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On the Zagreb Energy and Zagreb Estrada Index of Graphs

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Abstract

The (first) Zagreb matrix $Z(G) = (z_{ij})_{n\times n}$ of a graph G whose vertex v_i has degree d_i is defined by $z_{ij} = d_i + d_j$ if the vertices v_i and v_j are adjacent and $z_{ij} = 0$ otherwise. Let $\zeta_1, \zeta_2, \ldots, \zeta_n$ be the first Zagreb eigenvalues of $Z(G)$. The Zagreb energy ZE and the Zagreb Estrada index ZEE of a graph G are $ZE(G) = \sum\limits_{i=1}^{n} |\zeta_i|$ and $ZEE(G) = \sum\limits_{i=1}^{n} e^{\zeta_i}$, respectively. Very recently, Rad et al. [N. J. Rad, A. Jahanbani, I. Gutman, Zagreb Energy and Zagreb Estrada Index of Graphs, *MATCH Commun. Math. Comput. Chem.* **79** (2018) 371–386] introduced and investigated the Zagreb energy and Zagreb Estrada index of a graph. We found several errors in the results of the above paper. In this paper we correct these results and some of these results are presented in a revise form. Finally, we establish some new upper and lower bounds on ZE and ZEE. Moreover, we present some novel lower and upper bounds on the spectral radius of the (first) Zagreb matrix of the graph G.

1 Introduction

Let $G = (V, E)$ be a graph with a vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. The degree of a vertex $v_i \in V(G)$ is the number of vertices adjacent to v_i and is denoted by d_i. If the vertices v_i and v_j are adjacent we denote this as $v_iv_j \in E(G)$ or $i \sim j$. The Zagreb matrix of a graph G is a square matrix $Z(G) = (z_{ij})_{n\times n}$ of order n, defined in [2] as

$$z_{ij} = \begin{cases} d_i + d_j & \text{if } v_iv_j \in E(G), \\ 0 & \text{Otherwise.} \end{cases}$$

The eigenvalues of Z(G), labeled $\zeta_1 \geqslant \zeta_2 \geqslant \cdots \geqslant \zeta_n$, are known as the Zagreb eigenvalues or Z-*eigenvalues* of G and their collection is called the Zagreb spectrum or Z-spectrum of G. Several recent papers introduced hyper-Zagreb index and it is defined as

$$HM = HM(G) = \sum_{v_iv_j \in E(G)} (d_i + d_j)^2.$$

The Zagreb energy [2] of G is defined as

$$\mathrm{ZE} = \mathrm{ZE}(G) = \sum_{i=1}^{n} |\zeta_i|,$$

where $\zeta_1, \zeta_2, \ldots, \zeta_n$ are the eigenvalues of the Zagreb matrix of graph G.

The Zagreb Estrada index [2] of G, denoted by ZEE(G), is equal to

$$\mathrm{ZEE} = \mathrm{ZEE}(G) = \sum_{i=1}^{n} e^{\zeta_i},$$

where $\zeta_1 \geqslant \zeta_2 \geqslant \cdots \geqslant \zeta_n$ are the Z-*eigenvalues* of G. Let

$$N_k = \sum_{i=1}^{n} \zeta_i^k.$$

Then

$$\mathrm{ZEE}(G) = \sum_{k=0}^{\infty} \frac{N_k}{k!}.$$

This paper is organized as follows. In Section 2, we state some previously known results. In Section 3, we present some lower and upper bounds on the spectral radius of the Zagreb matrix of graphs. In Section 4, we have corrected several results from an earlier paper regarding the Zagreb energy ZE and the Zagreb Estrada index ZEE, and some of these results are presented in a revised form. Finally, we establish some new upper and lower bounds on ZE and ZEE.

2 Preliminaries

In this section we list some previously known results that will be needed in the next two sections. Horn and Johnson [1] presented the following result on the spectral radius of the irreducible nonnegative square matrix.

Lemma 1. [1] *Let $B = (B_{i,j})$ be an $n \times n$ irreducible nonnegative matrix with spectral radius λ and let $R_i(B) = \sum_{j=1}^{n} b_{i,j}$ be the ith row sum of B. Then*

$$\min\Big\{R_i(B)\ :\ 1 \leq i \leq n\Big\} \leq \lambda \leq \max\Big\{R_i(B)\ :\ 1 \leq i \leq n\Big\}.$$

Moreover, if the row sums of B are not all equal, then both of the inequalities are strict.

Lemma 2. [2] *For nonnegative $x_1, x_2, \ldots, x_n$ and $k \geqslant 2$,*

$$\sum_{i=1}^{n} x_i^k \leqslant \left(\sum_{i=1}^{n} {x_i}^2\right)^{\frac{k}{2}}. \tag{1}$$

In 1918, Szőkefalvi Nagy [3] proved the following result:

Lemma 3. *Let $a_1, a_2, \ldots, a_n$ be real numbers with the property $r \leq a_i \leq R$ $(1 \leq i \leq n)$. Then*

$$n \sum_{i=1}^{n} a_i^2 - \left(\sum_{i=1}^{n} a_i\right)^2 \geq \frac{n}{2}\,(R-r)^2.$$

Rad et al. [2] have proved some result in Lemma 1, but this result is not true. Here we have corrected this result as follows:

Lemma 4. *Let G be a graph of order n with the Zagreb matrix* $\mathrm{Z(G)}$. *Then*

$$(1)\quad N_1 = \sum_{i=1}^{n} \zeta_i = tr\Big(\mathrm{Z(G)}\Big) = 0, \tag{2}$$

$$(2)\quad N_2 = \sum_{i=1}^{n} {\zeta_i}^2 = tr\Big(\mathrm{Z(G)}^2\Big) = 2\sum_{i\sim j} (d_i+d_j)^2 = 2\,HM(G), \tag{3}$$

$$(3)\quad N_3 = \sum_{i=1}^{n} {\zeta_i}^3 = tr\Big(\mathrm{Z(G)}^3\Big) = 6 \sum_{i\sim j\sim k\sim i} (d_i+d_j)(d_j+d_k)(d_k+d_i), \tag{4}$$

$$(4)\quad N_4 = \sum_{i=1}^{n} {\zeta_i}^4 = tr\Big(\mathrm{Z(G)}^4\Big) = \sum_{i=1}^{n}\sum_{j=1}^{n}\left(\sum_{k:\, i\sim k\sim j} (d_i+d_k)(d_j+d_k)\right)^2, \tag{5}$$

where $i \sim j$ indicates a pair of adjacent vertices v_i and v_j.

Proof. By definition, the diagonal elements of $\mathrm{Z}(G)$ are equal to zero. Therefore the *trace* of $\mathrm{Z}(G)$ is zero.

Next, we calculate the matrix $\mathrm{Z}(G)^2$. For $i = j$

$$(\mathrm{Z}(G)^2)_{ii} = \sum_{j=1}^{n} \mathrm{z}_{ij}\mathrm{z}_{ji} = \sum_{j=1}^{n} (z_{ij})^2 = \sum_{j:\, j\sim i} (d_i+d_j)^2.$$

Moreover, for $i \neq j$

$$(\mathrm{Z}(G)^2)_{ij} = \sum_{k=1}^{n} z_{ik}\, z_{kj} = \sum_{k:\, i\sim k\sim j} z_{ik} z_{kj} = \sum_{k:\, i\sim k\sim j} (d_i + d_k)\,(d_j + d_k).$$

Therefore

$$tr(Z(G)^2) = \sum_{i=1}^{n} \sum_{j:\, j\sim i} (d_i + d_j)^2 = 2 \sum_{i\sim j} (d_i + d_j)^2 = 2\, HM(G).$$

Since the diagonal elements of Z^3 are

$$(Z(G)^3)_{ii} = \sum_{j=1}^{n} (Z^2)_{ij}\, z_{ji} = \sum_{j:\, j\sim i} \sum_{k:\, i\sim k\sim j} (d_i + d_k)\,(d_j + d_k)\,(d_i + d_j).$$

we obtain

$$\begin{aligned} tr(Z(G)^3) &= \sum_{i=1}^{n} \sum_{j:\, j\sim i} \sum_{k:\, i\sim k\sim j} (d_i + d_k)\,(d_j + d_k)\,(d_i + d_j) \\ &= 6 \sum_{i\sim j\sim k\sim i} (d_i + d_k)\,(d_j + d_k)\,(d_i + d_j). \end{aligned}$$

Since

$$(Z(G)^4)_{ii} = \sum_{j=1}^{n} (Z^2)_{ij}\,(Z^2)_{ji} = \sum_{j=1}^{n} \left(\sum_{k:\, i\sim k\sim j} (d_i + d_k)\,(d_j + d_k) \right)^2,$$

we have

$$tr(Z(G)^4) = \sum_{i=1}^{n} \sum_{j=1}^{n} (Z^2)_{ij}\,(Z^2)_{ji} = \sum_{i=1}^{n} \sum_{j=1}^{n} \left(\sum_{k:\, i\sim k\sim j} (d_i + d_k)\,(d_j + d_k) \right)^2.$$

■

Lemma 5. *Let G be a graph of order n. Then $|\zeta_1| = |\zeta_2| = \cdots = |\zeta_n|$ if and only if $G \cong \overline{K}_n$ or $G \cong \frac{n}{2} K_2$ (n is even).*

Proof. First we assume that G is connected. Then $\zeta_1 > 0$. By the Perron-Frobenius theorem, we have $\zeta_1 \geq |\zeta_i|$, $i = 2, 3, \ldots, n$. If $\zeta_2 > 0$, then $\zeta_1 = \zeta_2$. Then one can easily make one eigencomponent 0 of an eigenvector with a corresponding eigenvalue of ζ_1, a contradiction as G is connected. Otherwise, $\zeta_2 < 0$, that is, $\zeta_1 = -\zeta_2$. Since $\zeta_1 \geq \zeta_2 \geq \cdots \geq \zeta_n$ and $\sum_{i=1}^{n} \zeta_i = 0$, we must have $n = 2$ and $G \cong K_2$.

Next we assume that G is disconnected. For $\zeta_1 = 0$, we have $\zeta_1 = \zeta_2 = \cdots = \zeta_n = 0$ and hence $G \cong \overline{K}_n$. Otherwise, $\zeta_1 > 0$. For each connected component of G must be K_2. Hence $G \cong \frac{n}{2} K_2$ (n is even). ■

3 On the spectral radius of the Zagreb matrix of graphs

We present the upper and lower bounds on $\zeta_1(G)$ in terms of n, m, maximum degree Δ and minimum degree δ.

Theorem 6. *Let G be a graph of order n, m edges with a maximum degree Δ and minimum degree δ. Then*

$$2m-(n-1-\delta)\Delta+(\delta-1)\,\delta \leqslant \zeta_1(G) \leqslant 2m-(n-1-\Delta)\delta+(\Delta-1)\,\Delta \tag{6}$$

with both equalities hold if and only if G is a regular graph.

Proof. Let m_i be the average degree of the adjacent vertices of vertex v_i in G. Then $\delta \leqslant m_i \leqslant \Delta$. If G is r-regular, then $\zeta_1(G)=\lambda_1(Z(G))=\lambda_1(2r\,A(G))=2r\,\lambda_1(G)=2r^2$ ($\lambda_1(X)$ denotes the spectral radius of matrix X), both equalities hold in (6). Otherwise, G is a non-regular graph. We consider the following two cases.

Case 1 : G is connected.

Lower bound: Since $d_i m_i \geqslant 2m-d_i-(n-d_i-1)\Delta$, by Lemma 1, we have

$$\begin{aligned}\zeta_1(G) &\geqslant \min_{1\leq i\leq n} \sum_{v_j:\, v_iv_j\in E(G)} (d_i+d_j) = \min_{1\leq i\leq n} \left(d_i^2+d_im_i\right)\\ &\geqslant \min_{1\leq i\leq n} \left[d_i^2+2m-d_i-(n-d_i-1)\Delta\right]\\ &= \min_{1\leq i\leq n} \left[2m-(n-1)\Delta+(\Delta-1)\,d_i+d_i^2\right] \geqslant 2m-(n-1)\Delta+(\Delta+\delta-1)\,\delta,\end{aligned}$$

which gives the left inequality in (6).

Suppose that left equality holds in (6). Then all inequalities in the above argument must be equalities. By Lemma 1, we have

$$d_1^2+d_1m_1=d_2^2+d_2m_2=\cdots=d_n^2+d_nm_n, \text{ i.e., } d_1(d_1+m_1)=d_2(d_2+m_2)=\cdots=d_n(d_n+m_n).$$

Since G is non-regular, we have $\Delta>\delta$. From the above, we must have $d_1+m_1<d_n+m_n$ ($\Delta=d_1$ and $\delta=d_n$). Since $m_n\leqslant\Delta$ and $m_1\geqslant\delta$, we obtain $m_n-m_1\leqslant\Delta-\delta$, that is, $d_1+m_1\geqslant d_n+m_n$, a contradiction.

Upper bound: Since $d_im_i\leqslant 2m-d_i-(n-d_i-1)\delta$, by Lemma 1, we have

$$\begin{aligned}\zeta_1(G) &\leqslant \max_{1\leq i\leq n}\left(d_i^2+d_im_i\right) \leqslant \max_{1\leq i\leq n}\left[d_i^2+2m-d_i-(n-d_i-1)\delta\right]\\ &\leqslant 2m-(n-1)\delta+(\Delta+\delta-1)\,\Delta,\end{aligned}$$

which gives the right inequality in (6). Similarly, as before, we conclude that the right inequality in (6) is strict.

Case 2 : G is disconnected. Let G_i be the i-th connected component in G, $1 \leq i \leq k$. Denoted by, let n_i and m_i be the number of vertices and the number of edges in G_i, respectively. Then $n = n_1 + n_2 + \cdots + n_k$ and $m = m_1 + m_2 + \cdots + m_k$. Thus we have

$$n_i\delta \leq 2m_i \leq n_i\Delta,\ 1 \leq i \leq k.$$

Also let Δ_i and δ_i be the maximum degree and minimum degree of the i-th connected component G_i, $1 \leq i \leq k$. Therefore $\Delta \geq \Delta_i$ and $\delta \leq \delta_i$ for $1 \leq i \leq k$.
Lower bound: Using the above results, we have

$$\begin{aligned}\zeta_1(G) &= \max\Big\{\zeta_1(G_1),\, \zeta_1(G_2), \ldots,\, \zeta_1(G_k)\Big\} = \zeta_1(G_\ell),\ (\text{say}) \\ &\geqslant 2m_\ell - (n_\ell - 1 - \delta_\ell)\Delta_\ell + (\delta_\ell - 1)\,\delta_\ell \\ &\geqslant 2m_\ell - (n_\ell - 1 - \delta_\ell)\Delta + (\delta_\ell - 1)\,\delta_\ell - \sum_{i=1,\, i\neq \ell}^{k} \Big(n_i\Delta - 2m_i\Big) \\ &\geqslant 2m - (n - 1 - \delta)\Delta + (\delta - 1)\,\delta,\end{aligned}$$

which gives the left inequality in (6).

Suppose that left equality holds in (6). Then all inequalities in the above argument must be equalities. Thus, we conclude that G_ℓ is a regular graph and hence $\Delta_\ell = \delta_\ell$. Moreover, we have $\Delta = \Delta_\ell$, $\delta_\ell = \delta$ and $2m_i = n_i\Delta$, $1 \leq i \leq k$, $i \neq \ell$. Therefore $\Delta = \delta$, a contradiction as G is a non-regular graph.

Upper bound: Similarly, as before, we have

$$\begin{aligned}\zeta_1(G) &= \zeta_1(G_\ell),\ (\text{say}) \leqslant 2m_\ell - (n_\ell - 1 - \Delta_\ell)\delta_\ell + (\Delta_\ell - 1)\,\Delta_\ell \\ &\leqslant 2m_\ell - (n_\ell - 1 - \Delta_\ell)\delta + (\Delta - 1)\,\Delta + \sum_{i=1,\, i\neq \ell}^{k} \Big(2m_i - n_i\delta\Big) \\ &\leqslant 2m - (n - 1 - \Delta)\delta + (\Delta - 1)\,\Delta.\end{aligned}$$

Suppose that right equality holds in (6). Similarly, as before, we can get a contradiction. This completes the proof of the theorem. ■

Corollary 7. *Let G be a graph with maximum degree Δ and minimum degree δ. Then*

$$2\delta^2 \leqslant \zeta_1(G) \leqslant 2\Delta^2$$

with both equalities holding if and only if G is a regular graph.

Proof. Since $2\delta^2 \leq d_i^2 + d_i m_i \leq 2\Delta^2$, from Theorem 6, we get the required result. Moreover, both equalities hold if and only if G is a regular graph. ■

4 Main Results

We now give an upper bound on $\mathrm{ZEE}(G) - \mathrm{ZE}(G)$ in terms of n and the hyper-Zagreb index $HM(G)$.

Theorem 8. *Let G be a graph of order n with a hyper-Zagreb index $HM(G)$. Then*

$$\mathrm{ZEE}(G) - \mathrm{ZE}(G) \leqslant n - 1 - 2\sqrt{2HM(G)} + e^{\sqrt{2HM(G)}}$$

with equality holding if and only if $G \cong \overline{K}_n$.

Proof. One can easily see that the equality holds for $\overline{K}_n$. Otherwise, $G \ncong \overline{K}_n$. Then $\zeta_1 > 0$ and $\zeta_n < 0$. From the definition of the Zagreb Estrada index, we have

$$\mathrm{ZEE}(G) = \sum_{i=1}^{n} e^{\zeta_i} = \sum_{i=1}^{n}\sum_{k\geqslant 0}\frac{\zeta_i^k}{k!} = n + \sum_{i=1}^{n}\sum_{k\geqslant 2}\frac{\zeta_i^k}{k!} < n + \sum_{i=1}^{n}\sum_{k\geqslant 2}\frac{|\zeta_i|^k}{k!}.$$

Coupling this result with (1), we obtain

$$\begin{aligned} \mathrm{ZEE}(G) &< n + \sum_{k\geqslant 2}\frac{1}{k!}\sum_{i=1}^{n}|\zeta_i|^k \leqslant n + \sum_{k\geqslant 2}\frac{1}{k!}\left(\sum_{i=1}^{n}|\zeta_i|^2\right)^{k/2} \\ &= n + \sum_{k\geqslant 2}\frac{(\sqrt{2HM(G)})^k}{k!} \leqslant n - 1 - \sqrt{2HM(G)} + e^{\sqrt{2HM(G)}}. \end{aligned}$$

By Theorem 1 in [2], we have $\mathrm{ZE}(G) \geqslant \sqrt{2HM(G)}$. From these two results, we get the required result. This completes the proof of the theorem. ■

The following corollary is obtained in Theorem 12 [2]:

Corollary 9. [2] *Let G be a graph with n vertices. Then*

$$\mathrm{ZEE}(G) - \mathrm{ZE}(G) \leqslant n - 1 - \sqrt{2HM(G)} + e^{\sqrt{2HM(G)}}.$$

The following corollary is obtained from the upper bound in Theorem 7 [2], but no extremal graph is mentioned.

Corollary 10. [2] *Let G be a graph with n vertices and a hyper-Zagreb index $HM(G)$. Then*

$$\mathrm{ZEE}(G) \leqslant n - 1 + e^{\sqrt{2HM(G)}}$$

with equality holding if and only if $G \cong \overline{K}_n$.

Remark 11. In [2], it has been proved that $\mathrm{ZEE}(G) - \mathrm{ZE}(G) \leqslant n - 1 - \sqrt{2HM(G)} + e^{\sqrt{2HM(G)}}$. One can easily check that our result in Theorem 8 is always better than the previous results in Corollary 9 and Corollary 10.

Corollary 12. *Let G be a graph of order n. Then*

$$\mathrm{ZEE}(G) + \mathrm{ZE}(G) \leqslant n - 1 + e^{\mathrm{ZE}(G)}$$

with equality holding if and only if $G \cong \overline{K}_n$.

Proof. For $G \cong \overline{K}_n$, we have $\mathrm{ZEE}(G) = n$, $\mathrm{ZE}(G) = 0$ and $e^{\mathrm{ZE}(G)} = 1$. Hence the equality holds for $\overline{K}_n$. Otherwise, $G \ncong \overline{K}_n$. From the proof of Theorem 8, we have

$$\begin{aligned} \mathrm{ZEE}(G) &< n + \sum_{k\geqslant 2} \frac{1}{k!} \sum_{i=1}^{n} |\zeta_i|^k \leqslant n + \sum_{k\geqslant 2} \frac{1}{k!} \left(\sum_{i=1}^{n} |\zeta_i| \right)^k \\ &= n - 1 - ZE(G) + \sum_{k\geqslant 0} \frac{\left(\mathrm{ZE}(G)\right)^k}{k!} \end{aligned}$$

which implies

$$\mathrm{ZEE}(G) + \mathrm{ZE}(G) < n - 1 + e^{\mathrm{ZE}(G)}.$$

■

Remark 13. In Theorem 13 [2], it has been proved that $\mathrm{ZEE}(G) \leqslant n - 1 + e^{\mathrm{ZE}(G)}$. Clearly, the bound in Corollary 12 is better than the bound in [2].

The upper bound of Theorem 9 in [2] is the following:

$$\mathrm{ZEE}(G) \leqslant e^{\sqrt{2HM(G)}}.$$

This result is not correct. For $G \cong \overline{K}_n$ $(n > 1)$, we have $\mathrm{ZEE}(G) = n > 1 = e^{\sqrt{2HM(G)}}$.
The reason is the following:
From the first line of the proof of Theorem 9 [2], we have $n \leqslant 1$ for $k = 0$, which is not true. The corrected result is in the following:

Corollary 14. *Let G be a graph of order n with a hyper-Zagreb index $HM(G)$. Then*

$$\mathrm{ZEE}(G) \leqslant n - 1 - \sqrt{2HM(G)} + e^{\sqrt{2HM(G)}}$$

with equality holding if and only if $G \cong \overline{K}_n$.

The following result has been proved in Theorem 8 [2]:

$$ZEE(G) \leq n-1+e^{\sqrt[4]{N_4}}.$$

Lemma 2 is wrongly used in the proof of Theorem 8 [2], for example,

$$\sum_{i=1}^{n} \zeta_i^2 \leq \left(\sum_{i=1}^{n} \zeta_i^4\right)^{1/2} \quad \text{and} \quad \sum_{i=1}^{n} \zeta_i^3 \leq \left(\sum_{i=1}^{n} \zeta_i^4\right)^{3/4}.$$

Here we have corrected the result in the following:

Theorem 15. *Let G be a graph of order n with a hyper-Zagreb index $HM(G)$. Then*

$$\mathrm{ZEE}(G) \leqslant n-1+HM(G)+\frac{1}{6}\,N_3-N_4^{1/4}-\frac{1}{2}\,N_4^{1/2}-\frac{1}{6}\,N_4^{3/4}+e^{\sqrt[4]{N_4}},$$

where N_3 and N_4 are defined in Lemma 4.

Proof. By the definition of the Zagreb Estrada index with (2), we have

$$\begin{aligned}
\mathrm{ZEE}(G) &= \sum_{i=1}^{n} e^{\zeta_i} = \sum_{i=1}^{n}\sum_{k=0}^{\infty} \frac{\zeta_i^k}{k!} = n+\frac{1}{2}\sum_{i=1}^{n}\zeta_i^2+\frac{1}{6}\sum_{i=1}^{n}\zeta_i^3+\sum_{i=1}^{n}\sum_{k=4}^{\infty}\frac{\zeta_i^k}{k!}\\
&\leqslant n+\frac{1}{2}\,N_2+\frac{1}{6}\,N_3+\sum_{i=1}^{n}\sum_{k=4}^{\infty}\frac{|\zeta_i|^k}{k!} = n+HM(G)+\frac{1}{6}\,N_3+\sum_{k=4}^{\infty}\frac{1}{k!}\sum_{i=1}^{n}(\zeta_i^4)^{\frac{k}{4}}\\
&\leqslant n+HM(G)+\frac{1}{6}\,N_3+\sum_{k=4}^{\infty}\frac{1}{k!}\left(\sum_{i=1}^{n}\zeta_i^4\right)^{\frac{k}{4}}\\
&= n-1+HM(G)+\frac{1}{6}\,N_3-N_4^{1/4}-\frac{1}{2}\,N_4^{1/2}-\frac{1}{6}\,N_4^{3/4}+\sum_{k=0}^{\infty}\frac{\sqrt[4]{N_4^k}}{k!}\\
&= n-1+HM(G)+\frac{1}{6}\,N_3-N_4^{1/4}-\frac{1}{2}\,N_4^{1/2}-\frac{1}{6}\,N_4^{3/4}+e^{\sqrt[4]{N_4}}.
\end{aligned}$$

This completes the proof of the theorem. ∎

Theorem 16. *Let G be a graph of order n with a hyper-Zagreb index $HM(G)$. Then*

$$\mathrm{ZE}(G) \leqslant \sqrt{\frac{2(3n-1)}{3}\,HM(G)} \tag{7}$$

with equality holding if and only if $G \cong \overline{K}_n$.

Proof. For $G \cong \overline{K}_n$, we have $\mathrm{ZE}(G)=0$ and $HM(G)=0$. Hence the equality holds in (7). Otherwise, $G \ncong \overline{K}_n$. Setting $a_i=|\zeta_i|$ and $r=0 \leq |\zeta_i| \leq \zeta_1 = R$ in Lemma 3, we obtain

$$(n-1)\sum_{i=2}^{n}\zeta_i^2-\Big(\mathrm{ZE}(G)-\zeta_1\Big)^2 \geqslant \frac{n-1}{2}\,\zeta_1^2.$$

After simplifying, we get

$$\mathrm{ZE}(G) \leqslant \zeta_1 + \sqrt{(n-1)(2HM - \zeta_1^2) - \frac{n-1}{2}\,\zeta_1^2}.$$

Let us consider a function

$$h(x) = x + \sqrt{(n-1)(2HM - x^2) - \frac{n-1}{2}\,x^2}.$$

One can easily see that the function $h(x)$ is an increasing function on $x \leqslant \sqrt{\frac{8HM(G)}{3(3n-1)}}$ and a decreasing function on $x \geqslant \sqrt{\frac{8HM(G)}{3(3n-1)}}$. Hence

$$\mathrm{ZE}(G) \leqslant h\left(\sqrt{\frac{8HM(G)}{3(3n-1)}}\right) = \sqrt{\frac{2(3n-1)}{3}\,HM(G)}.$$

The first part of the proof is done.

Suppose that equality holds in (7). Then we have $\zeta_1 = \sqrt{\frac{8HM(G)}{3(3n-1)}}$. Since

$$n\,\zeta_1^2 \geq \sum_{i=1}^{n} \zeta_i^2 = 2HM(G),$$

we have

$$\frac{8n\,HM(G)}{3(3n-1)} \geq 2HM(G), \quad \text{that is,} \quad n \leq 3/5, \quad \text{a contradiction.}$$

This completes the proof of the theorem. ■

Here we give an upper bound on $\mathrm{ZE}(G)$.

Theorem 17. *Let G be a graph of order n with a hyper-Zagreb index $HM(G)$. Then*

$$\mathrm{ZE}(G) \leqslant e^{\sqrt{2HM(G)}} - 1 - \sqrt{2\,HM(G)} \tag{8}$$

with equality holding if and only if $G \cong \overline{K}_n$.

Proof. For $G \cong \overline{K}_n$, we have $\mathrm{ZE}(G) = 0 = e^{\sqrt{2HM(G)}} - 1 - \sqrt{2\,HM(G)}$ and hence the equality holds in (8). Otherwise, $G \not\cong \overline{K}_n$. Let p $(0 \leqslant p \leqslant n-2)$ be the number of isolated vertices in G. Suppose that $G \cong H \cup p\,K_1$. Let $k\,(\geq 1)$ be the number of connected components of the graph H. Also let n_i (≥ 2) be the number of vertices of the i-th connected component H_i of the graph H, where $i = 1, 2, \ldots, k$. Without loss of generality, we can assume that $n_1 \geq n_2 \geq \cdots \geq n_k \geq 2$. Then one can easily see that

$$HM(H_i) = \sum_{v_i v_j \in E(H_i)} (d_i + d_j)^2 \geqslant 4(n_i - 1) \geqslant 2n_i,\ i = 1, 2, \ldots, k.$$

Thus we have

$$HM(G) = HM(H) = \sum_{i=1}^{k} HM(H_i) \geq 2(n-p).$$

Using the above result with (7), we obtain

$$\begin{aligned} \mathrm{ZE}(G) &= \mathrm{ZE}(H) \leqslant \sqrt{\frac{2(3n-3p-1)}{3}\,HM(H)} < HM(H) = HM(G) \\ &< \sum_{k\geq 2} \frac{(\sqrt{2HM(G)})^k}{k!} = e^{\sqrt{2HM(G)}} - 1 - \sqrt{2\,HM(G)}. \end{aligned}$$

This completes the proof of the theorem. ■

Corollary 18. [2] *Let G be a graph with a hyper-Zagreb index $HM(G)$. Then*

$$\mathrm{ZE}(G) < e^{\sqrt{2HM(G)}}.$$

Remark 19. Our upper bound on ZE(G) in Theorem 17 is better than the previous upper bound in Theorem 2 [2].

Remark 20. In [2], two lower bounds on ZE(G) have been obtained in Theorems 2 and 3. These lower bounds are as follows:

$$\mathrm{ZE}(G) \geqslant e^{-\sqrt{2HM(G)}} \quad \text{and} \quad \mathrm{ZE}(G) \geqslant \frac{1}{2HM(G)}.$$

The first lower bound is not correct for $G \cong \overline{K}_n$. For $G \ncong \overline{K}_n$, both these results are trivial because

$$\mathrm{ZE}(G) > 1 > e^{-\sqrt{2HM(G)}} \quad \text{and} \quad \mathrm{ZE}(G) > 1 > \frac{1}{2HM(G)}.$$

The following three results are obtained in [2], but not determined extremal graphs. By Lemma 5, one can easily get the extremal graphs.

Remark 21. Let G be a graph of order n with a hyper-Zagreb index $HM(G)$. Then
(*i*) $\sqrt{2HM(G)} \leqslant \mathrm{ZE}(G) \leqslant \sqrt{2n\,HM(G)}$ with left (right) equality holding if and only if $G \cong \overline{K}_n$ ($G \cong \overline{K}_n$ or $G \cong \frac{n}{2}\,K_2$ (n is even)).

(*ii*) $\mathrm{ZE}(G) \geqslant \sqrt{2HM(G) + n(n-1)\,|\mathbf{det}\,Z(G)|^{\frac{2}{n}}}$ with equality holding if and only if $G \cong \overline{K}_n$ or $G \cong \frac{n}{2}\,K_2$.

(*iii*) $\mathrm{ZE}(G) \geqslant n\sqrt[n]{|\mathbf{det}\,Z(G)|}$ with equality holding if and only if $G \cong \overline{K}_n$ or $G \cong \frac{n}{2}\,K_2$.

In [2], Theorem 4 is not correct. One of the reason is that the incorrect Lemma 1 [2] has been used. Here we have corrected the lower bound on ZEE(G), which is as follows:

Theorem 22. *Let G be a graph of order n with a hyper-Zagreb index $HM(G)$. Then*

$$\mathrm{ZEE}(G) \geqslant n + HM(G) + 6\Bigg(\sinh(1) - 1\Bigg) \sum_{i\sim j\sim k\sim i} (d_i + d_j)(d_j + d_k)(d_k + d_i)$$

$$+ \Bigg(\cosh(1) - \frac{3}{2}\Bigg) \sum_{i=1}^{n} \sum_{j=1}^{n} \Bigg(\sum_{k:\, i\sim k\sim j} (d_i + d_k)(d_j + d_k)\Bigg)^2 .$$

Proof. Note that $N_2 = 2HM(G)$. By Lemma 2, we obtain

$$\begin{aligned}
\mathrm{ZEE}(G) &= n + HM(G) + \sum_{k\geqslant 1} \frac{N_{2k+1}}{(2k+1)!} + \sum_{k\geqslant 1} \frac{N_{2k+2}}{(2k+2)!} \\
&\geqslant n + HM(G) + \sum_{k\geqslant 1} \frac{N_3}{(2k+1)!} + \sum_{k\geqslant 1} \frac{N_4}{(2k+2)!} \\
&= n + HM(G) + 6\Bigg(\sinh(1) - 1\Bigg) \sum_{i\sim j\sim k\sim i} (d_i + d_j)(d_j + d_k)(d_k + d_i) \\
&+ \Bigg(\cosh(1) - \frac{3}{2}\Bigg) \sum_{i=1}^{n} \sum_{j=1}^{n} \Bigg(\sum_{k:\, i\sim k\sim j} (d_i + d_k)(d_j + d_k)\Bigg)^2 .
\end{aligned}$$

This completes the proof of the theorem. ■

The proof of the Theorem 5 in [2] is also not correct because the spectrum of K_2 is 2, −2, but the authors mentioned 1, −1. So we have corrected the result and it is a better upper bound than the previous one.

Theorem 23. *Let G be a graph of order n with a hyper-Zagreb index $HM(G)$. If G has at least one edge, then*

$$\mathrm{ZEE}(G) < n - 1 + e^{\sqrt{2HM(G)-4}}. \tag{9}$$

Proof. Let m and n_+ be the number of edges and the number of positive Zagreb eigenvalues of G, respectively. Since $f(x) = e^x$ monotonically increases in the interval $(-\infty, +\infty)$ and $m \geqslant 1$, from the proof of Theorem 5 in [2], we obtain

$$\mathrm{ZEE}(G) = \sum_{i=1}^{n} e^{\zeta_i} < n + \sum_{k\geqslant 1} \frac{1}{k!} \Bigg[\sum_{i=1}^{n_+} \zeta_i^2\Bigg]^{\frac{k}{2}}. \tag{10}$$

Since every (n, m)-graph with $m \neq 0$ has K_2 as its induced subgraph and the spectrum of K_2 is 2, −2 it follows from the interlacing inequalities that $\zeta_n \leqslant -2$, which implies that, $\sum\limits_{i=n_+ +1}^{n} \zeta_i^2 \geqslant 4$. Consequently,

$$\mathrm{ZEE}(G) < n + \sum_{k\geqslant 1} \frac{1}{k!} \Big[2HM(G) - 4\Big]^{\frac{k}{2}} = n - 1 + e^{\sqrt{2HM(G)-4}}.$$

■

The following result has been proved in Theorem 6 [2]:

$$\mathrm{ZEE}(G) \geqslant \sqrt{n^2(1+HM(G)) + 2n\,HM(G) + \frac{2HM(G)\Big(\sum\limits_{k\sim i,\,k\sim j} (d_k)^2\Big)}{3} + \frac{n}{12}\,N_4}.$$

This result is also not true. Since

$$\sum_{i=1}^{n}\sum_{j=1}^{n} \frac{\zeta_i^2\zeta_j^2}{4} = HM(G)^2 \quad\text{and}\quad \sum_{i=1}^{n}\sum_{j=1}^{n}\left(\frac{\zeta_i^3}{6}+\frac{\zeta_j^3}{6}\right) = \frac{n}{6}\sum_{i=1}^{n}\zeta_i^3 + \frac{n}{6}\sum_{j=1}^{n}\zeta_j^3 = \frac{n}{3}\,N_3,$$

the corrected result is in the following without proof.

Theorem 24. *Let G be a graph of order n with a hyper-Zagreb index $HM(G)$. Then*

$$\mathrm{ZEE}(G) \geqslant \sqrt{n^2 + HM(G)^2 + 2n\,HM(G) + \frac{n}{3}\,N_3 + \frac{n}{12}\,N_4}.$$

From the above result one can easily obtained a lower bound on ZEE(G) which is mentioned in Theorem 7 [2].

Corollary 25. [2] *Let G be an graph with n vertices. Then*

$$\mathrm{ZEE}(G) \geqslant \sqrt{n^2 + 4HM(G)}. \tag{11}$$

The following result is mentioned in Theorem 10 [2], but the extremal graph is not mentioned.

Theorem 26. *Let G be a graph of order n with the number of positive Zagreb eigenvalues n_+. Then*

$$\frac{1}{2}\,(e-1)\,\mathrm{ZE}(G) + n - n_+ \leqslant \mathrm{ZEE}(G) \leqslant n - 1 + e^{\mathrm{ZE}(G)/2}. \tag{12}$$

Moreover, both equalities hold if and only if $G \cong \overline{K}_n$.

Proof. For $G \cong \overline{K}_n$, we have $\zeta_i = 0$ for all i, $1 \le i \le n$ and $n_+ = 0$. Thus $\mathrm{ZEE}(G) = n = \frac{1}{2}\,(e-1)\,\mathrm{ZE}(G) + n - n_+ = n - 1 + e^{\mathrm{ZE}(G)/2}$ and hence both of the equalities hold. Otherwise, $G \not\cong \overline{K}_n$. Then $\zeta_1 > 0$ and $\zeta_n < 0$. Similarly, using the proof of Theorem 10 in [2], we get the required result. ■

Using Theorem 11 [2] with Corollary 7, we obtain the following result:

Theorem 27. *Let G be a graph with a minimum degree δ and let p, τ and q be, respectively, the number of positive, zero and negative Zagreb eigenvalues of G. Then*

$$\mathrm{ZEE}(G) \geqslant e^{2\delta^2} + \tau + (p-1)e^{\frac{\mathrm{ZE}(G)-4\delta^2}{2(p-1)}} + qe^{-\frac{\mathrm{ZE}(G)}{2q}}. \tag{13}$$

Proof. By Theorem 11 in [2], we obtain

$$\mathrm{ZEE}(G) \geqslant e^{\zeta_1} + \tau + (p-1)e^{\frac{\mathrm{ZE}(G)-2\zeta_1}{2(p-1)}} + qe^{-\frac{\mathrm{ZE}(G)}{2q}}.$$

Let us consider a function

$$f(x) = e^x + \tau + (p-1)e^{\frac{\mathrm{ZE}(G)-2x}{2(p-1)}} + qe^{-\frac{\mathrm{ZE}(G)}{2q}}, \quad x \geq 2\delta^2.$$

Since $\mathrm{ZE}(G) = 2\sum_{i=1}^{p} \zeta_i \leq 2p\,\zeta_1$, from the above, we get

$$f'(x) = e^x - e^{\frac{\mathrm{ZE}(G)-2x}{2(p-1)}} \geqslant 0.$$

Then $f(x)$ is an increasing function on $x \geqslant 2\delta^2$ and hence

$$\mathrm{ZEE}(G) \geqslant f(2\delta^2) = e^{2\delta^2} + \tau + (p-1)e^{\frac{\mathrm{ZE}(G)-4\delta^2}{2(p-1)}} + qe^{-\frac{\mathrm{ZE}(G)}{2q}},$$

which gives the required result. ■

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