 1$ and $d_2(v) = 1$. First, we show that $d_2(w) \geq 2$. Otherwise, $N[w] \cup \{v\} = V(G^*)$. Since $n \geq 9$, there is a vertex $x \in N(w)$ with $d(x) = 1$. Then we get the left inequality as desired by the proof of Case 1. Now we have $d_2(w) \geq 2$ and so $d_2(y) \geq 1$, for each $y \in V(G^*)$. Therefore,

$$\begin{aligned}
LM_2(G) \;\geq\; & LM_2(H) + LM_2(uv|G^*) + LM_2(uw|G^*) \\
& + \sum_{e \in (E(w|G^*) \setminus \{uw\})} LM_2(e) - \sum_{e \in (E(w|H) \setminus \{uw\})} LM_2(e) - LM_2(uw|H) \\
\geq\; & 4(n-1) - 13 + d_2(u) + d_2(u) * d_2(w) + \sum_{v \in N(w) \setminus \{u\}} d_2(v) \\
-\; & d_2(u)(d_2(w) - 1) \\
\geq\; & 4(n-1) - 13 + d(w) - 1 + d(w) - 1 + \sum_{v \in N(w) \setminus \{u\}} d_2(v)\,.
\end{aligned}$$

If there is a vertex $q \in N(w) - \{u\}$ with $d_2(q) \geq 2$ or $d(w) \geq 3$, then

$$\begin{aligned}
LM_2(G) \;\geq\; & 4(n-1) - 13 + d(w) - 1 + d(w) - 1 + \sum_{v \in N(w) \setminus \{u\}} d_2(v) \\
\geq\; & 4(n-1) - 13 + d(w) - 1 + d(w) - 1 + 2 \geq 4n - 13\,.
\end{aligned}$$

We now only consider the condition $d(w) = 2$ and $d_2(x) = 2$ for any $x \in N(w) - \{u\}$. Then all vertices except u, v, x are adjacent to x. Since $n \geq 9$, there is a leaf adjacent to x and $d(x) \geq 3$. Then we get the inequality by the proof of Case 1.
Now we prove the right inequality. Let G' be a unicyclic graph that maximizes $LM_2(G')$ and $C = v_1 v_2 \cdots v_k$ be the unique cycle of G'. Then

Claim 1. *For any $u \in V(G')$, $d(u, C) \leq 1$.*

Proof. Suppose to the contrary that there exists a vertex u such that $d(u, C) = p - 1 \geq 2$. Assume that $u_1 u_2 \cdots u_p$ is a shortest path from u_1 to C where $u_1 = u$ and $u_p = v_i$ for some $i = 1, 2, \ldots, k$.
If $p \geq 4$, then we construct a graph G'' such that $V(G'') = V(G')$ and $E(G'') = E(G') \cup \{u_{p-3}x | x \in L(u_{p-1})\} \setminus \{u_{p-1}x | x \in L(u_{p-1})\}$. Then $LM_2(G'') > LM_2(G')$, contradicting with the assumption that G' has maximum $LM_2(G')$.
If $p = 3$, then we construct a graph G'' such that $V(G'') = V(G')$ and $E(G'') = E(G') \cup \{v_{i-1}x | x \in L(u_{p-1})\} \setminus \{u_{p-1}x | x \in L(u_{p-1})\}$. Then $LM_2(G'') > LM_2(G')$, contradicting with the assumption that G' has maximum $LM_2(G')$. $\square$

For the upper bound, the proof is by induction on n. If $n = 8$, we can verify the result by computer search. Now we consider the case $n \geq 9$ and suppose that for any unicyclic graph G'' of order $n - 1$,

$$LM_2(G'') \leq LM_2(T_{r',s',t'}), \tag{4}$$

where $r' \geq s' \geq t'$, $r' + s' + t' + 3 = n - 1$ and $|r' - t'| \leq 1$.
It can be verified that $LM_2(C_n) < LM_2(T_{r,s,t})$, where $r \geq s \geq t$, $r + s + t + 3 = n$ and $|r - t| \leq 1$. Therefore, G' is not a cycle. Therefore, each vertex not in C of degree one and has a neighbor in C.
If $k = 3$,then by Lemmas 4 and 5, the right inequality holds.
If $k = 4$, then G' is a graph whose removal of all leaf vertices results in C_4. Then by analysis a function with three variables, we can obtain the desired result.
If $k = 5$, then G' is a graph whose removal of all leaf vertices results in C_5. Then by analysis a function with four variables, we can obtain the desired result.
Now we consider the case $k \geq 6$. Let v_i be a vertex in C with minimum degree. Construct a graph G'' such that $V(G'') = V(G') \setminus \{v_{i-1}\}$ and $E(G'') = E(G') \cup$

$\{v_{i-2}v_i\} \cup \{v_i x | x \in L(v_{i-1})\} \setminus \{v_{i-1}x | x \in L(v_{i-1})\}$. Let

$$\begin{aligned}
A_1 &= \{v_{i-1}u | u \in L(v_{i-1}|G')\},\\
B_1 &= \{v_{i-1}v_{i-2}\},\\
C_1 &= \{v_i u | u \in L(v_i|G')\},\\
D_1 &= E(G') \setminus (A_1 \cup B_1 \cup \{v_{i-1}v_i\} \cup C_1 \cup E_1),\\
E_1 &= \{v_i v_{i+1}\},\\
A_2 &= \{v_i u | u \in L(v_{i-1}|G')\},\\
B_2 &= \{v_{i-2}v_i\},\\
C_2 &= \{v_i u | u \in L(v_i|G'')\},\\
D_2 &= E(G'') \setminus (A_2 \cup B_2 \cup E_1).
\end{aligned}$$

We define a one-to-one mapping $h : E(G') \to E(G'')$ such that

$$\begin{aligned}
h(v_p v_q) &= v_p v_q \text{ if } v_p v_q \in D_1,\\
h(v_{i-1}u) &= v_i u \text{ if } u \in L(v_{i-1}|G'), i.e., v_{i-1}u \in A_1,\\
h(v_{i-1}v_{i-2}) &= v_{i-2}v_i, i.e., v_{i-1}u \in B_1.
\end{aligned}$$

Let

$$\Delta_1 = d_2(v_{i-2}|G')d_2(v_{i-1}|G') - d_2(v_{i-2}|G'')d_2(v_i|G'')\,.$$

Then by the choice of v_i and Lemma 6 we have

$$\begin{aligned}
\Delta_1 \;=\;& (d(v_{i-3}|G') + d(v_{i-1}|G') - 2)(d(v_{i-2}|G') + d(v_i|G') - 2)\\
-\;& (d(v_{i-3}|G'') + d(v_i|G'') - 2)(d(v_{i-2}|G'') + d(v_{i+1}|G'') - 2)\,.
\end{aligned}$$

Since $d(v_j|G') = d(v_j|G'')$ for any $j \in \{i-3, i-2, i+1\}$, $d(v_i|G') - 2 \geq 0$, and $d(v_i|G'') = d(v_i|G') + d(v_{i-1}|G') - 2$, we have $\Delta_1 \leq 0$, i.e., for any $e \in B_1$

$$LM_2(e|G') \leq LM_2(h(e)|G''). \tag{5}$$

For any vertex $u \in L(v_{i-1})$ in G',

$$\begin{aligned}
d_2(u|G')d_2(v_{i-1}|G') &= (d(v_i|G') - 1)d_2(v_i|G')\\
&= (d(v_i|G') - 1)(d(v_{i-2}|G') + d(v_i|G') - 2),
\end{aligned}$$

and

$$\begin{aligned}
d_2(u|G'')d_2(v_i|G'') &= (d(v_i|G'') - 1)d_2(v_i|G'')\\
&= (d(v_i|G'') - 1)(d(v_{i-2}|G'') + d(v_{i+1}|G'') - 2)\,.
\end{aligned}$$

Since $d(v_j|G') = d(v_j|G'')$ for any $j \in \{i-1, i+2\}$,

$$d_2(u|G')d_2(v_{i-1}|G') \leq d_2(u|G'')d_2(v_i|G'') \,.$$

Then for any $e \in A_1$, we have

$$LM_2(e|G') \leq LM_2(h(e)|G'') \,.$$

Now for any vertex $u \in L(v_i)$ in G', we have

$$\begin{aligned} d_2(u|G')d_2(v_i|G') &= (d(v_i|G') - 1)d_2(v_i|G') \\ &= (d(v_i|G') - 1)(d(v_{i-1}|G') + d(v_{i+1}|G') - 2), \end{aligned}$$

$$\begin{aligned} d_2(u|G'')d_2(v_i|G'') &= (d(v_i|G'') - 1)d_2(v_i|G'') \\ &= (d(v_i|G') + d(v_{i-1}) - 3)(d(v_{i-2}|G') + d(v_{i+1}|G') - 2) \,. \end{aligned}$$

Let $\Delta_2 = d_2(u|G'')d_2(v_i|G'') - d_2(u|G')d_2(v_i|G')$. Then

$$\begin{aligned} \Delta_2 &= (d(v_i|G') - 1)(d(v_{i-2}|G') - d(v_{i-1}|G')) + (d(v_{i-1}|G') - 2)(d(v_{i-2}|G') \\ &+ d(v_{i+1}|G') - 2) = (d(v_{i-1}|G') - 2)(d(v_{i+1}|G') - 1 - d(v_i|G') + 1) \\ &+ (d(v_{i-2}|G') - 2)(d(v_i|G') - 1) + (d(v_{i-1}|G') - 2)(d(v_{i-2}|G') - 1) \geq 0 \,. \end{aligned}$$

Then for any $e \in C_1$, we have

$$LM_2(e|G') \leq LM_2(h(e)|G'') \,.$$

Now for $e \in E_1$, we have

$$d_2(v_i|G')d_2(v_{i+1}|G') = (d(v_{i+1}|G') + d(v_{i-1}|G') - 2)(d(v_i|G') + d(v_{i+2}|G') - 2),$$

and

$$\begin{aligned} d_2(v_i|G'')d_2(v_{i+1}|G'') &= (d(v_{i+1}|G'') + d(v_{i-2}|G'') - 2)(d(v_i|G'') \\ &+ d(v_{i+2}|G'') - 2) = (d(v_{i+1}|G') + d(v_{i-2}|G') - 2)(d(v_i|G') \\ &+ d(v_{i-1}|G') - 2 + d(v_{i+2}|G') - 2) \,. \end{aligned}$$

Let $\Delta_3 = d_2(v_i|G')d_2(v_{i+1}|G') - d_2(v_i|G'')d_2(v_{i+1}|G'')$. Then

$$\begin{aligned} \Delta_3 &= -(d(v_{i+1}|G') - 2)(d(v_{i-1}|G') - 2) + (d(v_{i-2}|G') - d(v_{i-1}|G'))(d(v_i|G') \\ &+ d(v_{i+1}|G') - 2) - d(v_{i-2}|G')(d(v_{i-1}|G') - 2) \\ &\leq (d(v_{i-2}|G') - d(v_{i-1}|G'))(d(v_i|G') + d(v_{i+1}|G') - 2) \,. \end{aligned}$$

• If $d(v_{i-2}|G') - d(v_{i-1}|G') < 0$, then

$$(d(v_{i-2}|G') - d(v_{i-1}|G'))(d(v_i|G') + d(v_{i+1}|G') - 2) < 0\,.$$

• If $d(v_{i-2}|G') - d(v_{i-1}|G') > 0$, then

$$\begin{aligned}
\Delta_3 &\leq (d(v_{i-2}|G') - d(v_{i-1}|G'))(d(v_i|G') + d(v_{i+1}|G') - 2) \\
&\leq \left(\frac{d(v_{i-1}|G') - d(v_{i-2}|G') + d(v_i|G') + d(v_{i+1}|G') - 2}{2}\right)^2 \\
&\leq \left(\frac{d(v_i|G') + d(v_{i+1}|G') - 2}{2}\right)^2 \leq \left(\frac{n-2}{2}\right)^2 .
\end{aligned}$$

As above, for $e \in E_1$,

$$LM_2(e|G') - LM_2(e|G'') \leq \left(\frac{n-2}{2}\right)^2 .$$

Now we have

$$\begin{aligned}
LM_2(v_i v_{i-1}|G') &= (d(v_{i-1}|G') + d(v_{i+1}|G') - 2)(d(v_i|G') + d(v_{i-2}|G') - 2) \\
&\leq \left(\frac{d(v_{i-1}|G') + d(v_{i+1}|G') + d(v_i|G') + d(v_{i-2}|G') - 4}{2}\right)^2 \\
&\leq \left(\frac{n-2}{2}\right)^2 .
\end{aligned}$$

Finally, it is clear that for any $e \in D_1$

$$LM_2(e|G') \leq LM_2(h(e)|G'')\,. \tag{6}$$

Since $E(G') = A_1 \cup B_1 \cup D_1 \cup \{v_{i-1}v_i\}$, together with Eqs. (5)–(6) we obtain

$$\begin{aligned}
LM_2(G') &= \sum_{e\in A_1} LM_2(e|G') + \sum_{e\in B_1} LM_2(e|G') + \sum_{e\in D_1} LM_2(e|G') \\
&+ \sum_{e\in C_1} LM_2(e|G') + LM_2(v_iv_{i+1}|G') + LM_2(v_iv_{i-1}|G') \\
&\leq \sum_{e\in A_2} LM_2(e|G'') + \sum_{e\in B_2} LM_2(e|G'') + \sum_{e\in D_2} LM_2(e|G'') \\
&+ \sum_{e\in C_2} LM_2(e|G'') + LM_2(v_iv_{i+1}|G'') + LM_2(v_iv_{i+1}|G') \\
&- LM_2(v_iv_{i+1}|G'') + LM_2(v_iv_{i-1}|G') \\
&\leq LM_2(G'') + \left(\frac{n-2}{2}\right)^2 + \left(\frac{n-2}{2}\right)^2 \\
&< g(n-1) + \frac{2n^2-2n-21}{3} \text{ (apply induction assumption Eq. (4))} \\
&\leq g(n),
\end{aligned}$$

contradicting to the assumption made on the graph G'.
By this, the proof of Theorem 5 is completed. □

In a manner analogous to the proof of Theorem 5 we can establish the following:

Theorem 6. *Let G be an n-vertex unicyclic graph with $n \geq 6$. Then $4n-8 \leq LM_3(G) \leq (n-3)(n+2)$, where r, s, t are positive integers such that $r+s+t+3 = n$. The left equality holds if and only if $G \cong TP_n$ and the right equality holds if and only if $G \cong T_{r,s,t}$ for $r, s, t \geq 0$.*

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