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Applications of Neighbors Degree Sum of a Vertex on Zagreb Indices

Harishchandra S. Ramane[a], **Kartik S. Pise**[a],
Raju B. Jummannaver[b,†], **Daneshwari D. Patil**[a]

[a]*Department of Mathematics, Karnatak University, Dharwad - 580003, India*
hsramane@yahoo.com, pise.kartik@gmail.com, daneshwarip@gmail.com

[b]*P. G. Department of Mathematics, Karnatak Science College, Dharwad - 580001, India*
rajesh.rbj065@gmail.com

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Abstract

In this paper, we give the vertex versions of the re-defined third Zagreb index, reduced second Zagreb index and hyper Zagreb index by using the concept of neighbors degree sum. Further, by using the vertex version of re-defined third Zagreb index, explicit formulae for second Zagreb index of line graph, first Zagreb index of second iterated line graph, and also an explicit formula for second entire Zagreb index, which is free from auxiliary equations has been obtained. Also, the expressions for reduced second Zagreb and hyper-Zagreb indices of the line graph of a graph are obtained. Some noted results on comparisons between first and second Zagreb indices are presented. Flexibility in the computation of the results is due to the usage of neighbors degree sum concept. Hence, the present work can be considered as an application of concept of neighbors degree sum.

1 Introduction

Topological indices are numeric quantities in league with chemical constitutions for the intend of correlating chemical structures with numerous properties like physico-chemical properties, biological activity or chemical reactivity. Especially for the later purpose, namely quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR), topological indices hold good promise. So far tremendous work has been carried out on the topological indices. Zagreb indices are the most prominent molecular structure descriptors, also oldest among the topological indices, which were introduced in 1972 by Gutman and Trinajstić [20]. In 2004, Miličević et al. [27] reformulated the Zagreb indices in relating to edge-degrees instead of vertex-degrees. Later in 2012, Ilić and Zhou [22] established a set of bounds for the same, along with an exact formula for the first reformulated Zagreb index in terms of well known degree-based topological indices. Recently, Liu et al. [26] studied the reformulated Zagreb indices and obtained an expression for the first reformulated Zagreb index of the line graph of a graph, which includes both the vertex-degree and edge-degree based indices. Ranjini et al. [33] in 2013, introduced re-defined third Zagreb index, which is defined on the edge set. Recently, Alwardi et al. [1] defined entire Zagreb indices, in analog with Zagreb indices, which are defined over both the vertex set and edge set of a graph and obtained an expression for the second entire Zagreb index, which includes auxiliary equations. In 2014, Furtula et al. [14] studied differences of Zagreb indices and showed that this difference is in close connection with the reduced Zagreb index which is defined over the edge set. In the same paper, it was proposed that the comparision between first and second Zagreb indices appears to be prohibitively difficult task. In 2013, Shirdel et al. [34] defined the hyper-Zagreb index over the edge set and later, Kulli et al. [24] studied the same for derived graphs, deducing a formula for the hyper-Zagreb index of the line graph of regular graph. With the advent of research in the theory of topological indices, the concept of neighbors degree sum caught an attention of many researchers. Mondal et al. [29,30], introduced some neighbors degree based indices and discussed their mathematical properties. Related works can be seen in [2–7, 9–11, 16, 17, 23, 25, 28, 31, 32, 35].

In reality, it is noted that the first and second reformulated Zagreb indices of a graph G coincide with the first and second Zagreb indices of the line graph $L(G)$ of G, respectively. In the present work, we give two alternative definitions for the re-defined third Zagreb index by using the concept of neighbors degree sum, which includes a vertex set version and obtain an explicit formula for the second Zagreb index of $L(G)$ (or the second reformulated Zagreb index of G) in terms of well known degree-based topological indices. With interest to this, we make an attempt to express the first Zagreb index of the second iterated line graph of a graph G (or the first reformulated Zagreb index of $L(G)$) in terms of well known vertex-degree based topological indices only and a technique of drawing the second iterated line graph $L^2(G)$ without drawing its first iterated line graph. Further, we express the second entire Zagreb index of G in terms of well known degree-based topological indices of G, free from auxiliary equations. After this, we give the vertex set version of reduced Zagreb index, an explicit formula for reduced Zagreb index of $L(G)$, and some results on comparision between first and second Zagreb indices. Further, we give the vertex set version of hyper-Zagreb index and an explicit formula for the hyper-Zagreb index of $L(G)$. All these tasks are computed through the concept of neighbors degree sum of a vertex. Hence, we describe this paper as applications of neighbors degree sum of a vertex concept.

2 Preliminaries

All graphs taken into consideration here are simple, finite and undirected. A graph G contains a finite nonempty set of n vertices called the vertex set, denoted by $V(G)$, along with a pre-defined set of m unordered pairs of different vertices of $V(G)$ called the edge set, denoted by $E(G)$. Such each pair of vertices in $E(G)$ is termed as an edge of G. Whenever two vertices shares a common edge, those vertices are said to be adjacent and, such an edge is said to be incident on those vertices. If two edges have a common incident vertex then those edges are said to be adjacent. The number of elements of $E(G)$ having a common incident vertex v is called degree of the vertex v, denoted by $d_G(v)$. The degree of an edge e, whose end vertices are u and v, is $d_G(e) = d_G(u) + d_G(v) - 2$. Neighborhood of a vertex v and an edge e are defined as, $N_G(v) = \{u \in V(G) : u \text{ is adjacent to } v \text{ in } G\}$ and $N_G(e) = \{f \in E(G) : f \text{ is adjacent to } e \text{ in } G\}$, respectively. Neighbors degree sum of a vertex v and neighbors degree sum of an edge e are defined as, $\delta_G(v) = \sum\limits_{u \in N_G(v)} d_G(u)$ and $\delta_G(e) = \sum\limits_{f \in N_G(e)} d_G(f)$, respectively. For a graph G, its line graph $L(G)$ is the graph such that $V(L(G))$ is in bijection with $E(G)$, two members of $V(L(G))$ are adjacent in $L(G)$ if and only if their respective members of $E(G)$ are adjacent in G. The second iterarted line graph of G, deonted by $L^2(G)$, is defined as $L^2(G) = L(L(G))$. Let A be a nonempty set and $H = \{A_1, A_2, \ldots, A_k\}$ be a family of distinct nonempty subsets of A such that $\cup_{i=1}^{k} A_i = A$. Then the intersection graph of H, denoted by $\Omega(H)$, is the graph such that $V(\Omega(H)) = H$, with A_i and A_j are adjacent whenever $i \neq j$ and $A_i \cap A_j \neq \emptyset$. For graph theoretical definitions and notations, we follow the book [21].

The first Zagreb index $M_1(G)$ [20], second Zagreb index $M_2(G)$ [19], reformulated first Zagreb index $EM_1(G)$ [27], reformulated second Zagreb index $EM_2(G)$ [27], first entire

Zagreb index $M_1^{\varepsilon}(G)$ [1], second entire Zagreb index $M_2^{\varepsilon}(G)$ [1], forgotten topological index $F(G)$ [13], redefined third Zagreb index $ReZ(G)$ [33], reduced second Zagreb index $RM_2(G)$ [14], hyper-Zagreb index $HZ(G)$ [34], fifth Zagreb index $M'(G)$ [15], and first neighborhood Zagreb index $NM_1(G)$ [29] are defined respectively as:

$$M_1(G) = \sum_{u\in V(G)} d_G(u)^2 = \sum_{uv\in E(G)} [d_G(u) + d_G(v)] \tag{1}$$

$$M_2(G) = \sum_{uv\in E(G)} d_G(u)\ d_G(v) \tag{2}$$

$$EM_1(G) = \sum_{e\in E(G)} d_G(e)^2 \tag{3}$$

$$EM_2(G) = \sum_{e \text{ is adjacent to } f, \text{ where } e,f\in E(G)} d_G(e)\ d_G(f) \tag{4}$$

$$M_1^{\varepsilon}(G) = \sum_{x\in V(G)\cup E(G)} d_G(x)^2 \tag{5}$$

$$M_2^{\varepsilon}(G) = \sum_{x \text{ is either adjacent or incident to } y, \text{ where } x,y\in V(G)\cup E(G)} [d_G(x)\ d_G(y)] \tag{6}$$

$$F(G) = \sum_{u\in V(G)} d_G(u)^3 = \sum_{uv\in E(G)} \left[d_G(u)^2 + d_G(v)^2\right] \tag{7}$$

$$ReZ(G) = \sum_{uv\in E(G)} (d_G(u) + d_G(v))\ d_G(u)\ d_G(v) \tag{8}$$

$$RM_2(G) = \sum_{uv\in E(G)} (d_G(u) - 1)\,(d_G(v) - 1) \tag{9}$$

$$HZ(G) = \sum_{uv\in E(G)} [d_G(u) + d_G(v)]^2 \tag{10}$$

$$M'(G) = \sum_{uv\in E(G)} [\delta_G(u) + \delta_G(v)] \tag{11}$$

$$NM_1(G) = \sum_{u\in V(G)} \delta_G(u)^2. \tag{12}$$

Lemma 2.1. [30] *For a graph G,*

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

■

Lemma 2.2. [24] *Let G be a graph with m edges. Then,*

$$|E(L(G))| = \frac{1}{2}M_1(G) - m.$$

■

3 Redefined third Zagreb index

Here we present the re-defined third Zagreb index over the vertex set of G which is given by Theorem 3.1.

Theorem 3.1. *The vertex set version of the re-defined third Zagreb index of a graph G is given by*

$$ReZ(G) = \sum_{u \in V(G)} d_G(u)^2 \delta_G(u).$$

Proof. By definition,

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

■

Lemma 3.2. [12] *Let $TI(G)$ be a graph invarient, which is of the form*

$$TI(G) = \sum_{u \in V(G)} F_G(u).$$

Then

$$TI(G) = \sum_{uv \in E(G)} \left[\frac{F_G(u)}{d_G(u)} + \frac{F_G(v)}{d_G(v)} \right],$$

where F_G is a real valued function defined on the vertex set $V(G)$. ■

Following Theorem gives the edge set version of the re-defined third Zagreb index with respect to neighbors degree sum concept with the help of Lemma 3.2.

Theorem 3.3. *The edge set version of the re-defined third Zagreb index of a graph G with respect to neighbors degree sum concept is*

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

Proof. Proof follows by Theorem 3.1 and Lemma 3.2. ■

In the next section, the second Zagreb index of $L(G)$ (or the reformulated second Zagreb index of G) is computed with the help of above discussed new versions of re-defined Zagreb index.

4 Second Zagreb index of a line graph

We need the sum of neighbors degree of an edge in a graph G, as a vertex in $L(G)$ is in association with its corresponding edge in G.

Proposition 4.1. *Let $e = uv$ be an edge of a graph G. Then,*

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

Proof. Let f be an arbitrary edge of G which is adjacent to the edge $e = uv$ of G. Let u' be the vertex adjacent to u with $u' \neq v$ and v' be the vertex adjacent to v with $v' \neq u$. Then,

$$\begin{aligned}
\delta_G(e) &= \sum_{f \in N_G(e)} d_G(f) \\
&= \sum_{u' \in N_G(u)-\{v\}} d_G(uu') + \sum_{v' \in N_G(v)-\{u\}} d_G(vv') \\
&= \sum_{u' \in N_G(u)-\{v\}} \Big(d_G(u) + d_G(u') - 2\Big) + \sum_{v' \in N_G(v)-\{u\}} \Big(d_G(v) + d_G(v') - 2\Big) \\
&= \sum_{u' \in N_G(u)-\{v\}} \Big(d_G(u) - 2\Big) + \sum_{u' \in N_G(u)-\{v\}} d_G(u') + \sum_{v' \in N_G(v)-\{u\}} \Big(d_G(v) - 2\Big) \\
&\quad + \sum_{v' \in N_G(v)-\{u\}} d_G(v') \\
&= \left(d_G(u) - 2\right)\left(d_G(u) - 1\right) + \delta_G(u) - d_G(v) + \left(d_G(v) - 2\right)\left(d_G(v) - 1\right) \\
&\quad + \delta_G(v) - d_G(u) \\
&= \delta_G(u) + \delta_G(v) + d_G(u)^2 + d_G(v)^2 - 4\left(d_G(u) + d_G(v) - 1\right).
\end{aligned}$$

■

Now, we give an explicit formula for the second Zagreb index of a line graph.

Theorem 4.2. *Let G be a graph with n vertices and m edges. Then*

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

Proof. Applying Lemma 2.1 on the line graph of G, we have

$$\begin{aligned} M_2(L(G)) &= \frac{1}{2}M'(L(G)) \\ &= \frac{1}{2}\sum_{ef\in E(L(G))}\big(\delta_{L(G)}(e)+\delta_{L(G)}(f)\big) \\ &= \frac{1}{2}\sum_{uv,vw\in E(G)}[\delta_G(uv)+\delta_G(vw)] \end{aligned}$$

By Proposition 4.1, we have

$$\begin{aligned} M_2(L(G)) &= \frac{1}{2}\sum_{uv,vw\in E(G)}\big[\delta_G(u)+\delta_G(v)+d_G(u)^2+d_G(v)^2-4\,(d_G(u)+d_G(v)-1) \\ &\qquad +\delta_G(v)+\delta_G(w)+d_G(v)^2+d_G(w)^2-4\,(d_G(v)+d_G(w)-1)\big] \\ &= \frac{1}{2}\sum_{uv,vw\in E(G)}\big[\delta_G(u)+2\delta_G(v)+\delta_G(w)+\big(d_G(u)^2+2d_G(v)^2+d_G(w)^2\big) \\ &\qquad -4\,(d_G(u)+2d_G(v)+d_G(w)-2)] \\ &= \frac{1}{2}\left[\sum_{uv,vw\in E(G)}(\delta_G(u)+2\delta_G(v)+\delta_G(w))\right. \\ &\qquad +\sum_{uv,vw\in E(G)}\big(d_G(u)^2+2d_G(v)^2+d_G(w)^2\big) \\ &\qquad \left.-4\sum_{uv,vw\in E(G)}(d_G(u)+2d_G(v)+d_G(w))+\sum_{uv,vw\in E(G)}8\right] \\ &= \frac{1}{2}\left[\sum_{uv\in E(G)}(d_G(u)+d_G(v)-2)\,(\delta_G(u)+\delta_G(v))\right. \\ &\qquad +\sum_{uv\in E(G)}(d_G(u)+d_G(v)-2)\,\big(d_G(u)^2+d_G(v)^2\big) \\ &\qquad \left.-4\sum_{uv\in E(G)}(d_G(u)+d_G(v)-2)\,(d_G(u)+d_G(v))+\sum_{uv,vw\in E(G)}8\right] \end{aligned}$$

$$\begin{aligned} &= \frac{1}{2}\left[\sum_{uv\in E(G)}[(d_G(u)\delta_G(u)+d_G(v)\delta_G(v))+(d_G(u)\delta_G(v)+d_G(v)\delta_G(u))\right. \\ &\quad -2\,(\delta_G(u)+\delta_G(v))] \\ &\quad +\sum_{uv\in E(G)}\big[\big(d_G(u)^3+d_G(v)^3\big)+(d_G(u)+d_G(v))\,d_G(u)d_G(v) \end{aligned}$$

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

By Eqs. (1), (2), (7), (8), (11), (12), Theorem 3.3 and Lemma 2.2, we get

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

■

Now we have explicit formulae for the first and second Zagreb indices of the line graph of a graph G. This leads to curiosity of finding explicit formulae for the Zagreb indices of the second iterated line graph. In the next section, we give an explicit formula for the first Zagreb index of the second iterated line graph.

5 Second iterated line graph and its first Zagreb index

Recently, Liu et al. [26] computed the first reformulated Zagreb index of $L(G)$, which coincides with the first Zagreb index of $L^2(G)$, which is given in the following Theorem as:

Theorem 5.1. [26] *If $L(G)$ is the line graph of G, then*

$$EM_1(L(G)) = EF(G) + 2EM_2(G) - 4F(G) + 18M_1(G) - 8M_2(G) - 20m,$$

where

$$EF(G) = \sum_{e \in E(G)} d_G(e)^3 \quad \textit{and} \quad EM_2(G) = \sum_{e \text{ is adjacent to } f, \text{ where } e,f \in E(G)} d_G(e)d_G(f).$$

■

Expression for the reformulated first Zagreb index of $L(G)$ (or the first Zagreb index of $L^2(G)$) in Theorem 5.1 contains both the vertex-degree based and edge-degree based topological indices. Now, we establish a formula for the first Zagreb index of $L^2(G)$ in terms of vertex-degree based indices only.

During the task, we had a question: Is it possible to draw the second iterated line graph of G without drawing or considering the first line graph? The obtained affirmative answer to the thought with the concept of intersection graph can be seen through the following method.

METHOD: Let G be the graph with the edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$. Let $\mathcal{F}$ be a family of 2-subsets of $E(G)$ such that members of 2-subsets are adjacent in G, that is, $\mathcal{F} = \big\{\{e_i, e_j\} \subseteq E(G) \bigm| e_i \text{ is adjacent to } e_j \text{ in } G,\ i \neq j,\ 1 \leq i, j \leq m\big\}$. Then the intersection graph on the family $\mathcal{F}$ of the edge set $E(G)$ is the second iterated line graph of G.

Example 5.2. Consider the graph G in Fig. 1 with the edge set $E(G) = \{e_1, e_2, e_3, e_4\}$. Then, $\mathcal{F} = \{\{e_1, e_2\}, \{e_2, e_3\}, \{e_3, e_4\}, \{e_1, e_4\}, \{e_2, e_4\}\}$ and the intersection graph $\Omega(\mathcal{F})$ on the family $\mathcal{F}$ of the edge set $E(G)$, shown in Fig. 2, is the second iterated line graph of G.

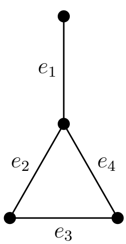

Figure 1. G

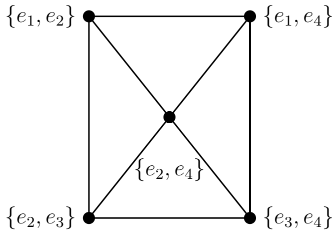

Figure 2. $\Omega(\mathcal{F}) \cong L^2(G)$

Clearly, one can observe that the vertices of $L^2(G)$ are due to the paths of length two present in G. Hence, the number of vertices of $L^2(G)$ is same as the number of paths of length two present in G, which is equal to the number of edges in $L(G)$.

Now we need the neighbors degree sum of a vertex of $L^2(G)$, which is given by following Proposition.

Proposition 5.3. *For $x \in V(L^2(G))$, where the vertex x is due to the path $uvw = ef$ in G, the neighbors degree sum of x in $L^2(G)$ is given by*

$$\begin{aligned}\delta_{L^2(G)}(x = uvw) &= \delta_G(u) + 2\delta_G(v) + \delta_G(w) + 2\left(d_G(u)^2 + 2d_G(v)^2 + d_G(w)^2\right)\\ &+ 2\left(d_G(u)d_G(v) + d_G(v)d_G(w)\right) - 12\left(d_G(u) + 2d_G(v) + d_G(w)\right) + 36.\end{aligned}$$

Proof.

$$\begin{aligned}\delta_{L^2(G)}(x) &= \delta_{L(G)}(ef)\\ &= \delta_{L(G)}(e) + \delta_{L(G)}(f) + d_{L(G)}(e)^2 + d_{L(G)}(f)^2 - 4\left(d_{L(G)}(e) + d_{L(G)}(f) - 1\right)\\ &= \delta_G(uv) + \delta_G(vw) + d_G(uv)^2 + d_G(vw)^2 - 4\left(d_G(uv) + d_G(vw) - 1\right)\\ &= \delta_G(u) + \delta_G(v) + d_G(u)^2 + d_G(v)^2 - 4\left(d_G(u) + d_G(v) - 1\right)\\ &\quad + \delta_G(v) + \delta_G(w) + d_G(v)^2 + d_G(w)^2 - 4\left(d_G(v) + d_G(w) - 1\right)\\ &\quad + \left(d_G(u) + d_G(v) - 2\right)^2 + \left(d_G(v) + d_G(w) - 2\right)^2\\ &\quad - 4\left(d_G(u) + d_G(v) - 2 + d_G(v) + d_G(w) - 2 - 1\right)\\ &= \delta_G(u) + 2\delta_G(v) + \delta_G(w) + 2\left(d_G(u)^2 + 2d_G(v)^2 + d_G(w)^2\right)\\ &\quad + 2\left(d_G(u)d_G(v) + d_G(v)d_G(w)\right) - 12\left(d_G(u) + 2d_G(v) + d_G(w)\right) + 36.\end{aligned}$$

∎

Theorem 5.4. *For a graph G with n vertices and m edges,*

$$M_1\left(L^2(G)\right) = 42M_1(G) - 32M_2(G) - 16F(G) + 5ReZ(G) + NM_1(G) + 2\sum_{u\in V(G)} d_G(u)^4 - 36m.$$

Proof. Applying Lemma 2.1 for $L^2(G)$, we have

$$M_1\left(L^2(G)\right) = \sum_{uvw\in V(L^2(G))} \delta_{L^2(G)}(uvw).$$

From Proposition 5.3,

$$\begin{aligned}
M_1\left(L^2(G)\right) &= \sum_{uv,vw\in E(G)}\Big[\delta_G(u)+2\delta_G(v)+\delta_G(w)+2\left(d_G(u)^2+2d_G(v)^2+d_G(w)^2\right) \\
&\quad + 2\left(d_G(u)d_G(v)+d_G(v)d_G(w)\right)-12\left(d_G(u)+2d_G(v)+d_G(w)\right)+36\Big] \\
&= \sum_{uv,vw\in E(G)}\left(\delta_G(u)+2\delta_G(v)+\delta_G(w)\right) \\
&\quad + 2\sum_{uv,vw\in E(G)}\left(d_G(u)^2+2d_G(v)^2+d_G(w)^2\right) \\
&\quad + 2\sum_{uv,vw\in E(G)}\left(d_G(u)d_G(v)+d_G(v)d_G(w)\right) \\
&\quad - 12\sum_{uv,vw\in E(G)}\left(d_G(u)+2d_G(v)+d_G(w)\right)+\sum_{uv,vw\in E(G)}36 \\
&= \sum_{uv\in E(G)}\left(d_G(u)+d_G(v)-2\right)\left(\delta_G(u)+\delta_G(v)\right) \\
&\quad + 2\sum_{uv\in E(G)}\left(d_G(u)+d_G(v)-2\right)\left(d_G(u)^2+d_G(v)^2\right) \\
&\quad + 2\sum_{uv\in E(G)}\left(d_G(u)+d_G(v)-2\right)\left(d_G(u)d_G(v)\right) \\
&\quad - 12\sum_{uv\in E(G)}\left(d_G(u)+d_G(v)-2\right)\left(d_G(u)+d_G(v)\right)+\sum_{uv,vw\in E(G)}36 \\
&= \sum_{uv\in E(G)}\left[\left(d_G(u)\delta_G(u)+d_G(v)\delta_G(v)\right)+\left(d_G(u)\delta_G(v)+d_G(v)\delta_G(u)\right)\right. \\
&\quad \left. - 2\left(\delta_G(u)+\delta_G(v)\right)\right] \\
&\quad + 2\sum_{uv\in E(G)}\Big[\left(d_G(u)^3+d_G(v)^3\right)+\left(d_G(u)+d_G(v)\right)d_G(u)d_G(v) \\
&\quad - 2\left(d_G(u)^2+d_G(v)^2\right)\Big] \\
&\quad + 2\sum_{uv\in E(G)}\left[\left(d_G(u)+d_G(v)\right)d_G(u)d_G(v)-2d_G(u)d_G(v)\right] \\
&\quad - 12\sum_{uv\in E(G)}\left[d_G(u)^2+d_G(v)^2+2d_G(u)d_G(v)-2\left(d_G(u)+d_G(v)\right)\right] \\
&\quad + \sum_{uv,vw\in E(G)}36.
\end{aligned}$$

By Eqs. (1), (2), (7), (8), (11), (12), Theorem 3.3 and Lemma 2.2,

$$\begin{aligned}
M_1\left(L^2(G)\right) &= ReZ(G)+NM_1(G)-2M'(G)+2\left[\sum_{u\in V(G)}d_G(u)^4+ReZ(G)-2F(G)\right] \\
&\quad + 2\left[ReZ(G)-2M_2(G)\right]-12\left[F(G)+2M_2(G)-2M_1(G)\right] \\
&\quad +36\left(\frac{1}{2}M_1(G)-m\right)
\end{aligned}$$

$$= 42M_1(G) - 32M_2(G) - 16F(G) + 5ReZ(G) + NM_1(G) + 2\sum_{u\in V(G)} d_G(u)^4 - 36m.$$

■

In the next section, we give application of neighbors degree sum concept over the entire Zagreb indices.

6 Second entire Zagreb index

In 2015, Alwardi et al. [1] obtained expressions for entire Zagreb indices which are as follows:

Theorem 6.1. [1] *For any graph G, the first and second entire Zagreb indices are*

$$M_1^\varepsilon(G) = 4m - 3M_1(G) + 2M_2(G) + \sum_{u\in V(G)} d_G(u)^3$$

and

$$\begin{aligned} M_2^\varepsilon(G) &= 4m - 2M_1^\varepsilon(G) - 2M_1(G) + M_2(G) + \frac{1}{2}\sum_{u\in V(G)} d_G(u)^4 \\ &+ \sum_{u\in V(G)} d_G(u)^2 \sum_{v\in N_G(u)} d_G(v) + \frac{1}{2}\sum_{u\in V(G)}\left(\sum_{v\in N_G(u)} d_G(v)\right)^2. \end{aligned}$$

■

It is noted that, the second entire Zagreb index in Theorem 6.1 contains auxiliary equations, to compute those one need to know the structure of the graph. In order to have an explicit formula for $M_2^\varepsilon(G)$ which to be free from the auxiliary equations, we apply the concept of neighbors degree sum. The improved version of second entire Zagreb index is given by Theorem 6.2 as:

Theorem 6.2. *For any graph G with m edges, the second entire Zagreb index is given by*

$$M_2^\varepsilon(G) = 4M_1(G) - 3M_2(G) - 2F(G) + ReZ(G) + \frac{1}{2}NM_1(G) + \frac{1}{2}\sum_{u\in V(G)} d_G(u)^4 - 4m.$$

Proof. From Theorem 6.1, we have

$$M_2^\varepsilon(G) = 4m - 2M_1^\varepsilon(G) - 2M_1(G) + M_2(G) + \frac{1}{2}\sum_{u\in V(G)} d_G(u)^4$$

$$
\begin{aligned}
&+ \sum_{u\in V(G)} d_G(u)^2 \sum_{v\in N_G(u)} d_G(v) + \frac{1}{2}\sum_{u\in V(G)}\left(\sum_{v\in N_G(u)} d_G(v)\right)^2 \\
= \;& 4m - 2\left(4m - 3M_1(G) + 2M_2(G) + \sum_{u\in V(G)} d_G(u)^3\right) - 2M_1(G) + M_2(G) \\
&+ \frac{1}{2}\sum_{u\in V(G)} d_G(u)^4 + \sum_{u\in V(G)} d_G(u)^2\delta_G(u) + \frac{1}{2}\sum_{u\in V(G)}\delta_G(u)^2
\end{aligned}
$$

By Eqns. (7), (12) and Theorem 3.1, we have

$$M_2^{\varepsilon}(G) = 4M_1(G) - 3M_2(G) - 2F(G) + ReZ(G) + \frac{1}{2}NM_1(G) + \frac{1}{2}\sum_{u\in V(G)} d_G(u)^4 - 4m.$$

■

7 Reduced Zagreb index and differences of Zagreb indices

In 2014, Furtula et al. [14] studied the difference of Zagreb indices $M_2(G) - M_1(G)$ which resulted in showing that this difference is in close connection with the reduced Zagreb index which is defined over edge set of a graph. In the same paper, they discribed that the characterization of graphs for which $M_1(G) < M_2(G)$ or for which $M_1(G) = M_2(G)$ or for which $M_1(G) > M_2(G)$ appears to be a prohibitively difficult task. In this section, we give the vertex set version of reduced Zagreb index, some results related to the comparision of Zagreb indices of a graph G and an explicit formula for the reduced Zagreb index of the line graph.

Theorem 7.1. *The vertex set version of reduced Zagreb index of a graph G is given by*

$$RM_2(G) = m + \frac{1}{2}\sum_{u\in V(G)} \delta_G(u)\left[d_G(u) - 2\right] \tag{13}$$

Proof. By the definition of reduced Zagreb index, we have

$$
\begin{aligned}
RM_2(G) &= \sum_{uv\in E(G)} \left(d_G(u) - 1\right)\left(d_G(v) - 1\right) \\
&= \sum_{uv\in E(G)} \left[d_G(u)d_G(v) - \left(d_G(u) + d_G(v)\right) + 1\right] \\
&= M_2(G) - M_1(G) + m
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{1}{2}\sum_{u\in V(G)} d_G(u)\delta_G(u) - \sum_{u\in V(G)} \delta_G(u) + m \\
&= m + \frac{1}{2}\sum_{u\in V(G)} \delta_G(u)\left[d_G(u) - 2\right].
\end{aligned}
$$

■

Now we study the difference of Zagreb indices with the help neighbors degree sum concept. The difference of Zagreb indices is

$$
M_2(G) - M_1(G) = \frac{1}{2}\sum_{u\in V(G)} d_G(u)\delta_G(u) - \sum_{u\in V(G)} \delta_G(u) = \frac{1}{2}\sum_{u\in V(G)} \delta_G(u)\left[d_G(u) - 2\right]. \quad (14)
$$

Some results relating to the comparision of Zagreb indices are given through the following theorems.

Theorem 7.2. *Let G be a nontrivial, connected, regular graph. Then $M_1(G) = M_2(G)$ if and only if $G \cong C_n$, a cycle on n vertices.*

Proof. Let G be a regular graph of degree r. Suppose $G \cong C_n$, then $d_G(u) = 2$ for all $u \in V(G)$. Substituting this in Eq. (14) gives

$$M_2(G) - M_1(G) = 0,$$

which follows the result.

Conversely, suppose $M_1(G) = M_2(G)$ then Eq. (14) implies that

$$\sum_{u\in V(G)} \delta_G(u)\left[d_G(u) - 2\right] = 0.$$

Since G is a regular of degree r, we have $\delta_G(u) = r^2$ for all $u \in V(G)$. Hence from the above equation we have,

$$nr^2(r-2) = 0.$$

Since G is nontrivial, connected graph, it follows that $r = 2$. Hence, $G \cong C_n$. ■

If G is totally disconnected, that is $G \cong \overline{K_n}$, a complement of a complete graph K_n, then also $M_1(G) = M_2(G)$.

Theorem 7.3. *If G is a graph with minimum degree $\delta(G) > 2$, then $M_1(G) < M_2(G)$. Hence, there exists no graph with minimum degree $\delta(G) > 2$ for which $M_1(G) = M_2(G)$.*

Proof. Since $\delta(G) > 2$, from Eq. (14) it is immediate that $M_2(G) - M_1(G) > 0$. Hence, $M_1(G) < M_2(G)$. ■

Corollary 7.4. *Neccessary condition for a connected graph G to satisfy $M_1(G) = M_2(G)$ is minimum degree $\delta(G) \leq 2$. Furthermore, if $G \ncong C_n$ then $M_1(G) = M_2(G)$ confirms the existence of at least one pendent vertex in G.*

Proof. Proof follows from Theorem 7.2 and Theorem 7.3. ■

Theorem 7.5. *If G is a graph with maximum degree $\Delta(G) \leq 2$ then $M_1(G) \geq M_2(G)$. Equality holds if and only if $G \cong C_n$.*

Proof. Suppose $\Delta(G) \leq 2$ then $G \cong P_n$, a path on n vertices or a cycle C_n. If $G \cong P_n$ then $M_1(G) = 4n - 6$ and $M_2(G) = 4n - 8$. Hence, $M_1(G) > M_2(G)$. If $G \cong C_n$ then result follows from Theorem 7.2. ■

Corollary 7.6. *For a path P_n, $M_1(P_n) > M_2(P_n)$. Moreover, $M_1(P_n) - M_2(P_n) = 2$.* ■

To find a formula for reduced Zagreb index of line graph we make use of the following proposition.

Proposition 7.7. [18] *For a graph G,*

$$M_1(L(G)) = F(G) - 4M_1(G) + 2M_2(G) + 4m.$$

■

Now we give an explicit formula for the reduced second Zagreb index of line graph as follows:

Thoerem 7.8. *Let G be a graph with n vertices and m edges. Then*

$$RM_2(L(G)) = \frac{21}{2}M_1(G) - 8M_2(G) - 4F(G) + ReZ(G) + \frac{1}{2}NM_1(G) + \frac{1}{2}\sum_{u \in V(G)} d_G(u)^4 - 9m.$$

Proof. Applying the definition of reduced Zagreb index for the line graph, we have

$$RM_2(L(G)) = M_2(L(G)) - M_1(L(G)) + m_L,$$

where m_L denotes the number of edges in $L(G)$. From Theorem 4.2, Proposition 7.7 and Lemma 2.2, the above equation becomes

$$\begin{aligned} RM_2(L(G)) &= 6M_1(G) - 6M_2(G) - 3F(G) + ReZ(G) + \frac{1}{2}NM_1(G) - 4m \\ &\quad + \frac{1}{2}\sum_{u \in V(G)} d_G(u)^4 - [F(G) - 4M_1(G) + 2M_2(G) + 4m] + \frac{1}{2}M_1(G) - m \end{aligned}$$

$$= \frac{21}{2}M_1(G) - 8M_2(G) - 4F(G) + ReZ(G) + \frac{1}{2}NM_1(G) + \frac{1}{2}\sum_{u\in V(G)} d_G(u)^4 - 9m.$$

■

8 Hyper–Zagreb index

In 2013, Shirdel et al. [34] defined the hyper-Zagreb index of a graph G over the edge set. Later in 2018, Kulli et al. [24] studied the same for derived graphs and deduced a formula for the hyper-Zagreb index of line graph of a regular graph. Now, we give the vertex set version of hyper-Zagreb index of a graph G and deduce hyper-Zagreb index of the line graph of all graphs.

Theorem 8.1. *The vertex set version of the hyper-Zagreb index of a graph G is given by,*

$$HZ(G) = \sum_{u\in V(G)} \left(d_G(u)^3 + d_G(u)\delta_G(u)\right).$$

Proof. By the definition of hyper-Zagreb index we have,

$$\begin{aligned} HZ(G) &= \sum_{uv\in E(G)} (d_G(u) + d_G(v))^2 \\ &= \sum_{uv\in E(G)} \left[d_G(u)^2 + d_G(v)^2 + 2d_G(u)d_G(v)\right] \\ &= F(G) + 2M_2(G) \\ &= \sum_{u\in V(G)} \left(d_G(u)^3 + d_G(u)\delta_G(u)\right). \end{aligned}$$

■

To find a formula for the hyper-Zagreb index of line graph we make use of the following proposition.

Proposition 8.2. [8] *For a graph G with n vertices and m edges,*

$$F(L(G)) = 12M_1(G) - 12M_2(G) - 6F(G) + 3ReZ(G) + \sum_{u\in V(G)} d_G(u)^4 - 8m.$$

■

The explicit formula for the hyper-Zagreb index of line graph is as follows:

Theorem 8.3. *Let G be a graph with n vertices and m edges. Then*

$$HZ(L(G)) = 24M_1(G) - 24M_2(G) - 12F(G) + 5ReZ(G) + NM_1(G) + 2\sum_{u\in V(G)} d_G(u)^4 - 16m.$$

Proof. By the definition of hyper-Zagreb index on the line graph, we have

$$HZ(L(G)) = F(L(G)) + 2M_2(L(G)).$$

From Proposition 8.2 and Theorem 4.2, the above equation becomes

$$\begin{aligned}
HZ(L(G)) &= 12M_1(G) - 12M_2(G) - 6F(G) + 3ReZ(G) + \sum_{u\in V(G)} d_G(u)^4 - 8m \\
&\quad + 2\Big(6M_1(G) - 6M_2(G) - 3F(G) + ReZ(G) + \frac{1}{2}NM_1(G) - 4m \\
&\quad + \frac{1}{2}\sum_{u\in V(G)} d_G(u)^4\Big) \\
&= 24M_1(G) - 24M_2(G) - 12F(G) + 5ReZ(G) + NM_1(G) \\
&\quad + 2\sum_{u\in V(G)} d_G(u)^4 - 16m.
\end{aligned}$$

■

9 Conclusion

Theorem 3.1, Theorem 7.1 and Theorem 8.1 gives the vertex versions of re-defined third Zagreb index, reduced Zagreb index and hyper-Zagreb index. These expressions helps in obtaining the explicit formulae for second Zagreb index of line graph, first Zagreb index of second iterated line graph and second entire Zagreb index (free from auxiliary equations). Comparisons between first and second Zagreb indices in terms of equality and inequality expressions is possible. To sum up, the concept of neighbors degree is more efficient for studying some of the well known topological indices.

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