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Zagreb Energy and Zagreb Estrada Index of Graphs

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Abstract

Let G be a graph of order n with vertices labeled as $v_1, v_2, \ldots, v_n$. Let d_i be the degree of the vertex v_i, for $i = 1, 2, \ldots, n$. The (first) Zagreb matrix of G is the square matrix of order n whose (i, j)-entry is equal to $d_i + d_j$ if v_i is adjacent to v_j, and zero otherwise. We introduce and investigate the Zagreb energy and Zagreb Estrada index of a graph, both base on the eigenvalues of the Zagreb matrix. In addition, we establish upper and lower bounds for these new graph invariants, and relations between them.

1 Introduction

All graphs considered in this paper are assumed to be simple. Let G be a (molecular) graph with vertex set $\mathbf{V}(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $\mathbf{E}(G)$. If v_i and v_j are adjacent vertices of G, then the edge connecting them is denoted by $v_i v_j$. By d_i we denote the degree of the vertex $v_i \in \mathbf{V}(G)$.

In mathematical chemistry, there is a large number of topological indices of the form

$$TI = TI(G) = \sum_{v_i v_j \in \mathbf{E}(G)} \mathcal{F}(d_i, d_j)$$

where F is a pertinently chosen function with the property $\mathcal{F}(x, y) = \mathcal{F}(y, x)$. The most popular topological indices of this kind are the:

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- first Zagreb index, $\mathcal{F} = x + y$,
- second Zagreb index, $\mathcal{F} = x \cdot y$,
- Randić connectivity index, $\mathcal{F} = 1/\sqrt{xy}$,
- harmonic index, $\mathcal{F} = 2/(x+y)$,
- atom–bond connectivity (ABC) index, $\mathcal{F} = \sqrt{(x+y-2)/(xy)}$,
- geometric–arithmetic index, $\mathcal{F} = 2\sqrt{xy}/(x+y)$.

Note that there are several more indices, see [11]. To each of such topological indices, a matrix **TI** can be associated, defined as

$$(\mathbf{TI})_{ij} = \begin{cases} \mathcal{F}(d_i, d_j) & \text{if } v_i v_j \in \mathbf{E}(G) \\ 0 & \text{otherwise}\,. \end{cases}$$

If $f_1, f_2, \ldots, f_n$ are the eigenvalues of the matrix **TI**, then an "*energy*" can be defined as

$$\mathcal{E}_{TI} = \mathcal{E}_{TI}(G) = \sum_{i=1}^{n} |f_i|\,.$$

The most extensively studied such graph energy is the *Randić energy* [4, 5, 8], based on the eigenvalues of the Randić matrix **R**, where

$$(\mathbf{R})_{ij} = \begin{cases} \frac{1}{\sqrt{d_i\, d_j}} & \text{if } v_i v_j \in \mathbf{E}(G) \\ 0 & \text{otherwise}\,. \end{cases}$$

Recently, the analogous concepts of *harmonic energy* [16], *ABC energy* [10], and *geometric–arithmetic energy* [23] were put forward.

Bearing this in mind, it seems to be purposeful to consider also the graph energies pertaining to the first and second Zagreb indices, especially in view of the fact that these are the oldest [13–15, 20] and most thoroughly examined vertex–degree–based topological indices, see the recent reviews [2, 3] and the references cited therein. If so, then we would have to introduce the *first Zagreb matrix* $\mathbf{Z^{(1)}}$ and the *second Zagreb matrix* $\mathbf{Z^{(2)}}$, respectively, defined as:

$$\left(\mathbf{Z^{(1)}}\right)_{ij} = \begin{cases} d_i + d_j & \text{if } v_i v_j \in \mathbf{E}(G) \\ 0 & \text{otherwise} \end{cases}$$

and

$$\left(\mathbf{Z^{(2)}}\right)_{ij} = \begin{cases} d_i \cdot d_j & \text{if } v_i v_j \in \mathbf{E}(G) \\ 0 & \text{otherwise}\,. \end{cases}$$

If the eigenvalues of $\mathbf{Z^{(1)}}$ are $\zeta_1^{(1)}, \zeta_2^{(1)}, \ldots, \zeta_n^{(1)}$, then the *first Zagreb energy* would be

$$ZE_1 = ZE_1(G) = \sum_{i=1}^{n} |\zeta_i^{(1)}|\,.$$

If the eigenvalues of $\mathbf{Z^{(2)}}$ are $\zeta_1^{(2)}, \zeta_2^{(2)}, \ldots, \zeta_n^{(2)}$, then the *second Zagreb energy* would be

$$ZE_2 = ZE_2(G) = \sum_{i=1}^{n} |\zeta_i^{(2)}|\,.$$

Remark. At this point it is worth noting that a quantity somewhat similar to the first Zagreb index was earlier examined under the name "*vertex sum energy*" [16,17,22]. It is defined as the sum of absolute values of the eigenvalues of the matrix whose (i,j)-element is equal to $d_i + d_j$ if $i \neq j$, and zero if $i = j$. Thus, the first Zagreb energy and the vertex sum energy coincide if and only if $G \cong K_n$ or $G \cong \overline{K_n}$.

2 First Zagreb index and first Zagreb energy

The first and second Zagreb index, usually denoted by M_1 and M_2, are defined as [14,15]

$$M_1 = M_1(G) = \sum_{v_i \in \mathbf{V}(G)} d_i^2 \qquad \text{and} \qquad M_2 = M_2(G) = \sum_{v_i v_j \in \mathbf{E}(G)} d_i\, d_j$$

whereas the first Zagreb index satisfies the identity

$$M_1 = \sum_{v_i v_j \in \mathbf{E}(G)} (d_i + d_j)\,.$$

In what follows, we shall be also concerned with the closely related quantity

$$HM = HM(G) = \sum_{v_i v_j \in \mathbf{E}(G)} (d_i + d_j)^2 \tag{1}$$

which is the so-called *hyper–Zagreb index*, recently introduced in [24], see also [1,12,21].

In this paper, we are concerned only with the first Zagreb index and the corresponding first Zagreb matrix and first Zagreb energy. The study of the analogous second–Zagreb quantities will be communicated in a forthcoming paper [18]. In view of this, in what follows, for the sake of simplicity, the indicator *first* will be omitted and we denote the (first) Zagreb matrix by $\mathbf{Z}$, its (i,j)-element by z_{ij}, its eigenvalues by $\zeta_1, \zeta_2, \ldots, \zeta_n$, and its energy by ZE. Thus,

$$z_{ij} = \begin{cases} d_i + d_j & \text{if the vertices } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{if the vertices } v_i \text{ and } v_j \text{ are not adjacent} \\ 0 & \text{if } i = j \end{cases}$$

and

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

This paper is organized as follows. In Section 3, we state some previously known results. In Section 4, we introduce and investigate the Zagreb energy and obtain lower and upper bounds for it. In Section 5, we put forward the concept of Zagreb Estrada index, and obtain lower and upper bounds for it. In Section 6, we investigate relations between Zagreb Estrada index and Zagreb energy.

3 Preliminaries and known results

In this section, we present previously known results that will be needed in the forthcoming sections. We first calculate $tr(\mathbf{Z}^2)$, $tr(\mathbf{Z}^3)$, and $tr(\mathbf{Z}^4)$, where tr denotes the trace of the respective matrix.

Denote by N_k the k-th spectral moment of the Zagreb matrix $\mathbf{Z}$, i. e.,

$$N_k = \sum_{i=1}^{n} (\zeta_i)^k \tag{2}$$

and recall that $N_k = tr(\mathbf{Z}^k)$.

Lemma 1. *Let G be a graph with n vertices and Zagreb matrix $\mathbf{Z}$. Then*

$$(1) \quad N_1 = tr(\mathbf{Z}) = 0 \tag{3}$$

$$(2) \quad N_2 = tr(\mathbf{Z}^2) = 2HM \tag{4}$$

$$(3) \quad N_3 = tr(\mathbf{Z}^3) = 2HM \sum_{\substack{i,j,k \in \{1,2,\ldots,n\} \\ i \sim j \sim k \,,\, i \sim k}} d_k^2 \tag{5}$$

$$(4) \quad N_4 = tr(\mathbf{Z}^4) = n(HM)^2 + \sum_{\substack{i,j \in \{1,2,\ldots,n\} \\ i \sim j}} (d_i + d_j)^2 \left(\sum_{\substack{k \in \{1,2,\ldots,n\} \\ i \sim k \sim j}} d_k^2 \right)^2 , \tag{6}$$

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

Proof. (1) By definition, the diagonal elements of $\mathbf{Z}$ are equal to zero. Therefore the *trace* of $\mathbf{Z}$ is zero.

(2) The diagonal elements of $\mathbf{Z}^2$ are

$$(\mathbf{Z}^2)_{ii} = \sum_{j=1}^{n} z_{ij}\, z_{ji} = \sum_{j=1}^{n} (z_{ij})^2 = \sum_{\substack{j \in \{1,2,\ldots,n\} \\ i \sim j}} (z_{ij})^2 = \sum_{\substack{j \in \{1,2,\ldots,n\} \\ i \sim j}} (d_i + d_j)^2$$

and therefore

$$tr(\mathbf{Z}^2) = \sum_{i=1}^{n} \sum_{\substack{j\in\{1,2,\dots,n\}\\ i\sim j}} (d_i+d_j)^2 = 2 \sum_{\substack{i,j\in\{1,2,\dots,n\}\\ i\sim j}} (d_i+d_j)^2 = 2HM\,.$$

In addition, for $i \neq j$

$$(\mathbf{Z}^2)_{ij} = \sum_{j=1}^{n} z_{ij}\, z_{ji} = z_{ii}\, z_{ij} + z_{ij}\, z_{jj} + \sum_{\substack{k\in\{1,2,\dots,n\}\\ i\sim k\sim j}} z_{ik}\, z_{kj} = (d_i+d_j) \sum_{\substack{k\in\{1,2,\dots,n\}\\ i\sim k\sim j}} (d_k)^2\,.$$

(3) Since the diagonal elements of $\mathbf{Z}^3$ are

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

we obtain

$$\begin{aligned} tr(\mathbf{Z}^3) &= \sum_{i=1}^{n} \sum_{\substack{j\in\{1,2,\dots,n\}\\ j\sim i}} (d_i+d_j)^2 \sum_{\substack{k\in\{1,2,\dots,n\}\\ i\sim k\sim j}} (d_k)^2 \\ &= 2 \sum_{\substack{i,j\in\{1,2,\dots,n\}\\ i\sim j}} (d_i+d_j)^2 \sum_{\substack{k\in\{1,2,\dots,n\}\\ i\sim k\sim j}} (d_k)^2 = 2HM \sum_{\substack{i,j,k\in\{1,2,\dots,n\}\\ i\sim j\sim k\,,\, i\sim k}} (d_k)^2. \end{aligned}$$

(4) The proof of formula (6) is analogous. ∎

Lemma 2. *For any non-negative real x, $e^x \geq 1 + x + \frac{x^2}{2} + \frac{x^3}{3} + \frac{x^4}{4}$. Equality holds if and only if $x = 0$.*

Lemma 3. *Let $x_1, x_2, \dots, x_n$ be positive numbers. Then*

$$\frac{n}{\frac{1}{x_1} + \cdots + \frac{1}{x_n}} \leq \sqrt[n]{x_1 x_2 \cdots x_n}\,.$$

Proof. By the arithmetic–geometric mean inequality, we have

$$\frac{1}{n}\left(\frac{1}{x_1} + \cdots + \frac{1}{x_n}\right) \geq \sqrt[n]{\frac{1}{x_1}\frac{1}{x_2}\cdots\frac{1}{x_n}}\,.$$

∎

Lemma 4. *(Chebishev's inequality [7]) Let $a_1 \leq a_2 \leq \cdots \leq a_n$ and $b_1 \leq b_2 \leq \cdots \leq b_n$ be real numbers. Then*

$$\left(\sum_{i=1}^{n} a_i\right)\left(\sum_{i=1}^{n} b_i\right) \leq n \sum_{i=1}^{n} a_i b_i\,.$$

Equality occurs if and only if $a_1 = a_2 = \cdots = a_n$ or $b_1 = b_2 = \cdots = b_n$.

Lemma 5. *For non-negative $x_1, x_2, \ldots, x_n$ and $k \geq 2$,*

$$\sum_{i=1}^{n} (x_i)^k \leq \left(\sum_{i=1}^{n} {x_i}^2 \right)^{k/2} . \tag{7}$$

Denote by M_k the number of closed walks of length k, equal to the k-th spectral moment of the adjacency matrix [6].

Lemma 6. [25] *Let G be a graph with m edges. Then for $k \geq 4$, $M_{k+2} \geq M_k$ with equality for all even $k \geq 4$ if and only if G consists of m copies of the complete graph on two vertices and possibly isolated vertices, and with equality for all odd $k \geq 5$ if and only if G is a bipartite graph.*

4 Bounds for Zagreb energy

Let n and m denote the number of vertices and edges of the graph under consideration. Recall that $\mathcal{E}$, the (ordinary) energy of a graph, is equal to the sum of absolute values of the eigenvalues of its adjacency matrix [19]. There exist several bounds on $\mathcal{E}$, depending on the parameters n and m [19].

Now, $2m$ is equal to the sum of the squares of the elements of the adjacency matrix. This implies that in the theory of Zagreb graph energy, the quantity $2\,HM$ will play the same role as $2m$ plays in the theory of ordinary graph energy, where HM is the hyper–Zagreb index, Eq. (1).

Bearing this in mind, we immediately arrive at the following estimates:

Theorem 1. *Let G be a graph with n vertices and hyper–Zagreb index HM. Then*

$$\sqrt{2HM} \leq ZE(G) \leq \sqrt{2nHM},$$

$$ZE(G) \geq \sqrt{2HM + n(n-1)\,|\det \mathbf{Z}(G)|^{2/n}},$$

$$ZE(G) \geq n\,\sqrt[n]{|\det \mathbf{Z}(G)|}\,.$$

Theorem 2. *Let G be a graph with hyper–Zagreb index HM. Then*

$$e^{-\sqrt{2HM}} \leq ZE(G) \leq e^{\sqrt{2HM}}\,. \tag{8}$$

Proof. For the sake of simplicity, we write $\xi_i = |\zeta_i|$.

Lower bound. By definition of the Zagreb energy and by the arithmetic–geometric mean inequality,

$$ZE(G) = \sum_{i=1}^{n} \xi_i = n \left(\frac{1}{n} \sum_{i=1}^{n} \xi_i \right) \geq n \left(\sqrt[n]{\xi_1 \xi_2 \cdots \xi_n} \right).$$

By Lemma 3, we have

$$\begin{aligned} n \sqrt[n]{\xi_1 \xi_2 \cdots \xi_n} &\geq n \left(\frac{n}{\sum_{i=1}^{n} \frac{1}{\xi_i}} \right) \geq n \left(\frac{n}{\sum_{i=1}^{n} \frac{1}{\xi_i} \sum_{i=1}^{n} \xi_i} \right) \geq n \left(\frac{n}{n \sum_{i=1}^{n} \frac{1}{\xi_i} \xi_i} \right) \qquad \text{(by Lemma 4)} \\ &\geq n \left(\frac{n}{n^2 \sum_{i=1}^{n} \xi_i} \right) > n \left(\frac{n}{n^2 \sum_{i=1}^{n} e^{\xi_i}} \right) = \frac{1}{\sum_{i=1}^{n} \sum_{k \geq 0} \frac{(\xi_i)^k}{k!}} \\ &= \frac{1}{\sum_{k \geq 0} \frac{1}{k!} \left(\sum_{i=1}^{n} (\xi_i)^k \right)} \geq \frac{1}{\sum_{k \geq 0} \frac{1}{k!} \left(\sum_{i=1}^{n} (\xi_i)^2 \right)^{k/2}} \qquad \text{(by inequality (7))} \\ &= \frac{1}{\sum_{k \geq 0} \frac{1}{k!} \left(\sum_{i=1}^{n} (\xi_i)^2 \right)^{k/2}} = \frac{1}{\sum_{k \geq 0} \frac{1}{k!} \left(\sqrt{2HM} \right)^k} \qquad \text{(by Eq. (4))}. \end{aligned}$$

Therefore, we have $ZE(G) \geq e^{-\sqrt{2HM}}$.

Upper bound. Starting with the definition of Zagreb energy, we get

$$ZE(G) = \sum_{i=1}^{n} \xi_i < \sum_{i=1}^{n} e^{\xi_i} = \sum_{i=1}^{n} \sum_{k \geq 0} \frac{(\xi_i)^k}{k!} = \sum_{k \geq 0} \frac{1}{k!} \sum_{i=1}^{n} (\xi_i)^k \leq \sum_{k \geq 0} \frac{1}{k!} \left(\sum_{i=1}^{n} (\xi_i)^2 \right)^{k/2}$$

by inequality (7), and

$$\begin{aligned} \sum_{k \geq 0} \frac{1}{k!} \left(\sum_{i=1}^{n} (\xi_i)^2 \right)^{k/2} &= \sum_{k \geq 0} \frac{1}{k!} \left(\sum_{i=1}^{n} (\xi_i)^2 \right)^{k/2} = \sum_{k \geq 0} \frac{1}{k!} \Big(2HM \Big)^{k/2}, \qquad \text{(by Eq. (4))} \\ &= \sum_{k \geq 0} \frac{1}{k!} \Big(\sqrt{2HM} \Big)^{k} = e^{\sqrt{2HM}}. \end{aligned}$$

■

Theorem 3. *Let G be a non-empty graph with hyper–Zagreb index HM. Then*

$$ZE(G) \geq \frac{1}{2HM}. \tag{9}$$

Proof. By definition of the Zagreb energy and by the arithmetic–geometric mean inequality, we have

$$ZE(G) = \sum_{i=1}^{n} \xi_i = n\left(\frac{1}{n}\sum_{i=1}^{n} \xi_i\right) \geq n\,\sqrt[n]{\xi_1\xi_2\cdots\xi_n}\,.$$

By Lemma 3,

$$n\,\sqrt[n]{\xi_1\xi_2\cdots\xi_n} \geq n\left(\frac{n}{\sum\limits_{i=1}^{n}\frac{1}{\xi_i}}\right) \geq n\left(\frac{n}{\sum\limits_{i=1}^{n}\frac{1}{\xi_i}\sum\limits_{i=1}^{n}\xi_i}\right) \geq n\left(\frac{n}{n\sum_{i=1}^{n}\frac{1}{\xi_i}\xi_i}\right)$$

by Lemma 4, and

$$\geq n\left(\frac{n}{n^2\sum\limits_{i=1}^{n}\xi_i}\right) \geq \frac{1}{\sum\limits_{i=1}^{n}(\xi_i)^k} \geq \frac{1}{\left(\sum\limits_{i=1}^{n}(\xi_i)^2\right)^{k/2}}$$

by inequality (7), and

$$= \frac{1}{\left(\sum\limits_{i=1}^{n}(\xi_i)^2\right)^{k/2}} = \frac{1}{(2HM)^{k/2}}$$

by Eq. (4). Hence, for $k = 2$, we arrive at (9). ■

5 Bounds on the Zagreb Estrada index

In this section, we consider the Zagreb Estrada index of a graph G, and give lower and upper bounds for it. We first recall that the Estrada index of a graph G is defined in [9] as

$$EE = EE(G) = \sum_{i=1}^{n} e^{\lambda_i},$$

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of the graph G, forming its spectrum [6]. Denoting by $M_k = M_k(G)$ the k-th spectral moment of the graph G,

$$M_k = M_k(G) = \sum_{i=1}^{n} (\lambda_i)^k,$$

we have

$$EE = \sum_{i=1}^{\infty} \frac{M_k(G)}{k!}\,.$$

Let thus G be a graph of order n whose Zagreb eigenvalues are $\zeta_1, \zeta_2, \dots, \zeta_n$. Then the *Zagreb Estrada index* of G, denoted by $ZEE(G)$, is defined to be

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

Recalling Eq. (2), it follows that

$$ZEE(G) = \sum_{i=1}^{\infty} \frac{N_k}{k!}.$$

Theorem 4. *Let G be a graph with n vertices. Then*

$$ZEE(G) \geq n + 2HM + 2HM\Big(\sinh(1) - 1\Big) \sum_{\substack{i,j,k \in \{1,2,\dots,n\} \\ i \sim k \sim j, i \sim j}} (d_k)^2$$
$$+ \Big(\cosh(1) - 1\Big) \left[n(HM)^2 + \sum_{\substack{i,j \in \{1,2,\dots,n\} \\ i \sim j}} (d_i + d_j)^2 \Big(\sum_{\substack{k \in \{1,2,\dots,n\} \\ i \sim k \sim j}} (d_k)^2 \Big)^2 \right].$$

Proof. Note that $N_2 = 2HM$. By Lemma 6,

$$\begin{aligned} ZEE(G) &= n + 2HM + \sum_{k \geq 1} \frac{N_{2k+1}}{(2k+1)!} + \sum_{k \geq 1} \frac{N_{2k+2}}{(2k+2)!} \\ &\geq n + 2HM + \sum_{k \geq 1} \frac{N_3}{(2k+1)!} + \sum_{k \geq 1} \frac{N_4}{(2k+2)!} \\ &= n + 2HM + 2HM\Big(\sinh(1) - 1\Big) \sum_{\substack{i,j,k \in \{1,2,\dots,n\} \\ i \sim k \sim j, i \sim j}} (d_k)^2 \\ &+ \Big(\cosh(1) - 1\Big) \left[n(HM)^2 + \sum_{\substack{i,j \in \{1,2,\dots,n\} \\ i \sim j}} (d_i + d_j)^2 \Big(\sum_{\substack{k \in \{1,2,\dots,n\} \\ i \sim k \sim j}} (d_k)^2 \Big)^2 \right]. \end{aligned}$$

■

Theorem 5. *Let G be a non-empty graph with hyper–Zagreb index HM. Then*

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

Proof. Let n_+ be the number of positive Zagreb eigenvalues of G. Since $f(x) = e^x$ monotonically increases in the interval $(\infty, +\infty)$ and $m \neq 0$, we get

$$ZEE = \sum_{i=1}^{n} e^{\zeta_i} < (n - n_+) + \sum_{i=1}^{n_+} e^{\zeta_i} = (n - n_+) + \sum_{i=1}^{n_+} \sum_{k \geq 0} \frac{(\zeta_i)^k}{k!}$$

$$= n + \sum_{k\geq 1} \frac{1}{k!} \sum_{i=1}^{n_+} (\zeta_i)^k \tag{10}$$

$$\leq n + \sum_{k\geq 1} \frac{1}{k!} \left(\sum_{i=1}^{n_+} \zeta_i^2 \right)^{k/2} = n + \sum_{k\geq 1} \frac{1}{k!} \left(\sum_{i=1}^{n_+} \zeta_i^2 \right)^{k/2}.$$

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

$$ZEE \geq n + \sum_{k\geq 1} \frac{1}{k!} (2HM - 1)^{k/2} = n - 1 + e^{\sqrt{2HM-1}}.$$

■

Theorem 6. *Let G be a graph with n vertices and hyper–Zagreb index HM. Then*

$$ZEE(G) \geq \sqrt{n^2(1 + HM) + 2nHM + \frac{2}{3} HM \sum_{\substack{i,j,k\in\{1,2,\dots,n\} \\ i\sim k\sim j, i\sim j}} (d_k)^2 + \frac{1}{12} n N_4}.$$

Proof. Suppose that $\zeta_1, \zeta_2, \dots, \zeta_n$ is the Zagreb spectrum of G. Using Lemma 2, we have

$$\begin{aligned} ZEE(G)^2 &= \sum_{i=1}^{n} \sum_{j=1}^{n} e^{\zeta_i + \zeta_j} \\ &\geq \sum_{i=1}^{n} \sum_{j=1}^{n} \left(1 + \zeta_i + \zeta_j + \frac{(\zeta_i + \zeta_j)^2}{2} + \frac{(\zeta_i + \zeta_j)^3}{6} + \frac{(\zeta_i + \zeta_j)^4}{24} \right) \\ &= \sum_{i=1}^{n} \sum_{j=1}^{n} \left(1 + \zeta_i + \zeta_j + \frac{\zeta_i^2}{2} + \frac{\zeta_j^2}{2} + \zeta_i \zeta_j + \frac{\zeta_i^3}{6} + \frac{\zeta_j^3}{6} + \frac{\zeta_i^2 \zeta_j}{2} + \frac{\zeta_i \zeta_j^2}{2} \right. \\ &\left. + \frac{\zeta_i^4}{24} + \frac{\zeta_j^4}{24} + \frac{\zeta_i^2 \zeta_j^2}{4} + \frac{\zeta_i^3 \zeta_j}{6} + \frac{\zeta_i \zeta_j^3}{6} \right). \end{aligned}$$

From Eqs. (3)–(6) it follows,

$$\sum_{i=1}^{n} \sum_{j=1}^{n} (\zeta_i + \zeta_j) = n \sum_{i=1}^{n} \zeta_i + n \sum_{j=1}^{n} \zeta_j = 0$$

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \zeta_i \zeta_j = \left(\sum_{i=1}^{n} \zeta_i \right)^2 = 0$$

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \left(\frac{\zeta_i^2}{2} + \frac{\zeta_j^2}{2} \right) = \frac{n}{2} \sum_{i=1}^{n} \zeta_i^2 + \frac{n}{2} \sum_{j=1}^{n} \zeta_j^2 = 2nHM$$

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \left(\frac{\zeta_i^3}{6} + \frac{\zeta_j^3}{6} \right) = \frac{n}{6} \sum_{i=1}^{n} \zeta_i^3 + \frac{n}{6} \sum_{j=1}^{n} \zeta_j^3 = \frac{2}{3} HM \sum_{\substack{i,j,k\in\{1,2,\dots,n\} \\ i\sim k\sim j, i\sim j}} (d_k)^2$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\frac{\zeta_i^4}{24}+\frac{\zeta_j^4}{24}\right)=\frac{n}{24}\sum_{i=1}^{n}\zeta_i^4+\frac{n}{24}\sum_{j=1}^{n}\zeta_j^4=\frac{1}{12}n\,N_4$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\zeta_i^2\zeta_j^2}{4}=n^2HM$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\zeta_i\zeta_j^3}{6}=\frac{1}{6}\sum_{i=1}^{n}\zeta_i\sum_{j=1}^{n}\zeta_j^3=0$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\zeta_i^3\zeta_j}{6}=\frac{1}{6}\sum_{i=1}^{n}\zeta_i^3\sum_{j=1}^{n}\zeta_j=0$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\zeta_i\zeta_j^2}{2}=\frac{1}{2}\sum_{i=1}^{n}\zeta_i\sum_{j=1}^{n}\zeta_j^3=0$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\zeta_i^2\zeta_j}{2}=\frac{1}{2}\sum_{i=1}^{n}\zeta_i^2\sum_{j=1}^{n}\zeta_j=0\,.$$

Combining the above relations, we get the inequality stated in Theorem 6. ∎

Theorem 7. *Let G be a graph with n vertices and hyper–Zagreb index HM. Then*

$$\sqrt{n^2+4HM}\leq ZEE(G)\leq n-1+e^{\sqrt{2HM}}\,. \tag{11}$$

Proof. **Lower bound**. Directly from the definition of the Zagreb Estrada index, we get

$$ZEE(G)^2=\sum_{i=1}^{n}e^{2\zeta_i}+2\sum_{i<j}e^{\zeta_i}e^{\zeta_j}\,. \tag{12}$$

In view of the inequality between the arithmetic and geometric means,

$$2\sum_{i<j}e^{\zeta_i}e^{\zeta_j}\geq n(n-1)\left(\prod_{i<j}e^{\zeta_i}e^{\zeta_j}\right)^{2/[n(n-1)]}=n(n-1)\left[\left(\prod_{i=1}^{n}e^{\zeta_i}\right)^{n-1}\right]^{2/[n(n-1)]}$$
$$=n(n-1)\left(e^{\sum_{i=1}^{n}\zeta_i}\right)^{2/n}=n(n-1)\,. \tag{13}$$

By means of a power-series expansion, and bearing in mind the properties of N_0, N_1, and N_2, we get

$$\sum_{i=1}^{n}e^{2\zeta_i}=\sum_{i=1}^{n}\sum_{k\geq 0}\frac{(2\zeta_i)^k}{k!}=n+4HM+\sum_{i=1}^{n}\sum_{k\geq 3}\frac{(2\zeta_i)^k}{k!}.$$

Because we are aiming at an (as good as possible) lower bound, it may look plausible to replace $\sum_{k\geq 3}\frac{(2\zeta_i)^k}{k!}$ by $8\sum_{k\geq 3}\frac{(\zeta_i)^k}{k!}$. However, instead of $8=2^3$ we shall use a multiplier $\omega\in[0,8]$, so as to arrive at

$$\sum_{i=1}^{n}e^{2\zeta_i}\geq n+4HM+\omega\sum_{i=1}^{n}\sum_{k\geq 3}\frac{(\zeta_i)^k}{k!}$$

$$= n + 4HM - \omega n - \omega HM + \omega \sum_{i=1}^{n} \sum_{k \geq 0} \frac{(\zeta_i)^k}{k!}$$

i.e.,

$$\sum_{i=1}^{n} e^{2\zeta_i} \geq (1-\omega)n + (4-\omega)HM + \omega ZEE(G)\,. \tag{14}$$

By substituting (13) and (14) back into (12), and solving for ZEE, we obtain

$$ZEE \geq \frac{\omega}{2} + \sqrt{\left(n - \frac{\omega}{2}\right)^2 + (4-\omega)HM}\,. \tag{15}$$

It is elementary to show that for $n \geq 2$ and $HM \geq 1$, the function

$$f(x) := \frac{x}{2} + \sqrt{\left(n - \frac{x}{2}\right)^2 + (4-x)HM}$$

monotonically decreases in the interval $[0, 8]$. Consequently, the best lower bound for ZEE is attained not for $\omega = 8$, but for $\omega = 0$. Setting $\omega = 0$ into (15) we arrive at the first half of Theorem 7.

Upper bound. By the definition of the Zagreb Estrada index,

$$\begin{aligned}
ZEE &= n + \sum_{i=1}^{n} \sum_{k \geq 1} \frac{(\zeta_i)^k}{k!} \leq n + \sum_{i=1}^{n} \sum_{k \geq 1} \frac{(\zeta_i)^k}{k!} \\
&= n + \sum_{k \geq 1} \frac{1}{k!} \sum_{i=1}^{n} \left[(\zeta_i)^2\right]^{k/2} \leq n + \sum_{k \geq 1} \frac{1}{k!} \left[\sum_{i=1}^{n} (\zeta_i)^2\right]^{k/2} \\
&= n + \sum_{k \geq 1} \frac{1}{k!} \Big(2HM\Big)^{k/2} = n - 1 + \sum_{k \geq 0} \frac{1}{k!} \Big(\sqrt{2HM}\Big)^k = n - 1 + e^{\sqrt{2HM}},
\end{aligned}$$

which directly leads to the right–hand side inequality in (11). Thus, the proof of Theorem 7 is completed. ■

Theorem 8. *Let G be a graph with n vertices. Then*

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

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

$$\begin{aligned}
ZEE(G) = \sum_{i=1}^{n} e^{\zeta_i} &= \sum_{i=1}^{n} \sum_{k=0}^{\infty} \frac{\zeta_i^k}{k!} \leq n + \sum_{i=1}^{n} \sum_{k=1}^{\infty} \frac{\zeta_i^k}{k!} \\
&= n + \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{i=1}^{n} (\zeta_i^4)^{k/4} \leq n + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\sum_{i=1}^{n} \zeta_i^4\right)^{k/4} = n + \sum_{k=1}^{\infty} \frac{1}{k!} (N_4)^{k/4} \\
&= n - 1 + \sum_{k=0}^{\infty} \frac{\sqrt[4]{N_4^k}}{k!} = n - 1 + e^{\sqrt[4]{N_4}}.
\end{aligned}$$

■

Theorem 9. *Let G be a graph with hyper–Zagreb index HM. Then*

$$ZEE(G) \leq e^{\sqrt{2MH}}\,. \tag{16}$$

Proof.

$$\begin{aligned}
ZEE(G) &= \sum_{k\geq 0} \frac{1}{k!} \sum_{i=1}^{n} (\zeta_i)^k \leq \sum_{k\geq 0} \frac{1}{k!} \left(\sum_{i=1}^{n} (\zeta_i)^2 \right)^{k/2} && \text{(by inequality (7))} \\
&= \sum_{k\geq 0} \frac{1}{k!} \left(\sum_{i=1}^{n} (\zeta_i)^2 \right)^{k/2} = \sum_{k\geq 0} \frac{1}{k!} (2MH)^{k/2} && \text{(by Eq. (4))} \\
&= \sum_{k\geq 0} \frac{1}{k!} (\sqrt{2MH})^k = e^{\sqrt{2MH}}.
\end{aligned}$$

■

6 Bounds for Zagreb Estrada index involving Zagreb energy

Theorem 10. *Let G be a graph on n vertices, with n_+ positive Zagreb eigenvalues. Then the Zagreb Estrada index $ZEE(G)$ and the graph Zagreb energy $ZE(G)$ satisfy the following inequalities:*

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

Proof. **Lower bound**. Note that $e^x \geq 1 + x$, with equality if and only if $x = 0$. Also, $e^x \geq ex$, with equality if and only if $x = 1$. Thus,

$$\begin{aligned}
ZEE(G) &= \sum_{i=1}^{n} e^{\zeta_i} = \sum_{\zeta_i > 0} e^{\zeta_i} + \sum_{\zeta_i \leq 0} e^{\zeta_i} \\
&\geq \sum_{\zeta_i > 0} e\zeta_i + \sum_{\zeta_i \leq 0} (1 + \zeta_i) \\
&= e(\zeta_1 + \zeta_2 + \cdots + \zeta_{n_+}) + (n - n_+) + (\zeta_{n_+ + 1} + \cdots + \zeta_n) \\
&= (e-1)(\zeta_1 + \zeta_2 + \cdots + \zeta_{n_+}) + (n - n_+) + \sum_{i=1}^{n} \zeta_i \\
&= \frac{1}{2} ZE(G)(e-1) + n - n_+\,.
\end{aligned}$$

Upper bound. From (10),

$$ZEE(G) \leq n + \sum_{k\geq 1} \frac{1}{k!} \sum_{i=1}^{n_+} (\zeta_i)^k \leq n + \sum_{k\geq 1} \frac{1}{k!} \left(\sum_{i=1}^{n_+} \zeta_i \right)^k = n - 1 + e^{ZE(G)/2}.$$

■

Theorem 11. *Let G be a graph with largest Zagreb eigenvalue ζ_1 and let p, τ and q be, respectively, the number of its positive, zero and negative Zagreb eigenvalues. Then*

$$ZEE(G) \geq e^{\zeta_1} + \tau + (p-1) e^{\frac{ZE(G)-2\zeta_1}{2(p-1)}} + q e^{-\frac{ZE(G)}{2q}}. \tag{17}$$

Proof. Let $\zeta_1, \ldots, \zeta_p$ be the positive, and $\zeta_{n-q+1}, \ldots, \zeta_n$ the negative eigenvalues of $\mathbf{Z}$. As the sum of eigenvalues is zero, one has

$$ZE(G) = 2 \sum_{i=1}^{p} \zeta_i = -2 \sum_{i=n-q+1}^{n} \zeta_i \, .$$

By the arithmetic–geometric mean inequality,

$$\sum_{i=2}^{p} e^{\zeta_i} \geq (p-1) e^{\frac{(\zeta_2 + \cdots + \zeta_p)}{(p-1)}} = (p-1) e^{\frac{ZE(G)-2\zeta_1}{2(p-1)}}.$$

Similarly,

$$\sum_{i=n-q+1}^{n} e^{\zeta_i} \geq q e^{-\frac{ZE(G)}{2q}}.$$

For the zero eigenvalues, we also have

$$\sum_{i=p+1}^{n-q} e^{\zeta_i} = \tau \, .$$

Thus, inequality (17) follows. ■

Theorem 12. *Let G be a graph with n vertices and hyper–Zagreb index HM. Then*

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

Proof. By the definitions of the Zagreb energy and Zagreb Estrada index, we have

$$\begin{aligned} ZEE(G) &= n + \sum_{i=1}^{n} \sum_{k\geq 1} \frac{(\zeta_i)^k}{k!} \leq n + \sum_{i=1}^{n} \sum_{k\geq 1} \frac{\zeta_i^k}{k!}, \\ ZEE(G) &\leq n + \mathcal{Z}E(G) + \sum_{i=1}^{n} \sum_{k\geq 2} \frac{\zeta_i^k}{k!} \end{aligned}$$

implying

$$ZEE(G) - ZE(G) \leq n + \sum_{i=1}^{n} \sum_{k\geq 2} \frac{\zeta_i^k}{k!} \leq n - 1 - \sqrt{2HM} + e^{\sqrt{2HM}}.$$

■

Theorem 13. *Let G be a graph with n vertices. Then*

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

Proof.

$$ZEE(G) = n + \sum_{i=1}^{n} \sum_{k \geq 1} \frac{\zeta_i^k}{k!} = n + \sum_{k \geq 1} \frac{1}{k!} \left(\sum_{i=1}^{n} \zeta_i^k \right) \leq n + \sum_{k \geq 1} \frac{(ZE(G))^k}{k!}.$$

■

7 Concluding Remarks

For a graph of order n, the first Zagreb matrix is defined as the square matrix whose (i, j)-element is equal to the sum of degrees of adjacent vertices v_i and v_j, and zero otherwise. The new concepts of first Zagreb energy and first Zagreb Estrada index are introduced. These graph invariants depend on the eigenvalues of the first Zagreb matrix in the same manner as the ordinary graph energy and Estrada index depend on the eigenvalues of the adjacency matrix. Their basic properties are determined. In particular, bounds for the Zagreb energy and for the Zagreb Estrada index are established, as well as relations between them.

The analogous second Zagreb energy and second Zagreb Estrada index, based on the eigenvalues of the second Zagreb matrix, are planned to be studied in a forthcoming paper [18].

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