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Leap neighbourhood Zagreb indices and coindices of graphs

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Abstract

This study investigates and defines a novel vertex degree-based topological index, specifically the Leap Neighbourhood Zagreb indices and coindices of a graph R. These indices are distance-degree-based topological indices derived from the second degrees of vertices, which refer to the number of second neighbours associated with each vertex. The precise formulas for certain standard graphs are computed. The relationships between

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the Leap Neighbourhood Zagreb Indices, each of the Leap Zagreb indices, and the Zagreb indices are established. Finally, the lower and upper bounds are determined.

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1. Introduction

This study focuses on simple connected graphs, where $R = (V, E)$ denotes a graph with vertex set $V(R)$ and edge set $E(R)$. The order $h = |V|$ represents the number of vertices, while the size $k = |E|$ indicates the number of edges in R. The distance $d(x, y)$ between any two vertices x and y in a graph R is delineated as the length of the shortest path connecting them, measured in edges.

Let x represent a vertex in $V(R)$ and i denote a positive integer. The open i-neighbourhood of x in the graph R, represented as $N_i(x/R)$, is delineated as the set

$$N_i(x/R) = \{y \in V(R): d(x, y) = i\}.$$

The i-distance degree of a vertex x in R, denoted as $d_i(x/R)$ (or $d_i(x)$), signifies the number of i-neighbours of vertex x in R, formally articulated as

$$d_i(x/R) = |N_i(x/R)|,$$

with the particular instance $d_1(x/R) = d(x/R)$ applicable to all $x \in V(R)$.

A graph with the same vertex set as a graph R is called its complement $\overline{R}$. Two vertices are adjacent in $\overline{R}$ if and only if they are not adjacent in R. The graph $\overline{K_n}$ denotes the null graph, characterised by the absence of edges connecting any pair of vertices.

For a vertex x in R, the eccentricity is delineated as $e(x) = \max\{d(x, y): y \in V(R)\}$. The diameter of R is delineated as $\operatorname{diam}(R) = \max\{e(x): x \in V(R)\}$, whereas the radius r of R is calculated as $r = \min\{e(x): x \in V(R)\}$.

For any definitions or notations not addressed above, we refer to [1].

The neighbourhood of a vertex x and an edge e in R are delineated respectively as $N_R(x) = \{y \in V(R): y$ is adjacent to x in $R\}$ and $N_R(e) = \{h \in E(R): h$ is adjacent to e in $R\}$.The closed neighbourhood of a vertex x is delineated as $N_R[x] = N_R(x) \cup \{x\}$. The neighbourhood degree sum of a vertex x is delineated as,

$$\delta_R(x) = \sum_{y \in N_R(x)} d_R(y).$$

Current mathematical and mathematical–chemical literature investigates various vertex-degree-based graph invariants [2, 3, 4, 5] and their applications in chemistry. The first (M_1) and second (M_2) Zagreb indices are the most thoroughly examined, having been established over forty years ago [6, 7], and are delineated as follows:

$$M_1 = M_1(R) = \sum_{x\in V(R)} d_1^2(x/R) = \sum_{xy\in E(R)} (d_R(x) + d_R(y))$$

and

$$M_2 = M_2(R) = \sum_{xy\in E(R)} d(x/R)\, d(y/R).$$

Refer to [8, 9, 10, 11] and the associated citations for the features of the two Zagreb indices. Recently, several new varieties of Zagreb indices have been introduced, including Zagreb coindices [12], reformulated Zagreb indices [13], reverse Zagreb indices [14], reverse Zagreb indices of F-sum of graphs [15], Leap Zagreb indices [16], and Leap Zagreb coindices [17], among others.

For a graph R, the first and second leap Zagreb indices are delineated as follows:

$$LM_1 = LM_1(R) = \sum_{x\in V(R)} d_2^2(x/R)\,,$$

$$LM_2 = LM_2(R) = \sum_{xy\in E(R)} d_2(x/R)\cdot d_2(y/R)\,.$$

The neighbourhood first Zagreb index $NM_1(R)$ [18] and the neighbourhood second Zagreb index $NM_2(R)$ [19] for a graph R are delineated as follows:

$$NM_1(R) = \sum_{x\in V(R)} \delta^2(x/R)$$

$$NM_2(R) = \sum_{xy\in E(R)} \delta(x/R)\, \delta_R(y/R)\,.$$

The fifth Zagreb index $M'(R)$[20], the first $\overline{M_1}(R)$, the second $\overline{M_2}(R)$, and the fifth $\overline{M'}(R)$ Zagreb coindex are delineated as follows:

$$M'(R) = \sum_{xy\in E(R)} (\delta_R(x) + \delta_R(y))\,,$$

$$\overline{M_1}(R) = \sum_{xy\notin E(R)} (d_R(x) + d_R(y))\,,$$

$$\overline{M_2}(R) = \sum_{xy\notin E(R)} d_1(x/R)\, d_1(y/R)\,,$$

$$\overline{M'}(R) = \sum_{xy\notin E(R)} (\delta_R(x) + \delta_R(y)).$$

This study seeks to expand the concept of Zagreb indices, particularly Leap Zagreb indices, to analogous graph invariants derived from second vertex degree neighbourhoods. We propose designating these graph invariants as the Leap Neighbourhood Zagreb Indices. The essential results enumerated below will be utilised in numerous subsequent analyses:

Lemma 1: [21] *If $R = (V, E)$ is a graph then,*

$$\overline{M_1}(R) = 2k(h-1) - M_1(R)$$

$$M_2(\overline{R}) = \tfrac{1}{2}h(h-1)^3 - 3k(h-1)^2 + 2k^2 + \tfrac{2h-3}{2}M_1(R) - M_2(R)$$

$$\overline{M_2}(R) = 2k^2 - \tfrac{1}{2}M_1(R) - M_2(R)$$

$$\overline{M_2}(\overline{R}) = k(h-1)^2 - (h-1)M_1(R) + M_2(R).$$

Lemma 2: [19] *For a Graph R,*

$$M_1(R) = \sum_{x\in V(R)} \delta(x/R)$$

and

$$M'(R) = \sum_{xy\in E(R)} (\delta(x/R) + \delta(y/R)) = 2M_2(R).$$

Lemma 3: [22, 23] *Let* $R = (V, E)$ *be a graph then,*

$$d_2(x/R) \le \left(\sum_{y\in N(x/R)} d_1(y/R)\right) - d_1(x/R)\,,$$

where equality holds in the particular inequality if and only if R is a $\{C_3, C_4\}$*-free.*

From lemma 3, it follows,

Corollary 1: *Let R be a graph with no cycles of* C_3 *and* C_4 *with* $h = |V(R)|$. *Then,*

$$d_2(x/R) = h(h-1)\,.$$

Lemma 4: [23] *For a graph R of order h. Then for any* $x \in V(R)$

$$d_2(x/R) \le h + 1 - d_1(x/R) - e(x/R)\,.$$

2. Leap Neighbourhood Zagreb Indices

Definition 1:

$$\delta_{L_N}(x/R) = \sum_{y\in N(x/R)} d_2(y/R)\,.$$

Based on this definition, the authors further propose a new family of topological indices delineated the leap neighbourhood Zagreb indices, denoted by $L_N M(R)$ is delineated as follows.

For a graph R, the Leap Neighbourhood Zagreb indices are

$$L_N M_1 = L_N M_1(R) = \sum_{x\in V(R)} \delta_{L_N}^2(x)\,,$$
$$L_N M_2 = L_N M_2(R) = \sum_{xy\in E(R)} \delta_{L_N}(x)\cdot\delta_{L_N}(y) \text{ and}$$
$$L_N M_3 = L_N M_3(R) = \sum_{xy\in E(R)} \delta_{L_N}(x) + \delta_{L_N}(y)\,.$$

Theorem 1: *Let R be a graph with h vertices; then, for any vertex* $x \in V(R)$*,*

$$\delta_{L_N}(x) \le d_1(x/R)(h+1) - \sum_{y\in N(x)} [d_1(y/R) + e(y/R)]\,.$$

Proof: Consider,

$$\begin{aligned}\delta_{L_N}(x) &= \sum_{y\in N(x)} d_2(y)\\ &\le \sum_{y\in N(x)} ((h+1) - d_1(y/R) - e(y/R))\\ &\le d_1(x/R)(h+1) - \sum_{y\in N(x)} [d_1(y/R) + e(y/R)].\end{aligned}$$

Corollary 2: *Let R be a graph with no cycles of C_3 and C_4 with $h = |V(R)|$. Then for any x ∈ V(R),*

$$\delta_{L_N}(x) \leq (h+1)(d_1(x/R)-1) + e(x/R) - \sum_{y \in N(x)} e(y/R)\,.$$

Corollary 3: *Let R be a graph with no cycles of C_3 and C_4 with $h = |V(R)|$. Then for any x ∈ V(R) with $diameter(R) \leq 2$*

$$\delta_{L_N}(x) \leq (h-1)\,[d_1(x/R)-1]\,.$$

Corollary 4: *Let R be a graph with no cycles of C_3 and C_4 with $h = |V(R)|$, $k = |E(R)|$ and radius r with $diameter(R) \geq 3$. Then*

$$\delta_{L_N}(x) \leq (h+1-r)(d_1(x/R)-1) + r\,.$$

3. Leap Neighbourhood Zagreb Indices of certain graph families

For the graphs K_n and $(\overline{K_n}), n \geq 1$, we get

$$L_N M_i(K_n) = L_N M_i(\overline{K_n}) = 0, \text{where } i = 1,2,3.$$

For the star $S_{1,r}, r \geq 3$, we get

$$\begin{aligned} L_N M_1(S_{1,r}) &= r^2(r-1)^2 \\ L_N M_2(S_{1,r}) &= 0 \\ L_N M_3(S_{1,r}) &= r^2(r-1). \end{aligned}$$

For the cycle C_h,

Case 1: If $h = 3$ then $C_3 = K_3$.

Case 2: If $h = 4$ then

$L_N M_1(C_4) = L_N M_2(C_4) = L_N M_3(C_4) = 16.$

Case 3: If $h > 4$ we get,

$$\begin{aligned} L_N M_1(C_h) &= 16h \\ L_N M_2(C_h) &= 16h \\ L_N M_3(C_h) &= 8h. \end{aligned}$$

For the path P_h, where $h \geq 3$, we obtain

$$L_N M_1(P_h) = \begin{cases} 4 & \text{if } h = 3 \\ 10 & \text{if } h = 4 \\ 24 & \text{if } h = 5 \\ 2(8h-29) & \text{if } h \geq 6 \end{cases}$$

$$L_N M_2(P_h) = \begin{cases} 0 & \text{if } h = 3 \\ 8 & \text{if } h = 4 \\ 3(5h-19) & \text{if } h = 5,6,7 \\ 16(h-4) & \text{if } h \geq 8 \end{cases}$$

$$L_N M_3(P_h) = \begin{cases} 4 & \text{if } h = 3 \\ 2(4h-11) & \text{if } h \geq 4\,. \end{cases}$$

For the complete bipartite graph, $K_{p,q}$ where $q \geq p \geq 1$, we get

$$\begin{aligned} L_N M_1(K_{p,q}) &= pq[q(q-1)^2 + p(p-1)^2] \\ L_N M_2(K_{p,q}) &= p^2 q^2 [(p-1)(q-1)] \\ L_N M_3(K_{p,q}) &= pq[p(p-1) + q(q-1)]\,. \end{aligned}$$

For the wheel graph $W_{1,h} = K_1 + C_h$, where $h \geq 3$, we get

$$\begin{aligned} L_N M_1(W_{1,h}) &= h(h+4)(h-3)^2 \\ L_N M_2(W_{1,h}) &= 2h(h+2)(h-3)^2 \\ L_N M_3(W_{1,h}) &= h(h+6)(h-3)\,. \end{aligned}$$

For a $\{C_3, C_4\}$-free m-regular graph of order h, we get

$$\begin{aligned} L_N M_1(R) &= hm^4(m-1)^2 \\ L_N M_2(R) &= \frac{hm^5}{2}(m-1)^2 \\ L_N M_3(R) &= hm^3(m-1)\,. \end{aligned}$$

4. Certain attributes of the Leap Neighbourhood Zagreb Indices

Theorem 2: *Let R be a graph of order h and size k. Then*

$$L_N M_1(R) \leq (h-1)^2[M_1(R) - 4k + h] \tag{1}$$

$$L_N M_2(R) \leq (h-1)^2[M_2(R) - M_1(R) + k] \tag{2}$$

$$L_N M_3(R) \leq (h-1)[M_1(R) - 2k] \tag{3}$$

equality is satisfied if and only if R is free of $\{C_3, C_4\}$ and has a diameter of at most two.

Proof: We prove the inequality (1). Consider ,

$$\begin{aligned} L_N M_1(R) &= \textstyle\sum_{x \in V(R)} \delta_{L_N}^2(x/R) \\ &\leq \textstyle\sum_{x \in V(R)} (h-1)^2[d_1(x/R) - 1]^2 \\ &= \textstyle\sum_{x \in V(R)} (h-1)^2[d_1^2(x/R) - 2\,d_1(x/R) + 1] \\ &= (h-1)^2[M_1(R) - 4k + h] \\ L_N M_1(R) &\leq (h-1)^2[M_1(R) - 4k + h]\,. \end{aligned}$$

The proofs of the inequalities (2) and (3) are analogous to that of (1).

Theorem 3: [23] *Let R be a graph with no cycles of C_3 and C_4 with $h = |V(R)|$, $k = |E(R)|$ and radius r. Then*

$$M_1(R) \leq h(h+1-r) \tag{4}$$

$$M_2(R) \leq k(h+1-r) \tag{5}$$

where equalities in (4) and (5) hold if and only if R is a Moore graph of diameter two or $R = C_6$.

Theorem 4: *Let R be a graph with h vertices, k edges and radius r. Then*

$$L_N M_1(R) \leq (h+1-r)^2 M_1(R) - 4k(h+1-r)(h+1-2r) + h(h+1-2r)^2.$$

Proof: From corollary 4,

$$\begin{aligned}
L_N M_1(R) &= \textstyle\sum_{x\in V(R)} \delta_{L_N}^2(x/R) \\
&\leq \textstyle\sum_{x\in V(R)} [(d_1(x/R)-1)(h+1-r)+r]^2 \\
&= \textstyle\sum_{x\in V(R)} [d_1(x/R)(h+1-r)-(h+1-r)+r]^2 \\
&= \textstyle\sum_{x\in V(R)} [d_1(x/R)(h+1-r)-(h+1-2r)]^2 \\
&= \textstyle\sum_{x\in V(R)} [d_1^2(x/R)(h+1-r)^2 \\
&\quad -2d_1(x/R)(h+1-r)(h+1-2r)+(h+1-2r)^2]
\end{aligned}$$

$$L_N M_1(R) \leq (h+1-r)^2 M_1(R) - 4k(h+1-r)(h+1-2r) + h(h+1-2r)^2.$$

Corollary 5: *Let R be a connected graph that contains no of cycles* C_3 *and* C_4*, with h vertices, k edges, and a radius r. Then*

$$L_N M_1(R) \leq (h+1-r)[h(h+1-r)^2 - 4k(h+1-2r)] + h(h+1-2r)^2.$$

Theorem 5: *Let R be a graph of order h, size k and radius r. Then*

$$\begin{aligned}
L_N M_2(R) &\leq (h+1-r)^2[M_2(R)-M_1(R)+k] \\
&\quad +r(h+1-r)[M_1(R)-2k]+kr^2.
\end{aligned}$$

Proof: From corollary 4,

$$\begin{aligned}
L_N M_2(R) &= \textstyle\sum_{xy\in E(R)} [\delta_{L_N}(x/R)\cdot\delta_{L_N}(y/R)] \\
&\leq \textstyle\sum_{xy\in E(R)} [(d_1(x/R)-1)(h+1-r)+r] \\
&\quad \times [(d_1(y/R)-1)(h+1-r)+r] \\
&= \textstyle\sum_{xy\in E(R)} (h+1-r)^2(d_1(x/R)-1)(d_1(y/R)-1) \\
&\quad +r(h+1-r)(d_1(x/R)-1) \\
&\quad +r(h+1-r)(d_1(x/R)-1)+r^2 \\
&= \textstyle\sum_{xy\in E(R)} (h+1-r)^2(d_1(x)\,d_1(y)-d_1(x)-d_1(y)+1) \\
&\quad +r(h+1-r)(d_1(x/R)+d_1(y/R)-2)+r^2 \\
L_N M_2(R) &\leq (h+1-r)^2[M_2(R)-M_1(R)+k] \\
&\quad +r(h+1-r)[M_1(R)-2k]+kr^2.
\end{aligned}$$

Corollary 6: *Let R be a graph that is free of cycles* C_3 *and* C_4 *with h vertices, k edges and radius r. Then*

$$\begin{aligned}
L_N M_2(R) &\leq k(h+1-r)^3 + (h+1-r)^2\left[\frac{-4k^2}{h}+k+hr\right] \\
&\quad +kr[r-2(h+1-r)]\,.
\end{aligned}$$

Theorem 6: *Let R be a graph with h vertices, k edges and radius r. Then*

$$L_N M_3(R) \leq (h+1-r)M_1(R) - 2k(h+1-r) + 2kr\,.$$

Proof: From corollary 4,

$$\begin{aligned} L_N M_3(R) &= \textstyle\sum_{xy\in E(R)} [\delta_{L_N}(x/R) + \delta_{L_N}(y/R)] \\ &\le \textstyle\sum_{xy\in E(R)} [(h+1-r)(d_1(x/R)-1)+r] \\ &+[(h+1-r)(d_1(y/R)-1)+r] \\ &= \textstyle\sum_{xy\in E(R)} (h+1-r)(d_1(x/R)+d_1(y/R)-2)+2r \\ L_N M_3(R) &\le (h+1-r)M_1(R) - 2k(h+1-r) + 2kr\,. \end{aligned}$$

Corollary 7: *Let R be a graph that is free of cycles* C_3 *and* C_4 *with h vertices, k edges and radius r. Then,*

$$L_N M_3(R) \le (h+1-r)[h(h+1-r)-2k] + 2kr\,.$$

5. Some observations and results regarding complementary graphs

Proposition 1: For the complete bipartite graph $(K_{h,g}), h, g \ge 1,$ we get

$$L_N M_1(R) = hg\; M_1(\overline{R}).$$

For the wheel graph $W_{1,h} = K_1 + C_h$, where, we get

$$L_N M_1(R) = (h+4)\; M_1(\overline{R}).$$

For the platonic graphs (i.e., cube, tetrahedron, octahedron, dodecahedron and icosahedron), we get

$$L_N M_1(R) \le (3h-2)\; M_1(\overline{R}).$$

The equality holds for tetrahedral and octahedral graphs.

For the crown graph $(C_{h,h}), h \ge 1,$ we get

$$L_N M_1(R) \le (h-1)^2\; M_1(\overline{R}).$$

For any other graph which is not mentioned above the following inequality holds,

$$L_N M_1(R) \le (h-1)\; M_1(\overline{R}).$$

Note that, $C_4 = K_{2,2}$, star graph of n vertices is $K_{1,h-1}$ complete bipartite graph and the above equality holds for Moore graph of diameter two

Theorem 7: [16] *Let R be a graph with h vertices. Then*

$$d_2(x/\overline{R}) \le d_1(x/R)\,.$$

Proof:

$$\begin{aligned} d_2(x/\overline{R}) &\le h-1-d_2(x/R) \\ &\le h-1-(h-1-d_1(x/R)) \\ &\le d_1(x/R)\,. \end{aligned}$$

Corollary 8: *Let R be a graph. Then*

$$\delta_{L_N}(x/\overline{R}) \le \delta_{\overline{N}}(x/R)\,.$$

and

$$\delta_{L_N}(x/R) \le \delta_{\overline{N}}(x/\overline{R}) .$$

Corollary 9: *Let R be a graph with h vertices and k edges. Then,*

$$\delta_{L_N}(x/\overline{R}) \le 2k - \delta_N(x/R) - d(x/R) .$$

and

$$\delta_{L_N}(x/R) \le h(h-1) - 2k - \delta_N(x/\overline{R}) - d(x/\overline{R}) .$$

Theorem 8: *Let* $R = (V, E)$ *be a graph, then*

$$\sum_{x\in\overline{R}} \delta_{L_N}(x) \le \overline{M_1}(R) .$$

The equality holds for all Path graphs (except P_3 and P_4), Cyclic graphs (except C_4), Platonic graphs (except octahedral), and Petersen graph.

Proof: From corollary 9,

$$\begin{aligned}
\sum_{x\in\overline{R}} \delta_{L_N}(x) &\le \sum_{x\in R} (2k - \delta_N(x/R) - d(x/R)) \\
&= \sum_{x\in R} 2k - \sum_{x\in R} \delta_N(x/R) - \sum_{x\in R} d(x/R) \\
&= 2hk - M_1(R) - 2k \\
&= 2k(h-1) - M_1(R) \\
\sum_{x\in\overline{R}} \delta_{L_N}(x) &\le \overline{M_1}(R) .
\end{aligned}$$

Theorem 9: *Let R be a graph with h vertices and k edges. Then,*

$$L_N M_1(\overline{R}) \le 4k^2(h-2) + NM_1(R) + 4M_2(R) - (4k-1)M_1(R) .$$

The equality holds for all Path graphs (except P_3 *and* P_4*), Cyclic graphs (except* C_4*), Platonic graphs (except octahedral), and Petersen graph.*

Proof: From corollary 9

$$\begin{aligned}
\delta_{L_N}^2(x/\overline{R}) &\le (2k - \delta_N(x/R) - d(x/R))^2 \\
&= 4k^2 + \delta_N^2(x) + d^2(x) - 4k\,\delta_N(x) \\
&\quad +2\,\delta_N(x)\,d(x) - 4k\,d(x)
\end{aligned}$$

$$\begin{aligned}
\sum_{x\in V(R)} \delta_{L_N}^2(x/\overline{R}) &\le \sum_{x\in V(R)} (4k^2 + \delta_N^2(x) + d^2(x) - 4k\,\delta_N(x) \\
&\quad +2\,\delta_N(x)\,d(x) - 4k\,d(x)) \\
&= 4k^2h + NM_1(R) + M_1(R)(1-4k) \\
&\quad +2(2M_2(R)) - 8k^2 \\
L_N M_1(\overline{R}) &\le (h-2)4k^2 + NM_1(R) + 4M_2(R) - (4k-1)M_1(R) .
\end{aligned}$$

Theorem 10: *Let R be a graph with h vertices and k edges. Then*

$$\sum_{x\in R} \delta_{L_N}(x) \le h(h-1)^2 - 2k(h-1) - M_1(\overline{R}) .$$

The equality holds for the graphs with $diameter \le 2$.

Proof: From corollary 9,

$$\begin{aligned}\textstyle\sum_{x\in R}\delta_{L_N}(x/R) &\le \textstyle\sum_{x\in\overline{R}}\left(h(h-1)-2k-\delta_N(x/\overline{R})-d(x/\overline{R})\right)\\ &= \textstyle\sum_{x\in\overline{R}}[h(h-1)-2k]-\sum_{x\in\overline{R}}\delta_N(x/\overline{R})-\sum_{x\in\overline{R}}d(x/\overline{R})\\ &= h[h(h-1)-2k]-M_1(\overline{R})-[h(h-1)-2k]\\ &= [h(h-1)-2k](h-1)-M_1(\overline{R})\end{aligned}$$

$$\textstyle\sum_{x\in R}\delta_{L_N}(x/R) \le h(h-1)^2-2k(h-1)-M_1(\overline{R})\,.$$

Theorem 11: *Let* $R=(V,E)$ *with* $h=|V(R)|$ *and* $k=|E(R)|$. *Then,*

$$\begin{aligned}L_NM_1(R) &\le (h-2)[h(h-1)-2k]^2+NM_1(\overline{R})+4M_2(\overline{R})\\ &\quad -M_1(\overline{R})\{2[h(h-1)-2k]-1\}\,.\end{aligned}$$

The equality holds for the graphs with $diameter \le 2$.

Proof: From corollary 9

$$\begin{aligned}\delta_{L_N}^2(x/R) &\le \left(h(h-1)-2k-\delta_N(x/\overline{R})-d(x/\overline{R})\right)^2\\ &\le [h(h-1)-2k]^2+\delta_N^2(x/\overline{R})+d^2(x/\overline{R})\\ &\quad -2[h(h-1)-2k]\,\delta_N(x/\overline{R})\\ &\quad +2\,\delta_N(x/\overline{R})\,d(x/\overline{R})-2[h(h-1)-2k]\,d(x/\overline{R})\end{aligned}$$

$$\begin{aligned}\textstyle\sum_{x\in V(R)}\delta_{L_N}^2(x/R) &\le \textstyle\sum_{x\in V(R)}[h(h-1)-2k]^2+\sum_{x\in V(R)}\delta_N^2(x/\overline{R})\\ &\quad +\textstyle\sum_{x\in V(R)}d^2(x/\overline{R})-2[h(h-1)-2k]\sum_{x\in V(R)}\delta_N(x/\overline{R})\\ &\quad +2\textstyle\sum_{x\in V(R)}\delta_N(x/\overline{R})\,d(x/\overline{R})\\ &\quad -2[h(h-1)-2k]\textstyle\sum_{x\in V(R)}d(x/\overline{R})\end{aligned}$$

$$\begin{aligned}L_NM_1(R) &\le h[h(h-1)-2k]^2+NM_1(\overline{R})+M_1(\overline{R})\\ &\quad -2[h(h-1)-2k]M_1(\overline{R})+2(2M_2(\overline{R}))\\ &\quad -2[h(h-1)-2k]^2\end{aligned}$$

$$\begin{aligned}L_NM_1(R) &\le (h-2)[h(h-1)-2k]^2+NM_1(\overline{R})+4M_2(\overline{R})\\ &\quad -M_1(\overline{R})\{2[h(h-1)-2k]-1\}\,.\end{aligned}$$

6. Leap Neighbourhood Zagreb coindices

Theorem 12: *Let R be a graph, then*

$$L_NM_1(R)=\textstyle\sum_{xy\in E(R)} d_2(x)\,\delta_{L_N}(y)+d_2(y)\,\delta_{L_N}(x)\,.$$

Proof:

$$\begin{aligned}L_NM_1(R) &= \textstyle\sum_{x\in V(R)}\delta_{L_N}^2(x)\\ &= \textstyle\sum_{x\in V(R)}\delta_{L_N}(x)\,\delta_{L_N}(x)\end{aligned}$$

$$= \sum_{x\in V(R)} \delta_{L_N}(x)\left(\sum_{y\in N(x/R)} d_2(y)\right)$$
$$= \sum_{xy\in E(R)} d_2(x)\,\delta_{L_N}(y) + d_2(y)\,\delta_{L_N}(x)\,.$$

Based on the above theorem, we define the Leap Neighbourhood Zagreb coindices as follows:
Let R be a graph,then

$$\overline{L_N M_1}(R) = \sum_{xy\notin E(R)} [d_2(x)\,\delta_{L_N}(y) + d_2(y)\,\delta_{L_N}(x)]\,,$$
$$\overline{L_N M_2}(R) = \sum_{xy\notin E(R)} \delta_{L_N}(x)\,\delta_{L_N}(y) \text{ and}$$
$$\overline{L_N M_3}(R) = \sum_{xy\notin E(R)} [\delta_{L_N}(x) + \delta_{L_N}(y)]\,.$$

7. Leap Neighbourhood Zagreb Coindices of certain graph families

For K_h, where $h \geq 1$ we obtain

$$\overline{L_N M_i}(K_h) = \overline{L_N M_i}(\overline{K_h}) = 0, \text{where } i = 1,2,3.$$

For the star $S_{1,r}, r \geq 3$, we get

$$\overline{L_N M_i}(S_{1,r}) = 0, \text{where } i = 1,2,3.$$

For the cycle C_h,

Case 1: If $h = 3$ then $C_3 = K_3$.

Case 2: If $h = 4$ then

$$L_N M_1(C_4) = L_N M_2(C_4) = L_N M_3(C_4) = 8.$$

Case 3: If $h > 4$ we get,

$$\overline{L_N M_1}(C_n) = 8h(h-3)$$
$$\overline{L_N M_2}(C_n) = 8h(h-3)$$
$$\overline{L_N M_3}(C_n) = 4h(h-3).$$

For the path $P_h, h \geq 3$, we get

$$\overline{L_N M_1}(P_h) = \begin{cases} 0 & \text{if } h = 3 \\ 8 & \text{if } h = 4 \\ (h-3)(7h-26)+6 & \text{if } 5 \leq h \leq 7 \\ 4(h-7)(2h-1)+98 & \text{if } h \geq 8\,. \end{cases}$$

$$\overline{L_N M_2}(P_h) = \begin{cases} 0 & \text{if } h = 3 \\ 5 & \text{if } h = 4 \\ \dfrac{h-5}{2}[15h-38]+20 & \text{if } h = 5,6,7 \\ 8(h-1)(h-7)+87 & \text{if } h \geq 8\,. \end{cases}$$

$$\overline{L_N M_3}(P_h) = \begin{cases} 0 & \text{if } h = 3 \\ 2[(h-3)(2h-5)]+2 & \text{if } h \geq 4\,. \end{cases}$$

For the complete bipartite graph, $K_{p,q}, q \geq p \geq 1$, we get

$$\overline{L_N M_1}(K_{p,q}) = pq[(p-1)(q-1)(p+q-2)]$$
$$\overline{L_N M_2}(K_{p,q}) = \frac{pq(p-1)(q-1)}{2}[q(q-1)+p(p-1)]$$
$$\overline{L_N M_3}(K_{p,q}) = 2pq(p-1)(q-1)\,.$$

For the wheel graph $W_{1,h} = K_1 + C_h$, where $h \geq 3$, we get

$$\overline{L_N M_1}(W_{1,h}) = 2h(h-3)^3$$
$$\overline{L_N M_2}(W_{1,n}) = 2h(h-3)^3$$
$$\overline{L_N M_3}(W_{1,n}) = 2h(h-3)^2\,.$$

Let R be a graph with no cycles of C_3 and C_4, m-regular of order h, then

$$\overline{L_N M_1}(R) = hm^3(h-m-1)(m-1)^2$$
$$\overline{L_N M_2}(R) = \frac{hm^4}{2}(h-m-1)(m-1)^2$$
$$\overline{L_N M_3}(R) = hm^2(h-m-1)(m-1)\,.$$

8. Certain attributes of the Leap Neighbourhood Zagreb Coindices

Lemma 5: [24] *Let R be a graph with h vertices and k edges. Then,*

$$\overline{NM_1}(R) = 2kM_1(R) - 2M_2(R) - NM_1(R)\,.$$

Lemma 6: [24] *Let R be a graph of order h and size k. Then,*

$$\overline{NM_2}(R) = \tfrac{1}{2}[M_1(R)^2 - NM_1(R)] - NM_2(R)\,.$$

Lemma 7: [24] *For a graph R with h vertices,*

$$\overline{M'}(R) = (h-1)M_1(R) - 2M_2(R)\,.$$

Theorem 13: *Let R be a graph with $V(R) = h$ and $E(R) = k$. Then,*

$$\overline{L_N M_1}(R) \leq [M_1(R) - 2k][h(h-1)^2 - 2k(h-1) - M_1(\overline{R})]$$
$$-2LM_2(R) - L_N M_1(R)\,.$$

Proof: Consider,

$$\begin{aligned}
L_N M_1(R) + \overline{L_N M_1}(R) &= \textstyle\sum_{\{x,y\}\subseteq V(R)} \left(d_2(x)\,\delta_{L_N}(y) + \delta_{L_N}(x)\,d_2(y)\right) \\
&= \textstyle\sum_{y\in V(R)} \delta_{L_N}(y)\left(\sum_{x\in V(R)} d_2(x) - d_2(y)\right) \\
&\leq \textstyle\sum_{y\in V(R)} \delta_{L_N}(y)[M_1(R) - 2k - d_2(y)] \\
&= \textstyle\sum_{y\in V(R)} \delta_{L_N}(y)[M_1(R) - 2k] \\
&\quad - \textstyle\sum_{y\in V(R)} \delta_{L_N}(y)\,d_2(y) \\
&= [M_1(R) - 2k]\textstyle\sum_{y\in V(R)} \delta_{L_N}(y) \\
&\quad - \textstyle\sum_{y\in V(R)} \delta_{L_N}(y)\,d_2(y) \\
&\leq [M_1(R) - 2k][h(h-1)^2 - 2k(h-1) \\
&\quad - M_1(\overline{R})] - 2LM_2(R)
\end{aligned}$$

$$\overline{L_N M_1}(R) \leq [M_1(R) - 2k][h(h-1)^2 - 2k(h-1) - M_1(\overline{R})]$$
$$-2LM_2(R) - L_N M_1(R)\,.$$

Theorem 14: *Let R be a graph with k edges. Then,*

$$\overline{L_N M_1}(\overline{R}) \leq 2kM_1(R) - NM_1(R) - 2M_2(R) = \overline{NM_1}(R)\,.$$

The equality holds for all Path graphs (except P_3 and P_4), Cyclic graphs (except C_4), Platonic graphs (except octahedral), and Petersen graph.

Proof:

$$\overline{L_N M_1}(\overline{R}) = \sum_{xy \notin E(\overline{R})} \left[d_2(x/\overline{R})\,\delta_{L_N}(y/\overline{R}) + d_2(y/\overline{R})\,\delta_{L_N}(x/\overline{R})\right]$$

$$\leq \sum_{xy \in E(R)} d(x/R)(2k - \delta_N(y/R) - d(y/R))$$
$$+d(y/R)(2m - \delta_N(x/R) - d(x/R))$$

$$= 2k \sum_{xy \in E(R)} d(x/R) + d(y/R)$$
$$-2\sum_{xy \in E(R)} d(x/R)d(y/R)$$
$$-\sum_{xy \in E(R)} (d(x/R)\,\delta_N(y/R) + d(y/R)\,\delta_N(x/R))$$

$$= 2k\,M_1(R) - NM_1(R) - 2M_2(R)$$

$$\overline{L_N M_1}(\overline{R}) \leq \overline{NM_1}(R).$$

Theorem 15: *Let $R = (V, E)$ with $h = |V(R)|$ and $k = |E(R)|$. Then,*

$$L_N M_2(\overline{R}) \leq 2k^2[(h-1)(h-2) - 2k + 1]$$
$$+M_1(R)\left[\tfrac{1}{2}(M_1(R) - 1) - 2k(h-3)\right]$$
$$+M_2(R)(4k - 3) - \tfrac{3}{2}NM_1(R) - NM_2(R)\,.$$

The equality holds for all Path graphs (except P_3 and P_4), Cyclic graphs (except C_4), Platonic graphs (except octahedral), and Petersen graph.

Proof:

$$L_N M_2(\overline{R}) = \sum_{xy \in E(\overline{R})} \left[\delta_{L_N}(x/\overline{R}) \cdot \delta_{L_N}(y/\overline{R})\right]$$
$$\leq \sum_{xy \notin E(R)} [2k - \delta_N(x/R) - d(x/R)][2k - \delta_N(y/R) - d(y/R)]$$
$$= \sum_{xy \notin E(R)} 4k^2 - \sum_{xy \notin E(R)} 2k[\delta_N(x/R) + \delta_N(y/R)]$$
$$-\sum_{xy \notin E(R)} 2k[d(x/R) + d(y/R)]$$
$$+\sum_{xy \notin E(R)} \delta_N(x/R)\,\delta_N(y/R) + \sum_{xy \notin E(R)} d(x/R)\,d(y/R)$$
$$+\sum_{xy \notin E(R)} [d(x/R)\delta_N(y/R) + d(x/R)\delta_N(x/R)]$$
$$= 4k^2\left(\frac{h(h-1)}{2} - k\right) - 2k\overline{M'}(R) - 2k\overline{M_1}(R)$$

$$+\overline{NM_2}(R) + \overline{M_2}(R) + \overline{NM_1}(R)$$

$$\leq 4k^2\left(\frac{h(h-1)}{2} - k\right) - 2k[(h-1)M_1(R) - 2M_2(R)]$$
$$-2k[2k(h-1) - M_1(R)] + \frac{1}{2}[M_1(R)^2 - NM_1(R)]$$
$$-NM_2(R) + 2k^2 - \frac{1}{2}M_1(R) - M_2(R)$$
$$+2kM_1(R) - 2M_2(R) - NM_1(R)$$
$$L_N M_2(\overline{R}) \leq 2k^2[(h-1)(h-2) - 2k + 1]$$
$$+M_1(R)\left[\frac{1}{2}(M_1(R) - 1) - 2k(h-3)\right]$$
$$+M_2(R)(4h-3) - \frac{3}{2}NM_1(R) - NM_2(R)\,.$$

Theorem 16: *Let R be a graph with h vertices and k edges. Then,*

$$\overline{L_N M_2}(R) \leq [h(h-1) - 2k]^2\left[\frac{h(h-1)}{2} - k\right]$$
$$-[h(h-1) - 2k][2M_2(\overline{R}) + M_1(\overline{R})]$$
$$+M_2(\overline{R}) + NM_1(\overline{R}) + NM_2(\overline{R})\,.$$

The equality holds for the graphs with $diameter \leq 2$.

Proof:

$$\overline{L_N M_2}(R) = \sum_{xy\notin E(R)} [\delta_{L_N}(x/R) \cdot \delta_{L_N}(y/R)$$

$$\leq \sum_{xy\notin E(R)} [h(h-1) - 2k - \delta_N(x/\overline{R}) - d(x/\overline{R})]$$
$$[h(h-1) - 2k - \delta_N(y/\overline{R}) - d(y/\overline{R})]$$

$$= \sum_{xy\notin E(R)} \{[h(h-1) - 2k]^2 - [h(h-1) - 2k]\,\delta_N(y/\overline{R})$$
$$-[h(h-1) - 2k]\,d(y/\overline{R})$$
$$-[h(h-1) - 2k]\,\delta_N(x/\overline{R}) + \delta_N(x/\overline{R}) \cdot \delta_N(y/\overline{R})$$
$$+\delta_N(x/\overline{R}).\,d(y/\overline{R}) - [h(h-1) - 2k]d(x/\overline{R})$$
$$+d(x/\overline{R}) \cdot \delta_N(y/\overline{R}) + d(x/\overline{R}) \cdot d(y/\overline{R})\}$$
$$= [h(h-1) - 2k]^2\left[\frac{h(h-1)}{2} - k\right]$$
$$-[h(h-1) - 2k]\sum_{xy\in E(\overline{R})} [\delta_N(x/\overline{R}) + \delta_N(y/\overline{R})]$$
$$-[h(h-1) - 2k]\sum_{xy\in E(\overline{R})} [d(x/\overline{R}) + d(y/\overline{R})]$$
$$+\sum_{xy\in E(\overline{R})} [\delta_N(x/\overline{R}) \cdot \delta_N(y/\overline{R})]$$
$$+\sum_{xy\in E(\overline{R})} [d(x/\overline{R}) \cdot d(y/\overline{R})]$$
$$+\sum_{xy\in E(\overline{R})} [\delta_N(x/\overline{R}) \cdot d(y/\overline{R}) + d(x/\overline{R} \cdot \delta_N(y/\overline{R})]$$

$$= [h(h-1)-2k]^2\left[\frac{h(h-1)}{2}-k\right]$$
$$-[h(h-1)-2k]M'(\overline{R})$$
$$-[h(h-1)-2k]M_1(\overline{R})+NM_2(\overline{R})+M_2(\overline{R})+NM_1(\overline{R})$$

$$= [h(h-1)-2k]^2\left[\frac{h(h-1)}{2}-k\right]$$
$$-[h(h-1)-2k][M'(\overline{R})+M_1(\overline{R})]$$
$$+NM_2(\overline{R})+M_2(\overline{R})+NM_1(\overline{R})$$

$$\overline{L_NM_2}(R) \le [h(h-1)-2k]^2\left[\frac{h(h-1)}{2}-k\right]$$
$$-[h(h-1)-2k][2M_2(\overline{R})+M_1(\overline{R})]+M_2(\overline{R})$$
$$+NM_1(\overline{R})+NM_2(\overline{R})\,.$$

Theorem 17: *Let R be a graph with k edges. Then,*

$$\overline{L_NM_2}(\overline{R}) \le 4k^3-2k[2M_2(R)+M_1(R)]+M_2(R)$$
$$+NM_1(R)+NM_2(R)\,.$$

The equality holds for all Path graphs (except P_3 and P_4), Cyclic graphs (except C_4), Platonic graphs (except octahedral), and Petersen graph.

Proof:

$$\overline{L_NM_2}(\overline{R}) = \sum_{xy\notin E(\overline{R})} \delta_{L_N}(x/\overline{R})\cdot\delta_{L_N}(y/\overline{R})$$

$$\le \sum_{xy\notin E(\overline{R})} [2k-\delta_N(x/R)-d(x/R)]$$
$$.[2k-\delta_N(y/R)-d(y/R)]$$
$$= \sum_{xy\in E(R)} 4k^2-\sum_{xy\in E(R)} 2k\,[\delta_N(y/R)+\delta_N(x/R)]$$
$$-\sum_{xy\in E(R)} 2k\,[d(x/R)+d(y/R)]$$
$$+\sum_{xy\in E(R)} [\delta_N(x/R)\cdot d(y/R)+\delta_N(y/R)\cdot d(x/R)]$$
$$+\sum_{xy\in E(R)} [\delta_N(x/R)\cdot\delta_N(y/R)]$$
$$+\sum_{xy\in E(R)} [d(x/R)\cdot d(y/R)]$$

$$= 4k^3-2k[M'(R)]-2k[M_1(R)]+NM_1(R)$$
$$+M_2(R)+NM_2(R)$$
$$\overline{L_NM_2}(\overline{R}) \le 4k^3-2k[2M_2(R)+M_1(R)]+M_2(R)$$
$$+NM_1(R)+NM_2(R)\,.$$

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