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ON NEIGHBORHOOD ZAGREB INDICES AND COINDICES OF GRAPHS

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Abstract. The second Zagreb index, the neighborhood first Zagreb index, and the neighborhood second Zagreb index are defined, respectively, as: $M_2(G) = \sum\limits_{uv\in E(G)} d_G(u)d_G(v)$, $NM_1(G) = \sum\limits_{u\in V(G)} \delta_G(u)^2$, and $NM_2(G) = \sum\limits_{uv\in E(G)} \delta_G(u)\delta_G(v)$. In this paper, we mainly focus on the expression of $M_2(G)$ on the vertex set and make an effort to express $NM_1(G)$ on the edge set of G, hence define the neighborhood first and second Zagreb coindices $\overline{NM_1}(G)$, $\overline{NM_2}(G)$ and establish a complete set of relations between these coindices with their respective indices. Remarkable result is that, the concept of neighborhood degree sum gives an explicit formula for the second Zagreb index of the line graph of a graph, which is free from auxiliary equations. Also, at the end we give some new upper bounds for $NM_1(G)$.

1. Introduction

Topological indices are numerical values associated with chemical constitutions for the purpose of correlating chemical structures with their properties, like physical properties, chemical reactivity, and biological activity. Especially for the later purpose, namely quantitative structure-activity relationships (QSAR), topological indices hold good promise. So far, tremendous work has been carried out on the topological indices. In 2015, Gutman et al. [**9**] studied the Zagreb indices and coindices for a graph and its complement, and established a set of relations between the first and second Zagreb indices and coindices. They remarked that the first Zagreb coindex for a graph and its complement are always equal. Further,

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Basavanagoud et al. [**1**] studied the second Zagreb index and coindex of some derived graphs and obtained an expression for the second Zagreb index of the line graph of a graph, which includes auxiliary equations. With the advent of research in the theory of topological indices, the concept of neighborhood degree sum caught the attention of many researchers. Mondal et al. [**14, 15**] introduced some neighborhood degree-based indices and discussed their mathematical properties. Related works can be seen in [**2, 4, 7, 8, 13, 17, 19**].

It is noted that the second Zagreb index and the neighborhood first Zagreb index are defined on the edge set and the vertex set of a graph, respectively. In the present work, we express the second Zagreb index on the vertex set of a graph and also express the neighborhood first Zagreb index on the edge set of a graph. Further, we define the neighborhood first and second Zagreb coindices for a graph and its complement, and hence establish a complete set of relations between these coindices and their respective indices. The remarkable result is due to an expression for the second Zagreb index of the line graph of a graph in terms of the well-known degree-based topological indices and neighborhood degree-based indices, which is free from auxiliary equations. Further, we establish some new bounds for the neighborhood first Zagreb index.

2. Preliminaries

Throughout this paper, we consider simple, finite, and undirected graphs. A graph G consists of a finite non-empty set $V(G)$ of n vertices together with a prescribed set $E(G)$ of m unordered pairs of distinct vertices of $V(G)$. Each pair of vertices in $E(G)$ is an edge of G. An edge is said to be incident on its end vertices. Two vertices are adjacent if they are the end vertices of the same edge. Two edges are said to be adjacent if they have a common incident point. The number of edges incident on a vertex v is called the degree of the vertex and is denoted by $d_G(v)$. For a graph G, the maximum degree Δ and the minimum degree δ are defined, respectively, as $\Delta = max\{d_G(u) : u \in V(G)\}$ and $\delta = min\{d_G(u) : u \in V(G)\}$. The neighbourhood of a vertex u and an edge e in G are defined, respectively, as $N_G(u) = \{\ v \in V(G) :\ v \text{ is adjacent to } u \text{ in } G\ \}$ and $N_G(e) = \{\ f \in E(G) : f \text{ is adjacent to } e \text{ in } G\ \}$. The closed neighborhood of a vertex u is defined as $N_G[u] = N_G(u) \cup \{u\}$. The neighborhood degree sum of a vertex u is defined as, $\delta_G(u) = \sum\limits_{v \in N_G(u)} d_G(v)$. For a graph G, the maximum neighbors degree sum Δ_N and the minimum neighbors degree sum δ_N are defined, respectively, as $\Delta_N = max\{\delta_G(u) : u \in V(G)\}$ and $\delta_N = min\{\delta_G(u) : u \in V(G)\}$. The complement $\overline{G}$ of a graph G has the same vertices as G, but two vertices are adjacent in $\overline{G}$ if and only if they are not adjacent in G. The line graph $L(G)$ of a graph G is the graph whose vertex set has one-to-one correspondence with the edge set of G, two vertices of $L(G)$ are adjacent if and only if the corresponding edges in G share an endpoint. For graph theoretical definitions and notations, we follow the book [**12**].

The first Zagreb index $M_1(G)$ [**11**], the second Zagreb index $M_2(G)$ [**10**], the forgotten index $F(G)$ [**5**], the re-defined third Zagreb index $ReZ(G)$ [**18**], the fifth

Zagreb index $M'(G)$ [**6**], the neighborhood first Zagreb index $NM_1(G)$ [**14**] and the neighborhood second Zagreb index $NM_2(G)$ [**15**] are defined, respectively, as:

$$M_1(G) = \sum_{u\in V(G)} d_G(u)^2 = \sum_{uv\in E(G)} \big(d_G(u)+d_G(v)\big) \tag{2.1}$$

$$M_2(G) = \sum_{uv\in E(G)} d_G(u)\ d_G(v) \tag{2.2}$$

$$F(G) = \sum_{u\in V(G)} d_G(u)^3 = \sum_{uv\in E(G)} \big(d_G(u)^2+d_G(v)^2\big) \tag{2.3}$$

$$ReZ(G) = \sum_{uv\in E(G)} \Big(d_G(u)+d_G(v)\Big)\ d_G(u)\ d_G(v) \tag{2.4}$$

$$M'(G) = \sum_{uv\in E(G)} \big(\delta_G(u)+\delta_G(v)\big) \tag{2.5}$$

$$NM_1(G) = \sum_{u\in V(G)} \delta_G(u)^2 \tag{2.6}$$

$$NM_2(G) = \sum_{uv\in E(G)} \delta_G(u)\ \delta_G(v). \tag{2.7}$$

The first Zagreb coindex $\overline{M_1}(G)$ [**3**], the second Zagreb coindex $\overline{M_2}(G)$ [**3**] and the fifth Zagreb coindex $\overline{M'}(G)$ are defined, respectively, as:

$$\overline{M_1}(G) = \sum_{uv\notin E(G)} \big(d_G(u)+d_G(v)\big) \tag{2.8}$$

$$\overline{M_2}(G) = \sum_{uv\notin E(G)} d_G(u)\ d_G(v) \tag{2.9}$$

$$\overline{M'}(G) = \sum_{uv\notin E(G)} \big(\delta_G(u)+\delta_G(v)\big). \tag{2.10}$$

LEMMA 2.1. [**1**] *If G is a graph on n vertices and m edges, then*

$$\begin{aligned}
\overline{M_1}(G) &= 2m(n-1) - M_1(G)\\
M_2\Big(\overline{G}\Big) &= \frac{1}{2}n(n-1)^3 - 3m(n-1)^2 + 2m^2 + \frac{2n-3}{2}M_1(G) - M_2(G)\\
\overline{M_2}(G) &= 2m^2 - \frac{1}{2}M_1(G) - M_2(G)\\
\overline{M_2}\Big(\overline{G}\Big) &= m(n-1)^2 - (n-1)M_1(G) + M_2(G).
\end{aligned}$$

LEMMA 2.2. [**15**] *For a graph G,*

$$\sum_{u\in V(G)} \delta_G(u) = M_1(G) \quad \textit{and} \quad M'(G) = \sum_{uv\in E(G)} \big(\delta_G(u)+\delta_G(v)\big) = 2M_2(G).$$

3. Neighborhood Zagreb indices and coindices

The neighborhood first Zagreb index is defined over the vertex set of G, which does not allow us to define its coindex. Hence, at first, we express the neighborhood first Zagreb index on the edge set of G, given by the following theorem:

THEOREM 3.1. *For a graph G,*

$$NM_1(G) = \sum_{uv \in E(G)} \big(d_G(u)\ \delta_G(v) + d_G(v)\ \delta_G(u) \big).$$

PROOF. By definition,

$$\begin{aligned} NM_1(G) &= \sum_{u \in V(G)} \delta_G(u)^2 \\ &= \sum_{u \in V(G)} \delta_G(u) \delta_G(u) \\ &= \sum_{u \in V(G)} \delta_G(u) \left(\sum_{v \in N_G(u)} d_G(v) \right) \\ &= \sum_{uv \in E(G)} \big(d_G(u)\ \delta_G(v) + d_G(v)\ \delta_G(u) \big). \end{aligned}$$

□

Now we define the neighborhood first and second Zagreb coindices, respectively, as:

$$\overline{NM_1}(G) = \sum_{uv \notin E(G)} \big(d_G(u)\ \delta_G(v) + d_G(v)\ \delta_G(u) \big)$$

and

$$\overline{NM_2}(G) = \sum_{uv \notin E(G)} \delta_G(u)\ \delta_G(v).$$

Propositions 3.1 and 3.2 are needful in establishing relations between the neighborhood Zagreb indices and their coindices.

PROPOSITION 3.1. *Let G be a graph on n vertices and m edges. Then,*

$$\delta_{\overline{G}}(u) = \delta_G(u) - (n-2)\ d_G(u) + (n-1)^2 - 2m.$$

PROOF. By the definition of the neighborhood degree sum of a vertex u in $\overline{G}$, we have

$$\begin{aligned}
\delta_{\overline{G}}(u) &= \sum_{v \in N_{\overline{G}}(u)} d_{\overline{G}}(v) \\
&= \sum_{v \notin N_G[u]} \Big(n-1-d_G(v)\Big) \\
&= \sum_{v \notin N_G[u]} (n-1) - \sum_{v \notin N_G[u]} d_G(v) \\
&= (n-1)\,\Big(n-1-d_G(u)\Big) - \left[\sum_{v \in V(G)} d_G(v) - \sum_{v \in N_G(u)} d_G(v) - d_G(u)\right] \\
&= (n-1)\,\Big(n-1-d_G(u)\Big) - [2m - \delta_G(u) - d_G(u)] \\
&= \delta_G(u) - (n-2)\; d_G(u) + (n-1)^2 - 2m.
\end{aligned}$$

□

PROPOSITION 3.2. *For a graph G with n vertices,*

$$\overline{M'}(G) = (n-1)M_1(G) - 2M_2(G).$$

PROOF.

$$\begin{aligned}
M'(G) + \overline{M'}(G) &= \sum_{\{u,v\} \subseteq V(G)} \Big[\delta_G(u) + \delta_G(v)\Big] \\
&= \sum_{u \in V(G)} (n-1)\; \delta_G(u).
\end{aligned}$$

By Lemma 2.2,

$$\overline{M'}(G) = (n-1)M_1(G) - 2M_2(G).$$

□

The section continues with the main results related to the neighborhood first and second Zagreb indices and coindices for a graph G and its complement $\overline{G}$.

THEOREM 3.2. *Let G be a graph with n vertices and m edges. Then,*

$$\begin{aligned}
(i)\overline{NM_1}(G) &= 2mM_1(G) - 2M_2(G) - NM_1(G) \\
(ii)NM_1\Big(\overline{G}\Big) &= \Big[(n-1)\;(3n-5) - 4m + 1\Big]M_1(G) - 4\;(n-2)\; M_2(G) \\
&\quad + NM_1(G) + n\;(n-1)^4 - 8m\;(n-1)^3 + 4m^2(3n-4) \\
(iii)\;\overline{NM_1}\Big(\overline{G}\Big) &= 2m(n-1)\Big[(n-1)^2 - 2m\Big] - \Big[(n-1)\;(2n-3) - 2m\Big]M_1(G) \\
&\quad + 2\;(2n-3)\; M_2(G) - NM_1(G).
\end{aligned}$$

PROOF. (i)

$$\begin{aligned}
NM_1(G)+\overline{NM_1}(G) &= \sum_{\{u,v\}\subseteq V(G)} [d_G(u)\ \delta_G(v)+d_G(v)\ \delta_G(u)]\\
&= \sum_{v\in V(G)} \left[\delta_G(v)\left(\sum_{u\in V(G)} d_G(u)-d_G(v)\right)\right]\\
&= \sum_{v\in V(G)} \Big[\delta_G(v)\Big(2m-d_G(v)\Big)\Big]\\
&= 2m\sum_{v\in V(G)} \delta_G(v)-\sum_{v\in V(G)} d_G(v)\ \delta_G(v)\\
&= 2m\ M_1(G)-M'(G)\\
&= 2m\ M_1(G)-2M_2(G).
\end{aligned}$$

On re-arrangement of the terms, the result follows.

(ii)

$$\begin{aligned}
NM_1\left(\overline{G}\right) &= \sum_{uv\in E\left(\overline{G}\right)} \Big[d_{\left(\overline{G}\right)}(u)\ \delta_{\left(\overline{G}\right)}(v)+d_{\left(\overline{G}\right)}(v)\ \delta_{\left(\overline{G}\right)}(u)\Big]\\
&= \sum_{uv\in E\left(\overline{G}\right)} \Big[\Big(n-1-d_G(u)\Big)\left((n-1)^2-2m+\delta_G(v)-(n-2)d_G(v)\right)\\
&\quad +\Big(n-1-d_G(v)\Big)\left((n-1)^2-2m+\delta_G(u)-(n-2)d_G(u)\right)\Big]\\
&= \sum_{uv\notin E(G)} \Big[2(n-1)\left((n-1)^2-2m\right)+(n-1)\Big(\delta_G(u)+\delta_G(v)\Big)\\
&\quad -\Big((n-1)\ (2n-3)-2m\Big)\ \Big(d_G(u)+d_G(v)\Big)\\
&\quad -\Big(d_G(u)\ \delta_G(v)+d_G(v)\ \delta_G(u)\Big)+2(n-2)\ d_G(u)\ d_G(v)\Big]\\
&= 2(n-1)\left((n-1)^2-2m\right)\left(\frac{n(n-1)}{2}-m\right)+(n-1)\ \overline{M'}(G)\\
&\quad -\Big[(n-1)(2n-3)-2m\Big]\ \overline{M_1}(G)-\overline{NM_1}(G)+2(n-2)\overline{M_2}(G).
\end{aligned}$$

From the above equation, Lemma 2.1 and Proposition 3.2 the result follows.
(iii)

$$\begin{aligned}
\overline{NM_1}(\overline{G}) &= \sum_{uv\notin E(\overline{G})} \Big[d_{(\overline{G})}(u)\delta_{(\overline{G})}(v) + d_{(\overline{G})}(v)\ \delta_{(\overline{G})}(u)\Big] \\
&= \sum_{uv\notin E(\overline{G})} \Big[(n-1-d_G(u))\left((n-1)^2-2m+\delta_G(v)-(n-2)d_G(v)\right) \\
&\quad +(n-1-d_G(v))\left((n-1)^2-2m+\delta_G(u)-(n-2)d_G(u)\right)\Big] \\
&= \sum_{uv\in E(G)} \Big[2(n-1)\Big((n-1)^2-2m\Big)+(n-1)\Big(\delta_G(u)+\delta_G(v)\Big) \\
&\quad -\Big((n-1)(2n-3)-2m\Big)\Big(d_G(u)+d_G(v)\Big) \\
&\quad -\Big(d_G(u)\ \delta_G(v)+d_G(v)\ \delta_G(u)\Big)+2(n-2)d_G(u)\ d_G(v)\Big] \\
&= 2m(n-1)\Big[(n-1)^2-2m\Big]+(n-1)M'(G) \\
&\quad -\Big[(n-1)(2n-3)-2m\Big]M_1(G)+2(n-2)M_2(G)-NM_1(G).
\end{aligned}$$

From the above equation and Lemma 2.2, the result follows. □

THEOREM 3.3. *Let G be graph on n vertices and m edges. Then,*

$$\begin{aligned}
(i)\overline{NM_2}(G) &= \frac{1}{2}\left[M_1(G)^2-NM_1(G)\right]-NM_2(G) \\
(ii)NM_2(\overline{G}) &= \overline{NM_2}(G)-(n-2)\,\overline{NM_1}(G)-(n-2)\left((n-1)^2-2m\right)\overline{M_1}(G) \\
&\quad +(n-2)^2\overline{M_2}(G)+\left((n-1)^2-2m\right)\overline{M'}(G) \\
&\quad +\left(\frac{n(n-1)}{2}-m\right)\left((n-1)^2-2m\right)^2 \\
(iii)\overline{NM_2}(\overline{G}) &= NM_2(G)-(n-2)\,NM_1(G)-(n-2)\left((n-1)^2-2m\right)M_1(G) \\
&\quad +\left(2(n-1)^2+(n-2)^2-4m\right)M_2(G)+m\left((n-1)^2-2m\right)^2.
\end{aligned}$$

PROOF. (i)

$$\begin{aligned}
[M_1(G)]^2 &= \sum_{u\in V(G)}\sum_{v\in V(G)} \delta_G(u)\delta_G(v) \\
&= 2\sum_{uv\in E(G)}\delta_G(u)\delta_G(v)+2\sum_{uv\notin E(G)}\delta_G(u)\delta_G(v)+\sum_{u\in V(G)}[\delta_G(u)]^2 \\
&= 2NM_2(G)+2\overline{NM_2}(G)+NM_1(G).
\end{aligned}$$

On re-arrangement, the result follows.

(*ii*)

$$
\begin{aligned}
NM_2(\overline{G}) &= \sum_{uv\in E(\overline{G})} \delta_{\overline{G}}(u)\delta_{\overline{G}}(v) \\
&= \sum_{uv\in E(\overline{G})} \left[\delta_G(u)-(n-2)d_G(u)+(n-1)^2-2m\right]\left[\delta_G(v)\right. \\
&\quad \left. -(n-2)d_G(v)+(n-1)^2-2m\right] \\
&= \sum_{uv\notin E(G)} \Bigg[\delta_G(u)\delta_G(v)-(n-2)\Big(d_G(u)\delta_G(v)+d_G(v)\delta_G(u)\Big) \\
&\quad +(n-2)^2 d_G(u)d_G(v)-(n-2)\left((n-1)^2-2m\right)\Big(d_G(u)+d_G(v)\Big) \\
&\quad +\left((n-1)^2-2m\right)\Big(\delta_G(u)+\delta_G(v)\Big)+\left((n-1)^2-2m\right)^2\Bigg] \\
&= \overline{NM_2}(G)-(n-2)\,\overline{NM_1}(G)+(n-2)^2\overline{M_2}(G) \\
&\quad -(n-2)\left((n-1)^2-2m\right)\overline{M_1}(G)+\left((n-1)^2-2m\right)\overline{M'}(G) \\
&\quad +\left((n-1)^2-2m\right)^2\left(\frac{n(n-1)}{2}-m\right).
\end{aligned}
$$

From the above equation and Lemma 2.2, the result follows.

(*iii*)

$$
\begin{aligned}
\overline{NM_2}(\overline{G}) &= \sum_{uv\notin E(\overline{G})} \delta_{\overline{G}}(u)\ \delta_{\overline{G}}(v) \\
&= \sum_{uv\notin E(\overline{G})} \left[\delta_G(u)-(n-2)d_G(u)+(n-1)^2-2m\right]\left[\delta_G(v)\right. \\
&\quad \left. -(n-2)d_G(v)+(n-1)^2-2m\right] \\
&= \sum_{uv\in E(G)} \Bigg[\delta_G(u)\delta_G(v)-(n-2)\Big(d_G(u)\delta_G(v)+d_G(v)\delta_G(u)\Big) \\
&\quad +(n-2)^2 d_G(u)d_G(v)-(n-2)\left((n-1)^2-2m\right)(d_G(u)+d_G(v)) \\
&\quad +\left((n-1)^2-2m\right)(\delta_G(u)+\delta_G(v))+\left((n-1)^2-2m\right)^2\Bigg] \\
&= NM_2(G)-(n-2)\,NM_1(G)+(n-2)^2M_2(G) \\
&\quad -(n-2)\left((n-1)^2-2m\right)M_1(G)+\left((n-1)^2-2m\right)M'(G) \\
&\quad +m\left((n-1)^2-2m\right)^2.
\end{aligned}
$$

From the above equation and Lemma 2.2, the result follows. □

The study related to the line graph of a graph has much significance. While studying the line graph of a graph, we noticed that the expression for $M_1(L(G))$ is explicitly available due to the vertex set version of $M_1(G)$. The study of $M_2(L(G))$

got struck due to the auxiliary equations involved in the expression, which is due to the unavailability of the vertex set version of $M_2(G)$. The astonishing fact is that a vertex set version of $M_2(G)$ is possible with the concept of neighborhood degree sum, which in turn resolves the auxiliary equations involved in $M_2(L(G))$ and leads to an explicit expression, which can be seen in the following section.

4. Second Zagreb index of line graph

Basavanagoud et al. [**1**], obtained an expression for the second Zagreb index of the line graph, which is as follows:

THEOREM 4.1. [**1**] *Let G be a graph on n vertices and m edges. Then,*

$$M_2\Big(L(G)\Big) = 2M_1(G) + M_3(G) - 2M_4(G) + M_5(G) - 4m$$

where $M_3(G)$, $M_4(G)$ and $M_5(G)$ are the auxiliary Zagreb–type indices given by,

$$\begin{aligned} M_3(G) &= \sum_{uv,vw\in E(G)} d_G(v)^2 \\ M_4(G) &= \sum_{uv,vw\in E(G)} \Big[d_G(u) + 2d_G(v) + d_G(w)\Big] \\ M_5(G) &= \sum_{uv,vw\in E(G)} \Big[d_G(u)d_G(v) + d_G(v)d_G(w) + d_G(w)d_G(u)\Big] \end{aligned}$$

with summation going over all paths of length two, contained in the graph G.

Theorem 4.1 contains auxiliary equations. In order to have an explicit formula for $M_2\Big(L(G)\Big)$ that is free from the auxiliary equations, we apply the concept of neighborhood degree sum. For this, we consider an expression for the second Zagreb index on the vertex set (vertex version) of a graph G which is given by:

$$M_2(G) = \frac{1}{2} \sum_{u\in V(G)} d_G(u)\delta_G(u), \tag{4.1}$$

which can be easily verified.

The re-defined third Zagreb index is alternately given as [**16**]

$$ReZ(G) = \sum_{uv\in E(G)} \Big[d_G(u)\ \delta_G(u) + d_G(v)\ \delta_G(v)\Big]. \tag{4.2}$$

The alternate form of the re-defined third Zagreb index given by Eqn. (4.2) is used in reformulating Theorem 4.1 along with the following proposition.

PROPOSITION 4.1. [**16**] *Let G be a graph on n vertices and m edges such that $e = uv$ is an edge of G. Then,*

$$\delta_G(e) = \delta_G(u) + \delta_G(v) + d_G(u)^2 + d_G(v)^2 - 4\Big(d_G(u) + d_G(v) - 1\Big).$$

THEOREM 4.2. *Let G be a graph on n vertices and m edges. Then,*

$$\begin{aligned} M_2\Big(L(G)\Big) &= 6M_1(G) - 6M_2(G) - 3F(G) + ReZ(G) + \frac{1}{2}NM_1(G) - 4m \\ &+\frac{1}{2}\sum_{u\in V(G)} d_G(u)^4. \end{aligned}$$

PROOF. From the definition of the second Zagreb index on the vertex set of $L(G)$, we have:

$$M_2(L(G)) = \frac{1}{2}\sum_{e=uv\in V(L(G))} d_{L(G)}(e)\delta_{L(G)}(e).$$

By Proposition 4.1,

$$\begin{aligned} M_2(L(G)) &= \frac{1}{2}\sum_{uv\in E(G)}\Big(d_G(u)+d_G(v)-2\Big)\Big(d_G(u)^2+d_G(v)^2 \\ &-4\left[d_G(u)+d_G(v)-1\right]+\delta_G(u)+\delta_G(v)\Big) \\ &= \frac{1}{2}\sum_{uv\in E(G)}\Big[\Big(d_G(u)^3+d_G(v)^3\Big)+\Big(d_G(u)+d_G(v)\Big)\Big(d_G(u)\ d_G(v)\Big) \\ &-6\Big(d_G(u)^2+d_G(v)^2\Big)-8\Big(d_G(u)\ d_G(v)\Big)+\Big(d_G(u)\delta_G(u)+d_G(v)\delta_G(v)\Big) \\ &+\Big(d_G(u)\delta_G(v)+d_G(v)\delta_G(u)\Big)+12\Big(d_G(u)+d_G(v)\Big) \\ &-2\Big(\delta_G(u)+\delta_G(v)\Big)-8\Big] \\ &= \frac{1}{2}\Big[\sum_{uv\in E(G)}\Big(d_G(u)^3+d_G(v)^3\Big)+\sum_{uv\in E(G)}\Big(d_G(u)+d_G(v)\Big)\ d_G(u)\ d_G(v) \\ &-6\sum_{uv\in E(G)}\Big(d_G(u)^2+d_G(v)^2\Big)-8\sum_{uv\in E(G)}\Big(d_G(u)\ d_G(v)\Big) \\ &+\sum_{uv\in E(G)}\Big(d_G(u)\ \delta_G(u)+d_G(v)\ \delta_G(v)\Big) \\ &+\sum_{uv\in E(G)}\Big(d_G(u)\ \delta_G(v)+d_G(v)\ \delta_G(u)\Big) \\ &+12\sum_{uv\in E(G)}\Big(d_G(u)+d_G(v)\Big)-2\sum_{uv\in E(G)}\Big(\delta_G(u)+\delta_G(v)\Big)-\sum_{uv\in E(G)} 8\ \Big]. \end{aligned}$$

By Eqns. (2.1), (2.2), (2.3), (2.4), (2.6), and (4.2) we get

$$\begin{aligned} M_2(L(G)) &= \frac{1}{2}\Bigg[\sum_{u\in V(G)} d_G(u)^4 + ReZ(G) - 6F(G) - 8M_2(G) + ReZ(G) + NM_1(G) \\ &\quad +12M_1(G) - 2M'(G) - 8m\Bigg] \\ &= 6M_1(G) - 6M_2(G) - 3F(G) + ReZ(G) + \frac{1}{2}NM_1(G) - 4m \\ &\quad +\frac{1}{2}\sum_{u\in V(G)} d_G(u)^4. \end{aligned}$$

□

The availability of expression for $M_2(G)$ over the vertex set leads to some new upper bounds for the neighborhood first Zagreb index, which can be seen in the following section.

5. Some new upper bounds for the neighborhood first Zagreb index

Lemma 5.1. *(Kantorovich inequality) Let x_i and y_i for $1 \leqslant i \leqslant n$ be positive real numbers such that $m \leqslant \frac{x_i}{y_i} \leqslant M$. Then*

$$\left(\sum_{i=1}^{n} x_i^2\right)\left(\sum_{i=1}^{n} y_i^2\right) \leqslant \frac{(M+m)^2}{4Mm}\left(\sum_{i=1}^{n} x_i y_i\right)^2.$$

Lemma 5.2. *(Diaz-Metcalf inequality) Let x_i and y_i for $1 \leqslant i \leqslant n$ be positive real numbers such that $m \leqslant \frac{x_i}{y_i} \leqslant M$. Then*

$$\sum_{i=1}^{n} x_i^2 + Mm\sum_{i=1}^{n} y_i^2 \leqslant (M+m)\sum_{i=1}^{n} x_i y_i$$

with equality if and only if $x_i = My_i$ or $x_i = my_i$, for $1 \leqslant i \leqslant n$.

Proposition 5.1. *For any vertex u in a graph G,*

$$\delta \leqslant \frac{\delta_G(u)}{d_G(u)} \leqslant \Delta.$$

Proof. For any vertex v in a graph G, we have

$$\delta \leqslant d_G(v) \leqslant \Delta.$$

Now taking summation over all the neighbors of vertex v in graph G throught the above inequality

$$\sum_{v\in N_G(u)} \delta \leqslant \sum_{v\in N_G(u)} d_G(v) \leqslant \sum_{v\in N_G(u)} \Delta$$

$$\delta\ d_G(u) \leqslant \delta_G(u) \leqslant \Delta\ d_G(u)$$

$$\delta \leqslant \frac{\delta_G(u)}{d_G(u)} \leqslant \Delta.$$

□

THEOREM 5.1. *For a graph G,*

$$NM_1(G) \leqslant \frac{(\Delta+\delta)^2}{\Delta\delta} \frac{M_2(G)^2}{M_1(G)}.$$

PROOF. Taking $x_i = \delta_G(v_i)$ and $y_i = d_G(v_i)$ in Lemma 5.1 and using Proposition 5.1, we get

$$\begin{aligned}
\left(\sum_{i=1}^{n} \delta_G(v_i)^2\right)\left(\sum_{i=1}^{n} d_G(v_i)^2\right) &\leqslant \frac{(\Delta+\delta)^2}{4\Delta\delta}\left(\sum_{i=1}^{n} \delta_G(v_i) d_G(v_i)\right)^2 \\
NM_1(G)\ M_1(G) &\leqslant \frac{(\Delta+\delta)^2}{4\Delta\delta}(2M_2(G))^2 \\
NM_1(G) &\leqslant \frac{(\Delta+\delta)^2}{\Delta\delta} \frac{M_2(G)^2}{M_1(G)}.
\end{aligned}$$

□

THEOREM 5.2. *For a graph G,*

$$NM_1(G) \leqslant 2(\Delta+\delta) M_2(G) - \Delta\delta M_1(G).$$

Equality holds if and only if $\delta_G(v_i) = \Delta d_G(v_i)$ or $\delta_G(v_i) = \delta d_G(v_i)$ for $1 \leqslant i \leqslant n$.

PROOF. Taking $x_i = \delta_G(v_i)$ and $y_i = d_G(v_i)$ in Lemma 5.2 and using Proposition 5.1, we get

$$\begin{aligned}
\sum_{i=1}^{n} \delta_G(v_i)^2 + \Delta\delta \sum_{i=1}^{n} d_G(v_i)^2 &\leqslant (\Delta+\delta) \sum_{i=1}^{n} \delta_G(v_i) d_G(v_i) \\
NM_1(G) + \Delta\delta M_1(G) &\leqslant (\Delta+\delta)\ 2M_2(G) \\
NM_1(G) &\leqslant 2(\Delta+\delta) M_2(G) - \Delta\delta M_1(G).
\end{aligned}$$

□

THEOREM 5.3. *For a graph G,*

$$NM_1(G) \leqslant (\Delta_N + \delta_N) M_1(G) - n\Delta_N\delta_N$$

where Δ_N and δ_N represents the maximum neighbors degree sum and minimum neighbors degree sum, respectively.

PROOF. Taking $x_i = \delta_G(v_i)$ and $y_i = 1$ in Lemma 5.2, we get

$$\begin{aligned}
\sum_{i=1}^{n} \delta_G(v_i)^2 + \Delta_N\delta_N \sum_{i=1}^{n} 1^2 &\leqslant (\Delta_N+\delta_N) \sum_{i=1}^{n} \delta_G(v_i) \\
NM_1(G) + \Delta_N\delta_N n &\leqslant (\Delta_N+\delta_N) M_1(G) \\
NM_1(G) &\leqslant (\Delta_N+\delta_N) M_1(G) - n\Delta_N\delta_N.
\end{aligned}$$

□

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