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Inverse Problem for Leap Zagreb Indices

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Abstract

The structure of a chemical compound is usually modeled as a graph, which is so-called a molecular graph. It has been found that some topological indices of a molecular graph are closely related to many physicochemical properties of its chemical compounds. From this relation, it arises the important inverse topological indices problem, that carry out a thorough search of the existence of a graph having its index value equal to a given integer. In this paper, we are interested in solving this problem for the first, second and third leap Zagreb indices of connected graphs. We are also restricting the solutions to trees and unicyclic graphs. It is shown that for every even non-negative integer k there exists a graph having its first leap Zagreb index value equal to k. For every non-negative integer k, except 2, there exists a graph having its second leap Zagreb index value equal to k and for every non-negative integer k, except $1, 3, 5, 7, 9, 11, 17$, there exists a graph having its third leap Zagreb index value equal to k. The general formulas of leap Zagreb indices values for some certain trees and unicyclic graphs which are useful in this work are presented.

Keywords: Second degree (of vertex); Leap Zagreb Indices; Inverse Problem.
2020 Mathematics Subject Classification: 05C07, 05C09, 05C12.

1. Introduction

Throughout this paper, we are concerned only with finite connected simple graphs $G = (V, E)$, such that graph is undirected with no loops, no weighted and multiple edges and there is a path joining any two vertices in it. As usual, $V = V(G)$ and $E = E(G)$ are the vertex and edge sets of G, whereas $n = |V|$ and $m = |E|$, indicate the number of vertices and edges in G, respectively. The distance $d(u, v)$ between two vertices u and v in G is the length (number of edges) of the shortest path connecting them. The eccentricity of $v \in V(G)$ is $e(v) = \max\{d(v, u) : u \in V(G)\}$, the radius of G is $rad(G) = \min\{e(v) : v \in V(G)\}$ and the diameter of G is $diam(G) = \max\{e(v) : v \in V(G)\}$. As usual, we denote a $K_n, P_n, C_n, K_{1,n-1}$, and $S_{r,s}$ by the complete, path, cycle, star and bistar of order n. A graph G

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is called F-free graph if no induced subgraph of G is isomorphic to F. The graph $G-e$ is the graph obtained from G by deleting the edge e, for $e \in E(G)$. For a vertex $v \in V(G)$, the open 2-distance neighborhood of v in a graph G, denoted by $N_2(v/G)$ (or $N_2(v)$ if not misunderstood), and defined as $N_2(v) = \{u \in V(G) : d(u,v) = 2\}$. The second degree of v, denoted by $d_k(v/G)$ (or $d_k(v)$), and is $d_2(v) = |N_2(v)|$. we denote by $E_2(G)$ to the set of all unordered pairs of vertices of G which the distance between them equal two, i.e., $E_2(G) = \Big\{\{u,v\} \subset V(G) : d(u,v) = 2\Big\}$ and let $m_2 = |E_2(G)|$. For any terminology or notation not mentioned here, we refer the reader to books [3,7].

A topological index (structure-descriptor) of a graph is a numerical parameter mathematically derived from the graph structure. It is a fixed invariant for any two isomorphic graphs. A graph invariant is any function on a graph that does not depend on labeling of its vertices. The topological indices of graphs are especially useful in establishing the mathematical basis for connections between the structure of molecular graph and the physicochemical properties or biological activity of its chemical compounds.

In the current mathematical and mathematico-chemical literature a large number of vertex-degree-based graph invariant are being studied. Among them, the first $M_1(G)$ and second $M_2(G)$ Zagreb indices are the far most extensively investigated ones. These have been introduced more than forty years ago [5,6], and are defined as:

$$\begin{aligned} M_1(G) &= \sum_{v \in V(G)} d^2(v), \\ M_2(G) &= \sum_{uv \in E(G)} d(u)d(v). \end{aligned}$$

Naji [13], introduced three new distance-degree-based topological indices conceived depending on the second degrees of vertices, and so-called leap Zagreb indices of a graph G are defined as:

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

The leap Zagreb indices have several chemical applications. Surprisingly, the first leap Zagreb index has very good correlation with physical properties of chemical compounds like boiling point, entropy, DHVAP, HVAP and accentric factor [2], hence attract the attention of many graph theorists and also other scientists including chemists. For properties and more details of leap Zagreb indices, we refer the readers to [1,2,9,11–17].

2. Preliminaries

The inverse problem for topological indices is the answer of the question "which integer number can be an index value of a graph?", It is about the existence of a graph having its index value equal to a given integer number. This problem was studied in due detail for the Wiener index [4,8,18–20]. Recently, Yurtas in [21], have been solved this problem for the first and second Zagreb indices, and they presented analogous results also for the forgotten and hyper-Zagreb index. They showed that, first Zagreb index of connected graphs can take any even positive integer value, except 4 and 8. The second Zagreb index of connected graphs can take any positive integer value, except $2, 3, 5, 6, 7, 10, 11, 13, 15$ and 17.

Motivated by these, we are interested in solving this problem for the first, second and third leap Zagreb indices of connected graphs. We begin with some old results which required to show the main results. Then, in sections 2.1 and 2.2, we present the general formulas of leap Zagreb indices for some certain trees and unicyclic graphs that will be useful. So also, the general formulas of leap Zagreb indices for some graphs are presented in section 2.3. In section 3, the possible values of the first leap Zagreb index of graphs and also of trees and unicyclic graphs are presented. In section 4, the possible values of the second leap Zagreb index of graphs as well as of trees and unicyclic graphs are presented. In section 5, the possible values of the third leap Zagreb index of graphs and so also of trees and unicyclic graphs are presented.

The following results will be useful.

Theorem 2.1 ([10]). *Let G be a connected graph with n vertices and m_2 second edges. Then*

$$\sum_{v\in V(G)} d_2(v) = 2m_2. \tag{1}$$

Corollary 2.2. *For a graph G, the number of vertices with odd second degree in G is even.*

Theorem 2.3 ([16]). *For any 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 $|r - s| \in \{0, 1\}$.

Lemma 2.4 ([14]). *For the path P_n, with n vertices.*

(1) $$LM_1(P_n) = \begin{cases} 0, & \text{if } n < 3; \\ 2, & \text{if } n = 3; \\ 4n - 12, & \text{if } n > 3. \end{cases}$$

(2) $LM_2(P_n) = \begin{cases} 0, & \text{if } n < 4; \\ 3, & \text{if } n = 4; \\ 4n - 14, & \text{if } n > 4. \end{cases}$

(3) $LM_3(P_n) = \begin{cases} 0, & \text{if } n < 3; \\ 2, & \text{if } n = 3; \\ 4n - 10, & \text{if } n > 3. \end{cases}$

Theorem 2.5 ([16]). *For a triangular unicyclic graph $P_{n-3}C_3$, with $n \geq 4$ vertices.*

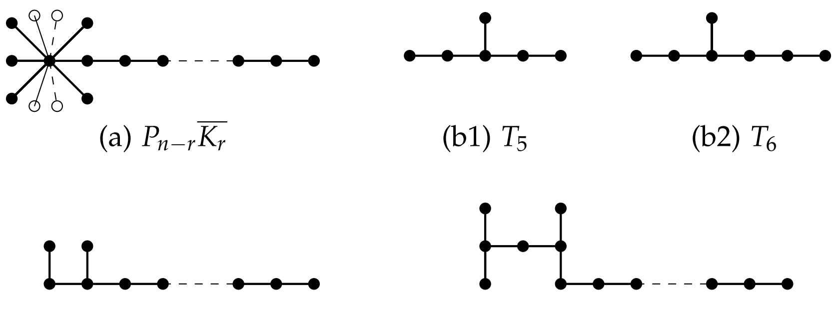
(1) $LM_1(P_{n-3}C_3) = 4n - 10$

(2) $LM_2(P_{n-3}C_3) = \begin{cases} 1, & \text{if } n = 4; \\ 7, & \text{if } n = 5; \\ 10, & \text{if } n = 6. \\ 4n - 13, & \text{if } n \geq 7. \end{cases}$

(3) $LM_3(P_{n-3}C_3) = \begin{cases} 6, & \text{if } n = 4; \\ 4n - 8, & \text{if } n \geq 5. \end{cases}$

2.1 The leap Zagreb indices for some trees

Recall that a vertex of a tree with one degree is called a leaf and its neighbor is called a support vertex. A vertex v of a tree T with $e(v) = rad(T)$ is called a central vertex, where a tree of even order have two central vertices, whereas a tree of odd order have only one. A tree with $n+1$ vertices obtained by joining a new vertex to any central vertex of a path P_n, will be denote T_n, figure1 (b1) and (b2), shows T_n for $n = 5, 6$. A tree that is obtained by joining $r \geq 2$ vertices to a leaf of a path P_n, is called a broom, as shown in figure 1.a, and denoted $P_{n-r}\overline{K_r}$. A tree which is constructed from the broom $P_{n-2}\overline{K_2}$, by joining a new vertex to any pendent vertex of $\overline{K_2}$ in the broom will be called an F-tree and denoted FT_n, for $n \geq 5$, see figure 1.c, whereas a tree which is constructed from the broom $P_{n-2}\overline{K_2}$, by joining a central vertex in P_3 to a pendent vertex of $\overline{K_2}$ in the broom will be called an H-tree and denoted HT_n, for $n \geq 7$, see figure 1.d).



(a) $P_{n-r}\overline{K_r}$ (b1) T_5 (b2) T_6

(c) FT_n (d) HT_n

Figure 1: The broom, T_n-, F- and H-trees.

Proposition 2.6. *The leap Zagreb indices of a T_n tree with $n \geq 3$ vertices, are given by*

$$(1)\ LM_1(T_n) = \begin{cases} 12, & \text{if } n = 3; \\ 14, & \text{if } n = 4; \\ 18, & \text{if } n = 5; \\ 24, & \text{if } n = 6; \\ 4n+2, & \text{if } n \geq 7. \end{cases}$$

$$(2)\ LM_2(T_n) = \begin{cases} 0, & \text{if } n = 3; \\ 8, & \text{if } n = 4; \\ 4(n-1), & \text{if } n = 5,6,7; \\ 29, & \text{if } n = 8; \\ 4n-2, & \text{if } n \geq 9. \end{cases}$$

$$(3)\ LM_3(T_n) = \begin{cases} 6, & \text{if } n = 3; \\ 12, & \text{if } n = 4; \\ 4n-2, & \text{if } n \geq 5. \end{cases}$$

Proposition 2.7. *For $r \geq 2$, the leap Zagreb indices of a broom $P_{n-r}\overline{K_r}$, with $n \geq 3$ vertices are given by*

$$(1)\ LM_1(P_{n-r}\overline{K_r}) = \begin{cases} r(r-1)^2, & \text{if } n = r+1; \\ r^2(r+1), & \text{if } n = r+2; \\ r^2(r+1)+2, & \text{if } n = r+3; \\ 4(n-r-3)+2r(r+1), & \text{if } n \geq r+4. \end{cases}$$

$$(2)\ LM_2(P_{n-r}\overline{K_r}) = \begin{cases} 0, & \text{if } n = r+1, r+2; \\ r(r+2), & \text{if } n = r+3; \\ r(r+2)+3, & \text{if } n = r+4; \\ 4(n-r)+r^2+3r-14, & \text{if } n \geq r+5. \end{cases}$$

$$(3)\ LM_3(P_{n-r}\overline{K_r}) = \begin{cases} r(r-1), & \text{if } n = r+1; \\ r(r+1), & \text{if } n = r+2; \\ 4(n-r)+r^2+3r-10, & \text{if } n \geq r+3. \end{cases}$$

Proposition 2.8. *The leap Zagreb indices of an F_n tree with $n \geq 5$ vertices, are given by*

$$(1)\ LM_1(FT_n) = \begin{cases} 14, & \text{if } n = 5; \\ 18, & \text{if } n = 6; \\ 4(n-1), & \text{if } n \geq 7. \end{cases}$$

$$(2)\ LM_2(FT_n) = \begin{cases} 8, & \text{if } n = 5; \\ 4n-8, & \text{if } n = 6,7; \\ 4n-7, & \text{if } n \geq 8. \end{cases}$$

(3) $LM_3(FT_n) = \begin{cases} 12, & \text{if } n = 5; \\ 4n-6, & \text{if } n \geq 6. \end{cases}$

Proposition 2.9. *The leap Zagreb indices of an H_n tree with $n \geq 7$ vertices, are given by*

(1) $LM_1(HT_n) = \begin{cases} 34, & \text{if } n = 7; \\ 38, & \text{if } n = 8; \\ 4n+8, & \text{if } n \geq 9. \end{cases}$

(2) $LM_2(HT_n) = \begin{cases} 16, & \text{if } n = 7; \\ 4n-6, & \text{if } n = 8, 9; \\ 4n-5, & \text{if } n \geq 10. \end{cases}$

(3) $LM_3(HT_n) = \begin{cases} 22, & \text{if } n = 7; \\ 4(n-1), & \text{if } n \geq 8. \end{cases}$

2.2 The leap Zagreb indices for some unicyclic graph

In this section, we will present the general formulas of the leap Zagreb indices for some special unicyclic graphs. Recall that the unicyclic graph UC_p with n vertices is a graph containing a cycle C_p with $3 \leq p \leq n$ vertices such that $d(v) \geq 2$, for every $v \in C_p$. If $UC_p - V(C_p) = P_{n-p}$, then UC_p will be denoted $P_{n-p}C_p$. A graph obtained from the triangle unicyclic graph $P_{n-3}C_3$ by joining a new vertex to any vertex of the triangle that has degree two in $P_{n-3}C_3$, is called an A-unicyclic graph and denote AU_n, see figure 2.c. While, a graph obtained from $P_{n-3}C_3$ by joining a new vertex to a neighbor of the support vertex of the pendent vertex in $P_{n-3}C_3$, is will be called F-unicyclic graph and denote FU_n, see figure 2.d. A graph obtained from the triangle or quadrangle unicyclic graph $P_{n-i}C_i$, for $i = 3, 4$, by joining a pendent vertex in $P_{n-i}C_i$ to a central vertex of P_3, is called a T_i-unicyclic graph and denote $T_{n-i}C_i$, see figure 2.e and 2.f.

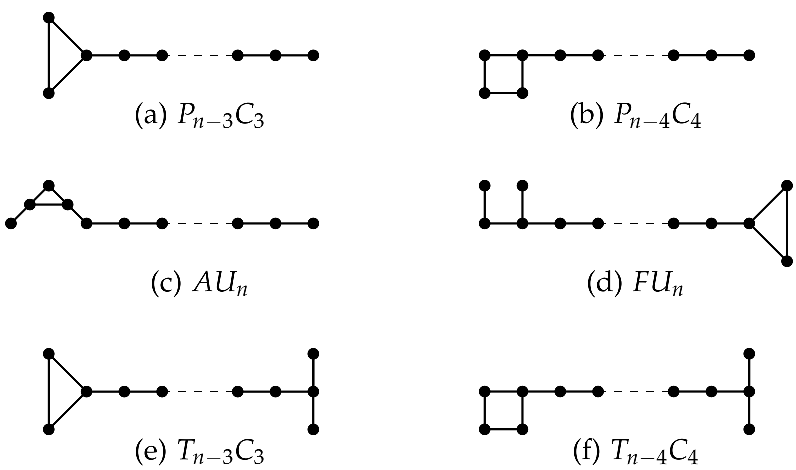


Figure 2: The triangle, quadrangle, A-, F- T_3- and T_4-unicyclic graphs.

Proposition 2.10. *For the quadrangle unicyclic $P_{n-4}C_4$ with $n \geq 4$ vertices, the leap Zagreb indices are given by*

$$(1)\ \ LM_1(P_{n-4}C_4) = \begin{cases} 4, & \textit{if } n = 4; \\ 14, & \textit{if } n = 5; \\ 18, & \textit{if } n = 6; \\ 4(n-1), & \textit{if } n \geq 7. \end{cases}$$

$$(2)\ \ LM_2(P_{n-4}C_4) = \begin{cases} 4, & \textit{if } n = 4; \\ 10, & \textit{if } n = 5; \\ 18, & \textit{if } n = 6; \\ 22, & \textit{if } n = 7; \\ 4n-5, & \textit{if } n \geq 8. \end{cases}$$

$$(3)\ \ LM_3(P_{n-4}C_4) = \begin{cases} 8, & \textit{if } n = 4; \\ 17, & \textit{if } n = 5; \\ 4n-3, & \textit{if } n \geq 6. \end{cases}$$

Proposition 2.11. *For the A-unicyclic graph AU_n with $n \geq 5$ vertices, the leap Zagreb indices are given by*

$$(1)\ \ LM_1(AU_n) = \begin{cases} 14, & \textit{if } n = 5; \\ 18, & \textit{if } n = 6; \\ 4(n-1), & \textit{if } n \geq 7. \end{cases}$$

$$(2)\ \ LM_2(AU_n) = \begin{cases} 9, & \textit{if } n = 5; \\ 16, & \textit{if } n = 6; \\ 20, & \textit{if } n = 7; \\ 4n-7, & \textit{if } n \geq 8. \end{cases}$$

$$(3)\ \ LM_3(AU_n) = \begin{cases} 14, & \textit{if } n = 5; \\ 24, & \textit{if } n = 6; \\ 4n, & \textit{if } n \geq 7. \end{cases}$$

Proposition 2.12. *For the F-unicyclic graph FU_n with $n \geq 5$ vertices, the leap Zagreb indices are given by*

$$(1)\ \ LM_1(FU_n) = \begin{cases} 24, & \textit{if } n = 8; \\ 32, & \textit{if } n = 9; \\ 4n-2, & \textit{if } n \geq 10. \end{cases}$$

$$(2)\ \ LM_2(FU_n) = \begin{cases} 5, & \textit{if } n = 8; \\ 31, & \textit{if } n = 9; \\ 4n-6, & \textit{if } n \geq 10. \end{cases}$$

$$(3)\ \ LM_3(FU_n) = \begin{cases} 26, & \textit{if } n = 8; \\ 4(n-1), & \textit{if } n \geq 9. \end{cases}$$

Proposition 2.13. *For the T_3-unicyclic graph $T_{n-3}C_3$ with $n \geq 6$ vertices, the leap Zagreb indices are given by*

(1) $LM_1(T_{n-3}C_3) = \begin{cases} 18, & \text{if } n = 6; \\ 28, & \text{if } n = 7; \\ 4n-2, & \text{if } n \geq 8. \end{cases}$

(2) $LM_2(T_{n-3}C_3) = \begin{cases} 17, & \text{if } n = 6; \\ 15, & \text{if } n = 7; \\ 22, & \text{if } n = 8; \\ 4n-11, & \text{if } n \geq 9. \end{cases}$

(3) $LM_3(T_{n-3}C_3) = \begin{cases} 20, & \text{if } n = 6; \\ 4n-6, & \text{if } n \geq 7. \end{cases}$

Proposition 2.14. *For the T_4-unicyclic graph $T_{n-4}C_4$ with $n \geq 7$ vertices, the leap Zagreb indices are given by*

(1) $LM_1(T_{n-4}C_4) = \begin{cases} 30, & \text{if } n = 7; \\ 38, & \text{if } n = 8; \\ 4n+4, & \text{if } n \geq 9. \end{cases}$

(2) $LM_2(T_{n-4}C_4) = \begin{cases} 30, & \text{if } n = 7; \\ 28, & \text{if } n = 8; \\ 34, & \text{if } n = 9; \\ 4n-3, & \text{if } n \geq 10. \end{cases}$

(3) $LM_3(T_{n-4}C_4) = \begin{cases} 29, & \text{if } n = 7; \\ 4n-1, & \text{if } n \geq 8. \end{cases}$

2.3 The leap Zagreb indices of some graphs

In this section, we present the general formulas of the leap Zagreb indices values for some graphs, which required to solve the main problem. The special case of these graphs are shown in the following figure.

$P_{n-4}\tilde{C}_4$ $P_{n-4}K_4$

Figure 3: The graphs $P_{n-4}\tilde{C}_4$ and $P_{n-q}K_q$.

Proposition 2.15. *For a graph $P_{n-4}\tilde{C}_4$ with $n \geq 4$ vertices, the leap Zagreb indices are given by*

(1) $LM_1(P_{n-4}\tilde{C}_4) = \begin{cases} 2, & \text{if } n = 4; \\ 8, & \text{if } n = 5; \\ 12, & \text{if } n = 6; \\ 4n-10, & \text{if } n \geq 7. \end{cases}$

(2) $LM_2(P_{n-4}\tilde{C}_4) = \begin{cases} 0, & \text{if } n = 4; \\ 7, & \text{if } n = 5; \\ 13, & \text{if } n = 6; \\ 17, & \text{if } n = 7; \\ 4n-10, & \text{if } n \geq 8. \end{cases}$

(3) $LM_3(P_{n-4}\tilde{C}_4) = \begin{cases} 4, & \text{if } n = 4; \\ 13, & \text{if } n = 5; \\ 4n-5, & \text{if } n \geq 6. \end{cases}$

Proposition 2.16. *For $q \geq 3$, the leap Zagreb indices of a graph $P_{n-q}K_q$ with $n \geq q+1$ vertices, are given by*

(1) $LM_1(P_{n-q}K_q) = \begin{cases} q^2-q, & \text{if } n = q+1; \\ q^2-q+2, & \text{if } n = q+2; \\ nq+4(n-q)-10, & \text{if } n \geq q+3. \end{cases}$

(2) $LM_2(P_{n-q}K_q) = \begin{cases} \frac{1}{2}(q-1)(q-2), & \text{if } n = q+1; \\ \frac{1}{2}(q-1)(q+4), & \text{if } n = q+2; \\ \frac{1}{2}q(q-1)+2q+1, & \text{if } n = q+3; \\ \frac{1}{2}q(q-1)+3(q+1)+4(n-q-4), & \text{if } n \geq q+4. \end{cases}$

(3) $LM_3(P_{n-q}K_q) = \begin{cases} q(q-1), & \text{if } n = q+1; \\ q(q+1)+4(n-q-2), & \text{if } n \geq q+2. \end{cases}$

3. Possible Values of the First Leap Zagreb Index of Graphs

By the Corollary 2.2, any graph G have to possess an even number of vertices of odd second degree. Since the square of an integer number is odd, if and only if the number itself is odd. Then the sum of squares of vertex second degrees, Equation (1), there is an even number of odd terms. Therefore, the values of the first leap Zagreb index of a graph G must be an even integer number.

Theorem 3.1. *For every non-negative even integer k, there exists a graph G, with $LM_1(G) = k$.*

Proof. For a graph G, let $LM_1(G) = k$. Since for any even non-negative integer number n, either $n \equiv 0 \ (mod\ 4)$ or $n \equiv 2 \ (mod\ 4)$. Then we consider the following two cases.

Case 1: For every non-negative integer $k \equiv 0 \ (mod\ 4)$, by Lemma 2.4, we have $LM_1(P_2) = 0$ and $LM_1(P_n) = 4(n-3)$, for every $n \geq 4$. Thus for every integer number$k \geq 4$ and $k \equiv 0 \ (mod\ 4)$, the Path P_n is the desired graph, which for it $LM_1(P_{\frac{k+12}{4}}) = k$.

Case 2: For every non-negative integer $k \equiv 2 \ (mod\ 4)$, we have the following subcases:

Subcase 2.1: For $k = 2$, by Lemma 2.4, $LM_1(P_3) = 2$.

Subcase 2.2: For $k = 6$, by Theorem 2.5, if $n = 4$, then $LM_1(P_1C_3) = 6$.

Subcase 2.3: For $k = 10$, it is easy to check that $LM_1(K_1 + P_4) = 10$.

Subcase 2.4: For $k \geq 14$, by Theorem 2.5, $LM_1(P_{n-3}C_3) = 4n - 13$. That is

$$LM_1(P_{\frac{k+13}{4}}C_3) = k.$$

Therefore, The value of the first leap Zagreb index of graphs can be any non-negative even integer. □

In the following result we investigate which integer number can be a value for the first leap Zagreb index of a tree.

Theorem 3.2. *For every non-negative even integer k, such that* $k \notin \{6, 10, 22, 26\}$, *there exists a tree T, with* $LM_1(T) = k$.

Proof. By similar arguments as in the proof of Theorem 3.1, we have the following two cases

Case 1: For every non-negative integer $k \equiv 0 \ (mod\ 4)$. By Lemma 2.4, $LM_1(P_2) = 0$ and $LM_1(P_{\frac{k+12}{4}}) = k$, for every positive integer $k \geq 4$. Thus the path P_n is the required tree.

Case 2: For every non-negative integer $k \equiv 2 \ (mod\ 4)$, we have $LM_1(P_3) = 2$ and from Proposition 2.6, $LM_1(T_4) = 14, LM_1(T_5) = 18, LM_1(T_7) = 30$ and $LM_1(T_{\frac{k-2}{4}}) = k$, for every $k \geq 32$, and $k \equiv 2 \ (mod\ 4)$.

Therefore, the value of the first leap Zagreb index of a tree can be any non-negative even integer number except $6, 10, 22, 26$. □

Theorem 3.3. *For every non-negative even integer k, such that* $k \notin \{2, 8, 12, 16\}$, *there exists a unicyclic graph G, with* $LM_1(G) = k$.

Proof. We consider the following two cases.

Case 1: For $k \equiv 0 \ (mod\ 4)$ and $k \in \{8, 12, 16\}$, we have $LM_(K_3) = 0, LM_1(C_4) = 4$ and since $LM_1(C_n) = 4n$, for every $n \geq 5$. Then $LM_1(C_{\frac{k}{4}}) = k$, for every $k \geq 20$ and $k \equiv 0 \ (mod\ 4)$.

Case 2: For $k \equiv 2 \ (mod\ 4)$. Firstly, for $k = 2$ there is no unicyclic graph UC_n, with $LM_1(UC_n) = 2$. Then for $k \geq 6$ and $k \equiv 2 \ (mod\ 4)$, the triangle unicyclic $P_{n-3}C_3$ is the desired graph. That is, by Theorem 2.5, $LM_1(P_{n-3}C_3) = 4n - 10$, for $n \geq 4$. Thus for every even integer $k \geq 6$ and $k \equiv 2 \ (mod\ 4)$, $LM_1(P_{\frac{k-2}{4}}C_3) = k$.

Therefore, for every non-negative integer k except $2, 8, 12, 16$, there are a unicyclic graph G with $LM_1(G) = k$. □

4. Possible values of the second leap Zagreb index of graphs

In this section, we solve the inverse problem for the second leap Zagreb index for graphs, where the second leap index value can be any non-negative integer except 2. Analogously, the solution of this problem for trees and unicyclic graphs are being presented.

Theorem 4.1. *For every non-negative integer k, such that $k \neq 2$, there exists a graph G, with $LM_2(G) = k$.*

Proof. Let k be a non-negative integer, such that $k \neq 2$. Then we consider the following cases.

Case 1: For $k \equiv 0\,(mod\,4)$, we have $LM_2(K_n) = 0$, for every $n \geq 0$, $LM_2(C_4) = 4$, by Proposition 2.16, $LM_2(P_2K_4) = 12$, and from Propositions 2.7, $LM_2(P_3\overline{K_2}) = 8$ and for every $k \geq 16$, $LM_2(P_{\frac{k+4}{4}}\overline{K_2}) = k$.

Case 2: For $k \equiv 1\,(mod\,4)$, by Proposition 2.5, $LM_2(P_1C_3) = 1$, so one can easy check that $LM_2(P_4 + K_1) = 5$, by Proposition 2.11, $LM_2(AU_5) = 9$, by Proposition 2.15, $LM_2(P_2\tilde{C}_4) = 13, LM_2(P_3\tilde{C}_4) = 17$, and by Propositions 2.16, $LM_2(P_{\frac{k-5}{4}}K_4) = k$, for every $k \geq 21$.

Case 3: For $k \equiv 2\,(mod\,4)$ and $k \geq 6$, by Lemma 2.4, $LM_2(P_{\frac{k+14}{4}}) = k$.

Case 4: For $k \equiv 3\,(mod\,4)$, we have $LM_2(P_4) = 3$, by Proposition 2.5, $LM_2(P_2C_3) = 7$, by Proposition 2.7, $LM_2(P_4\overline{K_2}) = 11$, and from Proposition 2.5, $LM_2(P_{\frac{k+4}{4}}C_3) = k$, for $k \geq 19$.

Therefore, For every integer $0 \leq k \neq 2$, there exists a graph G, with $LM_2(G) = k$. □

Theorem 4.2. *For every non-negative integer k, such that $k \notin \{1, 2, 4, 5, 7, 9, 13, 17, 19, 21, 31\}$, there exists a tree T, with $LM_2(T) = k$.*

Proof. For every non-negative integer k, we consider the following cases.

Case 1: For $k \equiv 0\,(mod\,4)$. Firstly, for $k = 0$, we have $LM_2(T) = 0$, for every tree T with diameter at most two. For $k = 4, 12$, by Theorem 2.3, and check all tree with $n \leq 6$, there is no any tree T, with $LM_2(T) = k$. For $k = 8$, by Proposition 2.7, with set $r = 2$, we obtained $LM_2(P_3\overline{K_2}) = 8$. Finlay, For every $k \geq 16$, the broom $P_{n-2}\overline{K_2}$, for $n \geq 7$ is the desired tree. That is by proposition 2.7, $LM_2(P_{\frac{k+12}{4}}\overline{K_2}) = k$.

Case 2: For $k \equiv 1\,(mod\,4)$, we consider the following: For $k \leq 21$, by Theorem 2.3, for every tree T, $LM_2(T) \geq LM_2(P_n)$, and by Lemma 2.4, $LM_(P_9) = 22$. Thus one can easily compute the second leap index for all tree with $n \leq 8$ vertices and check that there is no any tree T with $L_2(T) = k$. For $k \geq 25$, by Proposition 2.8, $LM_2(FT_n = 4n - 7)$ for $n \geq 8$. That is $LM_2(FT_{\frac{k+7}{4}} = k)$.

Case 3: For $k \equiv 2\,(mod\,4)$. By Theorem 4.1, there is no any graph and so, any tree T with $LM_2(T) = 2$. For $k \geq 6$, the path P_n, for $n \geq 4$ is the desired tree. That is by Lemma 2.4, $LM_2(P_{\frac{k+14}{4}}) = k$.

Case 4: For $k \equiv 3\,(mod\,4)$. Firstly, for $k = 3$, $LM_2(P_4) = 3$. For $k = 7, 19, 31$, there is no any tree T, with $LM_2(T) = k$. For $k = 11, 15, 27$, by Proposition 2.7, with set $r = 2, 3, 4$, we obtained, $LM_2(P_4\overline{K_2}) = 11$, $LM_2(P_3\overline{K_3}) = 15$ and $LM_2(P_4\overline{K_4}) = 27$. For $k = 23$, the tree shown in figure 4, is the desired tree.

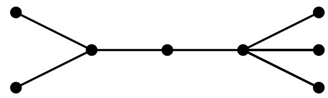


Figure 4: A tree T with $LM_2(T) = 23$.

Finally, For every $k \geq 35$, the H_n-tree with $n \geq 10$ vertices, is the desired tree, where from Proposition 2.9, for $n \geq 10$, $LM_2(HT_n) = 4n - 5$. That is $LM_2(HT_{\frac{k+5}{4}}) = k$, for every $k \geq 35$ and $k \equiv 3\,(mod 4)$. □

Theorem 4.3. *For every non-negative integer k, such that $k \notin \{2, 3, 5, 6, 8, 11, 12, 13, 14\}$, there exists a unicyclic graph UC_p, with $LM_2(UC_p) = k$.*

Proof. For every non-negative integer k, we consider the following cases.

Case 1: For $k \equiv 0\,(mod\,4)$, we obtained the following: for $k = 0$, the triangle is the desired graph. i.e., $LM_2(C_3) = 0$. For $k = 4$, $LM_2(C_4) = 4$. For $k = 8, 12$, there is no unicyclic graph G with $LM_2(G) = k$. For $k = 16$, by Proposition 2.11, $LM_2(AU_6) = 16$. Finally, for every $K \geq 20$, the cycles C_n, for $n \geq 5$ are the desired graphs. That is $LM_2(C_{\frac{k}{4}}) = k$.

Case 2: For $k \equiv 1\,(mod\,4)$, we obtained the following: for $k = 5, 13$, there is no unicyclic graph. For $k = 9$, by Proposition 2.11, $LM_2(AU_5) = 9$. For $k = 17$, by Proposition 2.13, $LM_2(T_3C_3) = 17$. For $k = 21$, the desired graph shown in figure 5,

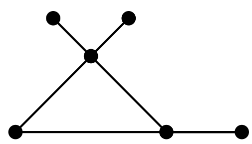


Figure 5: A unicyclic UC_3 with $LM_2(UC_3) = 21$.

For $k \geq 25$, the AU_n, for $n \geq 8$, is the desired unicyclic graph. That is by Proposition 2.11, $LM_2(AU_{\frac{k+7}{4}}) = k$.

Case 3: For $k \equiv 2\,(mod\,4)$, we obtained the following: when $k = 2, 6, 14$, there is no unicyclic graph UC_n with $LM_2(UC_n) = k$. For $k = 10, 18, 22$, by Proposition 2.10, $LM_2(P_1C_4) = 10, LM_2(P_2C_4) = 18, LM_2(P_3C_4) = 22$. For $k = 26, 30$, the desired graphs shown in the following figure.

Figure 6: The unicyclic graphs with $LM_2(G_1) = 26, LM_2(G_2) = 30$

For $k \geq 34$, by Proposition 2.12, FU_n, for $n \geq 10$, is the desired graph. That is $LM_2(FU_{\frac{k+6}{4}}) = k$.

Case 4: For $k \equiv 3\,(mod\,4)$, we obtained the following: when $k = 3, 11$, there is no unicyclic graph UC_n with $LM_2(UC_n) = k$. By proposition 2.5, for $k = 7$, $LM_2(P_2C_3) = 7$ whereas for $k \geq 15$, $LM_2(P_{\frac{k+13}{4}}C_3) = k$. □

5. Possible Values of the Third Leap Zagreb Index of Graphs

In this section, we solve the inverse problem for the third leap Zagreb index for graphs. Analogously, the solution of this problem for trees and unicyclic graphs are being presented.

Theorem 5.1. *For every non-negative integer k, such that $k \notin \{1, 3, 5, 7, 9, 11, 17\}$, there exists a graph G, such that $LM_3(G) = k$.*

Proof. Let k be a non-negative integer number. Then we have the following cases:

Case 1: For every even non-negative integer number k, since $LM_3(K_n - e) = 2(n-2)$, for $n \geq 2$, where $K_n - e$ is graph obtained from the complete graph K_n, by deleting an edge e from it. Then the graph $K_n - e$, for $n \geq 2$ is the desired graph. That is $LM_3(K_{\frac{k+4}{2}}) = k$, for every even non-negative integer k.

Case 2: For $k \equiv 1\,(mod 4)$, there is no graph G, with $LM_3(G) = k$, for $k = 1, 5, 9, 17$. For $k = 13$, by Proposition 2.15, $LM_3(P_1\tilde{C_4}) = 13$. For $k \geq 21$, by Proposition 2.10, $LM_3(P_{n-4}C_4) = 4n - 3$, for every $n \geq 6$. That is $LM_3(P_{\frac{k+3}{4}}C_4) = k$.

Case3: For $k \equiv 3\,(mod 4)$, there is no graph G, with $LM_3(G) = k$, for $k = 3, 7, 11$. For $k = 15$, by Proposition 2.10, $LM_3(P_1C_4) = 15$. For $k \geq 19$ by Proposition 2.15, $LM_3(P_{n-4}\tilde{C_4}) = 4n - 5$, for every $n \geq 6$. That is $LM_3(P_{\frac{k+5}{4}}\tilde{C_4}) = k$, for every $k \geq 19$. □

From Theorem 10 in [14], if G is a C_3, C_4-free graph, then $LM_3(G) = 2M_2(G) - M_1(G)$, and since the value of $M_1(G)$ is even. Then the third leap Zagreb index of any triangle- and quadrangle-free graph is always even. Hence the following result follows.

Theorem 5.2. *For every even non-negative integer k, such that $k \notin \{4, 8\}$, there exists a tree T, with $LM_3(T) = k$.*

Proof. For every even non-negative integer k, we have the following two cases.

Case 1: For $k \equiv 0\,(mod\,4)$, we have $LM_3(P_2) = 0$. For $k = 4, 8$, there is no tree with $LM_3(T) = k$. For $k \geq 12$, the broom $P_{n-2}\overline{K_2}$, for $n \geq 5$ and $r = 2$, is the desired tree, where from Proposition 2.7, by setting $r = 2$, we have $LM_3(P_{n-2}\overline{K_2}) = 4n - 8$. That is $LM_3(P_{\frac{k}{4}}\overline{K_2}) = k$, for every $k \geq 12$.

Case 2: For $k \equiv 2\,(mod\,4)$, the path P_n, for $n \geq 3$, is the desired tree, where from Lemma 2.4, $LM_3(P_3) = 2$ and $LM_3(\frac{k+10}{4}) = k$. □

Theorem 5.3. *For every non-negative integer k, such that $k \notin \{1,2,3,4,5,7,9,10,11,13,17,18,19,23,27\}$, there exists a unicyclic graph UC_n, with $LM_3(UC_n) = k$.*

Proof. For every non-negative integer k, we consider the following cases.

Case 1: For $k \equiv 0\,(mod\,4)$, we have $LM_3(C_3) = 0$. For $k = 4$, there is no unicyclic graph UC_n with $LM_3(UC_n) = 4$. For $k = 8$, $LM_3(C_4) = 8$. For $k \geq 12$, the triangle unicyclic $P_{n-2}C_3$, for $n \geq 5$, is the desired tree, where from Theorem 2.5, we have $LM_3(P_{n-3}C_3) = 4n - 8$. That is $LM_3(P_{\frac{k}{4}}C_3) = k$, for every $k \geq 12$.

Case 2: For $k \equiv 1\,(mod\,4)$, there is no a unicyclic graph with $LM_3(UC_n) = k$ for every $k \in \{1,5,9,13,17\}$, whereas for $k \geq 21$, the quadrangle unicyclic $P_{n-4}C_4$, for $n \geq 6$, is the desired unicyclic, where from Proposition 2.10, $LM_3(P_{n-4}C_4) = 4n - 3$. That is $LM_3(P_{\frac{k+3}{4}}C_4) = k$, for every $k \geq 21$.

Case 3: For $k \equiv 2\,(mod\,4)$, there is no unicyclic graph with $LM_3(UC_n) = k$, for $k \in \{2,10,18\}$. For $k = 6$, by Theorem 2.5, $LM_3(P_1C_3) = 6$. For $k = 14$, by Proposition 2.11, $LM_3(AU_5) = 14$. For $k \geq 22$, the T_3-unicyclic is the desired graphs, where from proposition 2.13, $LM_3(T_{n-3}C_3) = 4n - 6$, for $n \geq 7$. That is $LM_3(T_{\frac{k-6}{4}}C_3) = k$, for every $k \geq 22$.

Case 4: For $k \equiv 3\,(mod\,4)$, there is no unicyclic graph with $LM_3(UC_n) = k$, for every $k \in \{3,7,11,19,23,27\}$. For $k \geq 31$, the T_4-unicyclic graph with $n \geq 8$ vertices is the desired graph,where from Proposition 2.14, we have $LM_3(T_{n-4}C_4) = 4n - 1$, for $n \geq 8$. That is $LM_3(T_{\frac{k-15}{4}}C_4) = k$, for every $k \geq 31$. □

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