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Zagreb Energy of Weighted Graphs

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Abstract. In this paper, first Zagreb and second Zagreb matrices are defined for weighted graphs and accordingly the first Zagreb and second Zagreb energy of weighted graphs are introduced. Moreover, some upper and lower bounds are presented for Zagreb energy of positive definite matrix weighted graphs. Also some bounds are obtained for number weighted and unweighted graphs.

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1. Introduction and Preliminaries

Let $G = (V(G), E(G))$ be a graph with vertex set $V(G)$ and edge set $E(G)$. If u, v are adjacent vertices, it is denoted by $u \sim v$ or $uv \in E(G)$. Degree of a vertex u is denoted by d_u. The concept of topological index of a graph is a numerical value which is invariant under graph isomorphism is arisen from the work of famous chemist Wiener [19]. Degree based topological indices plays an essential role in chemical graph theory (see [15]). One of these are *first Zagreb* and *second Zagreb* indices of a graph G which are defined by

$$\begin{aligned} M_1(G) &= \sum_{u\in V(G)} d_u^2 = \sum_{uv\in E(G)} d_u + d_v, \\ M_2(G) &= \sum_{uv\in E(G)} d_u d_v, \end{aligned}$$

respectively (see [4, 5]). There are many generalizations of Zagreb indices. In [10, 11], for $\alpha \in \mathbb{R}$, the following generalizations of the first Zagreb and second Zagreb index are introduced as

$$\begin{aligned} M_1^{(\alpha)}(G) &= \sum_{u\in V(G)} d_u^{\alpha} = \sum_{uv\in E(G)} \left(d_u^{\alpha-1} + d_v^{\alpha-1}\right), \\ M_2^{(\alpha)}(G) &= \sum_{uv\in E(G)} (d_u d_v)^{\alpha}, \end{aligned}$$

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which are called *general Zagreb indices* or *variable Zagreb indices,* nowadays. $M_2^{(\alpha)}(G)$ is known as *general Randić index*. In [21], another generalization is defined as

$$H_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha, \quad \alpha \in \mathbb{R}$$

and called *general sum-connectivity index*. For $\alpha = 2$, $H_\alpha(G)$ is called *hyper-Zagreb index* and denoted by $HM(G)$, namely

$$HM = HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2,$$

which is introduced by Shirdel et al. in [16].

In [6], energy of a graph is defined as sum of the absolute values of the eigenvalues of adjacency matrix. It is an attractive concept for chemists and mathematicians (see [3,7,9,17]).

Let $G = (V(G), E(G))$ be a graph with n vertices. In [14], the first Zagreb $\left(Z^{(1)}(G)\right)_{n\times n}$ and second Zagreb $\left(Z^{(2)}(G)\right)_{n\times n}$ matrices of a graph G are respectively defined such that the $(i, j) - th$ element of $Z^{(1)}(G)$ is $d_i + d_j$, if $v_iv_j \in E(G)$ and 0, otherwise and the $(i, j) - th$ element of $Z^{(2)}(G)$ is d_id_j, if $v_iv_j \in E(G)$ and 0, otherwise. The eigenvalues of $Z^{(1)}(G)$ and $Z^{(2)}(G)$ are called first Zagreb and second Zagreb eigenvalues of G which can be arranged as in non-increasing order $\lambda_1^{(1)} \geq \lambda_2^{(1)} \geq ... \geq \lambda_n^{(1)}$ and $\lambda_1^{(2)} \geq \lambda_2^{(2)} \geq ... \geq \lambda_n^{(2)}$, respectively. The first Zagreb energy $E_{Z^{(1)}}(G)$ and second Zagreb energy $E_{Z^{(2)}}(G)$ are defined as $E_{Z^{(1)}}(G) = \sum_{i=1}^{n} \left|\lambda_i^{(1)}\right|$ and $E_{Z^{(2)}}(G) = \sum_{i=1}^{n} \left|\lambda_i^{(2)}\right|$, respectively.

An edge weighted graph is a graph that has a numeric label w_{ij} associated with each edge ij, called the weight of the edge ij. In many applications, the weights are usually represented by nonnegative integers or square matrices. If each edge weight is 1, then the graph is called unweighted graph. We consider edge weighted graphs with edge weights of which have been assigned a positive definite matrix. Let w_{ij} be $t \times t$ positive definite weight matrix of the edge ij, assume that $w_{ij} = w_{ji}$ and for all $i \in V$, $w_i = \sum_{j:\, j\sim i} w_{ij}$.

Eigenvalue bounds of graph matrices of weighted graphs are widely studied by many mathematicians (see [2,8,18, 20]). Energy and distance energy of weighted graphs are considered in [1] and [2], respectively. By this motivation, we will define Zagreb energy of edge weighted graphs without loops and parallel edges. For this purpose, we firstly introduce weighted first Zagreb matrix $Z_w^{(1)}(G) = \left(z_{ij}^{(1)}\right)_{nt\times nt}$ of G and weighted second Zagreb matrix $Z_w^{(2)}(G) = \left(z_{ij}^{(2)}\right)_{nt\times nt}$ of G respectively as

$$z_{ij}^{(1)} = \begin{cases} w_i + w_j, & \text{if } i \sim j \\ 0 \quad , & \text{otherwise} \end{cases}, \tag{1.1}$$

$$z_{ij}^{(2)} = \begin{cases} w_iw_j, & \text{if } i \sim j \\ 0 \quad , & \text{otherwise} \end{cases}, \tag{1.2}$$

where 0 denotes $t \times t$ zero matrix. Since $Z_w^{(1)}(G)$ and $Z_w^{(2)}(G)$ are real symmetric matrices, weighted first Zagreb eigenvalues and weighted second Zagreb eigenvalues are real and can be arranged respectively as $\lambda_{w,1}^{(1)} \geq \lambda_{w,2}^{(1)} \geq ... \geq \lambda_{w,nt}^{(1)}$ and $\lambda_{w,1}^{(2)} \geq \lambda_{w,2}^{(2)} \geq ... \geq \lambda_{w,nt}^{(2)}$ in non-increasing order. Also we can define the first Zagreb and second Zagreb energy of a weighted graph G as

$$E_{Z_w^{(1)}} = E_{Z_w^{(1)}}(G) = \sum_{i=1}^{nt} \left|\lambda_{w,i}^{(1)}\right|,$$

$$E_{Z_w^{(2)}} = E_{Z_w^{(2)}}(G) = \sum_{i=1}^{nt} \left|\lambda_{w,i}^{(2)}\right|,$$

respectively. $E_{Z_w^{(1)}}$ and $E_{Z_w^{(2)}}$ can also be called as weighted first Zagreb energy and weighted second Zagreb energy. In above definition, setting $t = 1$ gives the first Zagreb and second Zagreb energy of number weighted graphs. By setting $t = 1, w_{ij} = 1$ for all i, j and $i \sim j$, we have $w_i = d_i$, thus an unweighted graph is obtained. If we consider (1.1) and (1.2) for an unweighted graph, then $Z^{(1)}(G)$ and $Z^{(2)}(G)$ matrices are obtained and also Zagreb energies $E_{Z^{(1)}}(G)$ and $E_{Z^{(2)}}(G)$.

In this paper, first Zagreb and second Zagreb energy of edge weighted graphs are introduced and some bounds are presented for the first Zagreb and second Zagreb energy for positive definite matrix weighted graphs. By means of these bounds some results are also obtained for number weighted and unweighted graphs. Firstly, we give the following known inequalities.

Lemma 1.1 (Pólya and Szegő, [13])**.** *If x_i and y_i $(1 \leq i \leq n)$ are positive real numbers, then*

$$\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i^2 \leq \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}}+\sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2\left(\sum_{i=1}^{n} x_i y_i\right)^2,$$

where $M_1 = \max_{1\leq i\leq n}\{x_i\}$, $M_2 = \max_{1\leq i\leq n}\{y_i\}$; $m_1 = \min_{1\leq i\leq n}\{x_i\}$, $m_2 = \min_{1\leq i\leq n}\{y_i\}$.

Lemma 1.2 (Ozeki, [12])**.** *If x_i and y_i $(1 \leq i \leq n)$ are non-negative real numbers, then*

$$\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i^2 - \left(\sum_{i=1}^{n} x_i y_i\right)^2 \leq \frac{n^2}{4}\left(M_1M_2 - m_1m_2\right)^2,$$

where M_i and m_i defined in Lemma 1.1.

2. Bounds for Weighted First Zagreb Energy

In this section, we present upper and lower bounds for the first Zagreb energy of matrix weighted graphs and assume that all of the matrix weighted graphs have $t\times t$ positive definite matrix edge weights. Further some bounds are obtained for number weighted and unweighted graphs. Fundamental properties will be given in the following lemma.

Lemma 2.1. *If G is a matrix weighted graph of order $n\,(\geq 3)$, then*

(1) $\sum\limits_{i=1}^{nt} \lambda_{w,i}^{(1)} = 0$ and $\sum\limits_{i=1}^{nt} \lambda_{w,i}^{(2)} = 0$,

(2) $\sum\limits_{i=1}^{nt} \left(\lambda_{w,i}^{(1)}\right)^2 = 2\mathcal{W}_1$ and $\sum\limits_{i=1}^{nt} \left(\lambda_{w,i}^{(2)}\right)^2 = 2\mathcal{W}_2$,

where $\mathcal{W}_1 = \sum\limits_{\substack{j:\ j\sim i\\ i,j\in\{1,2,\ldots,n\}}} \left(w_i + w_j\right)^2$ and $\mathcal{W}_2 = \sum\limits_{\substack{j:\ j\sim i\\ i,j\in\{1,2,\ldots,n\}}} \left(w_iw_j\right)^2$.

Proof. (1) Since diagonal elements of $Z_w^{(1)}(G)$ and $Z_w^{(2)}(G)$ matrices are equal to zero, obviously we have

$$\begin{aligned}\sum_{i=1}^{nt} \lambda_{w,i}^{(1)} &= tr\left[Z_w^{(1)}(G)\right] = 0,\\ \sum_{i=1}^{nt} \lambda_{w,i}^{(2)} &= tr\left[Z_w^{(2)}(G)\right] = 0,\end{aligned}$$

where $tr(.)$ stands for trace of a matrix.

(2) Also we have

$$\begin{aligned}\sum_{i=1}^{nt} \left(\lambda_{w,i}^{(1)}\right)^2 &= tr\left[\left(Z_w^{(1)}(G)\right)^2\right] = \sum_{i=1}^{n}\sum_{j:\ j\sim i}\left(w_i + w_j\right)^2 \\ &= 2\sum_{\substack{j:\ j\sim i\\ i,j\in\{1,2,\ldots,n\}}}\left(w_i + w_j\right)^2 = 2\mathcal{W}_1,\end{aligned} \tag{2.1}$$

and

$$\begin{aligned}\sum_{i=1}^{nt} \left(\lambda_{w,i}^{(2)}\right)^2 &= tr\left[\left(Z_w^{(2)}(G)\right)^2\right] = \sum_{i=1}^{n}\sum_{j:\ j\sim i}\left(w_iw_j\right)^2 \\ &= 2\sum_{\substack{j:\ j\sim i\\ i,j\in\{1,2,\ldots,n\}}}\left(w_iw_j\right)^2 = 2\mathcal{W}_2.\end{aligned} \tag{2.2}$$

□

Remark 2.2. Let G be an unweighted graph. By setting $t = 1$, $w_{ij} = 1$, for all i, j and $i \sim j$, we have $w_i = d_i$ and consider (2.1) and (2.2). Then

$$2 \sum_{\substack{j:\ j\sim i \\ i,j\in\{1,2,\ldots,n\}}} \left(w_i + w_j\right)^2 = 2 \sum_{\substack{j:\ j\sim i \\ i,j\in\{1,2,\ldots,n\}}} \left(d_i + d_j\right)^2 = 2HM = tr\left[\left(Z_w^{(1)}(G)\right)^2\right] \tag{2.3}$$

yields the result which is presented in [14] (see Lemma 1), where HM is the *hyper-Zagreb* index of G and

$$2 \sum_{\substack{j:\ j\sim i \\ i,j\in\{1,2,\ldots,n\}}} \left(w_i w_j\right)^2 = 2 \sum_{\substack{j:\ j\sim i \\ i,j\in\{1,2,\ldots,n\}}} \left(d_i d_j\right)^2 = 2M_2^{(2)} = tr\left[\left(Z_w^{(2)}(G)\right)^2\right], \tag{2.4}$$

where $M_2^{(2)}$ is the general Randić index of G with $\alpha = 2$. Thus in unweighted case $\mathcal{W}_1 = HM$ and $\mathcal{W}_2 = M_2^{(2)}$.

Theorem 2.3. *If G is a matrix weighted graph of order $n\,(\geq 3)$, then*

$$E_{Z_w^{(1)}}(G) \leq \left|\lambda_{w,1}^{(1)}\right| + \sqrt{(nt-1)\left(2\mathcal{W}_1 - \left(\lambda_{w,1}^{(1)}\right)^2\right)}, \tag{2.5}$$

where $\lambda_{w,1}^{(1)}$ is the largest eigenvalue of $Z_w^{(1)}(G)$.

Proof. It is obvious that

$$E_{Z_w^{(1)}} - \left|\lambda_{w,1}^{(1)}\right| = \sum_{i=2}^{nt} \left|\lambda_{w,i}^{(1)}\right|.$$

Setting $x_i = 1$ and $y_i = \left|\lambda_{w,i}^{(1)}\right|$ $(1 \leq i \leq nt)$, applying Cauchy-Schwarz inequality and using (2.1) yields

$$\begin{aligned}
\left(E_{Z_w^{(1)}} - \left|\lambda_{w,1}^{(1)}\right|\right)^2 &= \left(\sum_{i=2}^{nt} \left|\lambda_{w,i}^{(1)}\right|.1\right)^2 \leq \sum_{i=2}^{nt} \left(\lambda_{w,i}^{(1)}\right)^2 \sum_{i=2}^{nt} 1^2 \\
&= (nt-1) \sum_{i=2}^{nt} \left(\lambda_{w,i}^{(1)}\right)^2 \\
&= (nt-1)\left(\sum_{i=1}^{nt} \left(\lambda_{w,i}^{(1)}\right)^2 - \left(\lambda_{w,1}^{(1)}\right)^2\right) \\
&= (nt-1)\left(2 \sum_{\substack{j:\ j\sim i \\ i,j\in\{1,2,\ldots,n\}}} \left(w_i + w_j\right)^2 - \left(\lambda_{w,1}^{(1)}\right)^2\right),
\end{aligned}$$

since $\mathcal{W}_1 = \sum_{\substack{j:\ j\sim i \\ i,j\in\{1,2,\ldots,n\}}} \left(w_i + w_j\right)^2$, we get the required result. □

Corollary 2.4. *If G is a number weighted graph of order n $(n \geq 3)$ with positive edge weights, then*

$$E_{Z_w^{(1)}}(G) \leq \left|\lambda_{w,1}^{(1)}\right| + \sqrt{(n-1)\left(2\mathcal{W}_1 - \left(\lambda_{w,1}^{(1)}\right)^2\right)}, \tag{2.6}$$

where $\lambda_{w,1}^{(1)}$ is the largest eigenvalue of $Z_w^{(1)}(G)$.

Proof. For a number weighted graph, if we take $t = 1$ in (2.5), then proof is completed. □

Corollary 2.5. *If G is an unweighted graph of order $n\,(\geq 3)$, then*

$$E_{Z^{(1)}}(G) \leq \left|\lambda_1^{(1)}\right| + \sqrt{(n-1)\left(2HM - \left(\lambda_1^{(1)}\right)^2\right)},$$

where HM is the hyper-Zagreb index of G and $\lambda_1^{(1)}$ is the largest first Zagreb eigenvalue of G.

Proof. For an unweighted graph, $t = 1$, $w_{ij} = 1$ and for all i, j and $i \sim j$, we have $w_i = d_i$ in (2.5). Using (2.3),

$$\begin{aligned} E_{Z^{(1)}} &\leq \left|\lambda_1^{(1)}\right| + \sqrt{(n-1)\left(2\sum_{\substack{j:\ j\sim i \\ i,j\in\{1,2,\ldots,n\}}} \left(d_i + d_j\right)^2 - \left(\lambda_1^{(1)}\right)^2\right)} \\ &\leq \left|\lambda_1^{(1)}\right| + \sqrt{(n-1)\left(2HM - \left(\lambda_1^{(1)}\right)^2\right)}, \end{aligned}$$

completes proof. □

Theorem 2.6. *If G is a matrix weighted graph of order $n\,(\geq 3)$, then*

$$\sqrt{2\mathcal{W}_1} \leq E_{Z_w^{(1)}}(G) \leq \sqrt{(2nt)\,\mathcal{W}_1}. \tag{2.7}$$

Proof. Taking $x_i = 1$ and $y_i = \left|\lambda_{w,i}^{(1)}\right|$ $(1 \leq i \leq nt)$ in Cauchy-Schwarz inequality, we get

$$\left(E_{Z_w^{(1)}}\right)^2 = \left(\sum_{i=1}^{nt} 1.\left|\lambda_{w,i}^{(1)}\right|\right)^2 \leq \sum_{i=1}^{nt} 1^2 \sum_{i=1}^{nt} \left(\lambda_{w,i}^{(1)}\right)^2 = nt \sum_{i=1}^{nt} \left(\lambda_{w,i}^{(1)}\right)^2.$$

From (2.1), we have

$$\left(E_{Z_w^{(1)}}\right)^2 \leq 2nt \sum_{\substack{j:\ j\sim i \\ i,j\in\{1,2,\ldots,n\}}} \left(w_i + w_j\right)^2 = (2nt)\,\mathcal{W}_1,$$

which determines the upper bound. On the other hand, if we use (2.1) then

$$\begin{aligned} \left(E_{Z_w^{(1)}}\right)^2 &= \left(\sum_{i=1}^{nt} \left|\lambda_{w,i}^{(1)}\right|\right)^2 \geq \sum_{i=1}^{nt} \left(\lambda_{w,i}^{(1)}\right)^2 \\ &= 2 \sum_{\substack{j:\ j\sim i \\ i,j\in\{1,2,\ldots,n\}}} \left(w_i + w_j\right)^2 = 2\mathcal{W}_1, \end{aligned}$$

so, proof is completed. □

Corollary 2.7. *If G is a number weighted graph of order $n\,(\geq 3)$ with positive edge weights, then*

$$\sqrt{2\mathcal{W}_1} \leq E_{Z_w^{(1)}}(G) \leq \sqrt{(2n)\,\mathcal{W}_1}. \tag{2.8}$$

Proof. If we take $t = 1$ in (2.7), then proof is obvious. □

The following bounds are presented in Theorem 1 in [14].

Corollary 2.8. *If G is an unweighted graph of order $n\,(\geq 3)$, then*

$$\sqrt{2HM} \leq E_{Z^{(1)}}(G) \leq \sqrt{2nHM},$$

where HM is the hyper-Zagreb index of G.

Proof. In an unweighted graph, $t = 1$, $w_{ij} = 1$ and for all i, j and $i \sim j$, $w_i = d_i$. Thus from (2.7)

$$\sqrt{2 \sum_{\substack{j:\ j\sim i \\ i,j\in\{1,2,\ldots,n\}}} \left(d_i + d_j\right)^2} \leq E_{Z^{(1)}} \leq \sqrt{2n \sum_{\substack{j:\ j\sim i \\ i,j\in\{1,2,\ldots,n\}}} \left(d_i + d_j\right)^2},$$

by (2.3), we have

$$\sqrt{2HM} \leq E_{Z^{(1)}} \leq \sqrt{2nHM},$$

completes proof. □

Theorem 2.9. *If G is a matrix weighted graph of order $n\,(\geq 3)$ and zero is not an eigenvalue of $Z_w^{(1)}(G)$, then*

$$E_{Z_w^{(1)}}(G) \geq \frac{2\sqrt{\lambda_{w,1}^{(1)}\lambda_{w,nt}^{(1)}}\sqrt{(2nt)\mathcal{W}_1}}{\lambda_{w,1}^{(1)}+\lambda_{w,nt}^{(1)}}, \tag{2.9}$$

where $\lambda_{w,1}^{(1)}$ and $\lambda_{w,nt}^{(1)}$ are maximum and minimum of the absolute value of $\lambda_{w,i}^{(1)}$s, respectively.

Proof. Assume that $x_i = \left|\lambda_{w,i}^{(1)}\right|$ and $y_i = 1$ $(1 \leq i \leq nt)$ and applying Pólya-Szegő inequality, we have

$$\sum_{i=1}^{nt}\left|\lambda_{w,i}^{(1)}\right|^2 \sum_{i=1}^{nt} 1^2 \leq \frac{1}{4}\left(\sqrt{\frac{\lambda_{w,nt}^{(1)}}{\lambda_{w,1}^{(1)}}}+\sqrt{\frac{\lambda_{w,1}^{(1)}}{\lambda_{w,nt}^{(1)}}}\right)^2\left(\sum_{i=1}^{nt}\left|\lambda_{w,i}^{(1)}\right|\right)^2.$$

By (2.1)

$$2nt\sum_{\substack{j:\ j\sim i\\ i,j\in\{1,2,\dots,n\}}}\left(w_i+w_j\right)^2 \leq \frac{1}{4}\frac{\left(\lambda_{w,1}^{(1)}+\lambda_{w,nt}^{(1)}\right)^2}{\lambda_{w,1}^{(1)}\lambda_{w,nt}^{(1)}}\left(E_{Z_w^{(1)}}\right)^2,$$

and

$$\begin{aligned} E_{Z_w^{(1)}} &\geq \frac{2\sqrt{\lambda_{w,1}^{(1)}\lambda_{w,nt}^{(1)}}\sqrt{2nt\sum\limits_{\substack{j:\ j\sim i\\ i,j\in\{1,2,\dots,n\}}}\left(w_i+w_j\right)^2}}{\lambda_{w,1}^{(1)}+\lambda_{w,nt}^{(1)}} \\ &= \frac{2\sqrt{\lambda_{w,1}^{(1)}\lambda_{w,nt}^{(1)}}\sqrt{(2nt)\mathcal{W}_1}}{\lambda_{w,1}^{(1)}+\lambda_{w,nt}^{(1)}}. \end{aligned}$$

□

Corollary 2.10. *If G is a number weighted graph of order $n\,(\geq 3)$ with positive edge weights and zero is not an eigenvalue of $Z_w^{(1)}(G)$, then*

$$E_{Z_w^{(1)}}(G) \geq \frac{2\sqrt{\lambda_{w,1}^{(1)}\lambda_{w,n}^{(1)}}\sqrt{(2n)\mathcal{W}_1}}{\lambda_{w,1}^{(1)}+\lambda_{w,n}^{(1)}},$$

where $\lambda_{w,1}^{(1)}$ and $\lambda_{w,n}^{(1)}$ are maximum and minimum of the absolute value of $\lambda_{w,i}^{(1)}$s, respectively.

Proof. If we write $t = 1$ in (2.9), then proof is obvious. □

Corollary 2.11. *If G is an unweighted graph of order $n\,(\geq 3)$ and zero is not an eigenvalue of $Z^{(1)}(G)$, then*

$$E_{Z^{(1)}}(G) \geq \frac{2\sqrt{2n\lambda_1^{(1)}\lambda_n^{(1)}HM}}{\lambda_1^{(1)}+\lambda_n^{(1)}},$$

where $\lambda_1^{(1)}$ and $\lambda_n^{(1)}$ are maximum and minimum of the absolute value of $\lambda_i^{(1)}$s, respectively.

Proof. Assume that $t = 1$ and $w_{ij} = 1$ for all i, j and $i \sim j$, we have $w_i = d_i$ in (2.9), then

$$E_{Z^{(1)}} \geq \frac{2\sqrt{\lambda_1^{(1)}\lambda_n^{(1)}}\sqrt{2n\sum\limits_{\substack{j:\ j\sim i\\ i,j\in\{1,2,\dots,n\}}}\left(d_i+d_j\right)^2}}{\lambda_1^{(1)}+\lambda_n^{(1)}}.$$

From (2.3), we have

$$E_{Z^{(1)}} \geq \frac{2\sqrt{2n\lambda_1^{(1)}\lambda_n^{(1)}HM}}{\lambda_1^{(1)}+\lambda_n^{(1)}},$$

thus we get the required result. □

Theorem 2.12. *If G is a matrix weighted graph of order $n\,(\geq 3)$, then*

$$E_{Z_w^{(1)}}(G) \geq \sqrt{2nt\mathcal{W}_1 - \frac{n^2t^2}{4}\left(\lambda_{w,1}^{(1)} - \lambda_{w,nt}^{(1)}\right)^2}, \tag{2.10}$$

where $\lambda_{w,1}^{(1)}$ and $\lambda_{w,nt}^{(1)}$ are maximum and minimum of the absolute value of $\lambda_{w,i}^{(1)}$s, respectively.

Proof. By substituting $x_i = \left|\lambda_{w,i}^{(1)}\right|$ and $y_i = 1$ $(1 \leq i \leq nt)$ in Ozeki inequality, then

$$\sum_{i=1}^{nt}\left|\lambda_{w,i}^{(1)}\right|^2 \sum_{i=1}^{nt} 1^2 - \left(\sum_{i=1}^{nt}\left|\lambda_{w,i}^{(1)}\right|\right)^2 \leq \frac{n^2t^2}{4}\left(\lambda_{w,1}^{(1)} - \lambda_{w,nt}^{(1)}\right)^2.$$

From (2.1), we have

$$2nt \sum_{\substack{j:\ j\sim i \\ i,j\in\{1,2,\ldots,n\}}} \left(w_i + w_j\right)^2 - \left(E_{Z_w^{(1)}}\right)^2 \leq \frac{n^2t^2}{4}\left(\lambda_{w,1}^{(1)} - \lambda_{w,nt}^{(1)}\right)^2,$$

and

$$E_{Z_w^{(1)}} \geq \sqrt{2nt\mathcal{W}_1 - \frac{n^2t^2}{4}\left(\lambda_{w,1}^{(1)} - \lambda_{w,nt}^{(1)}\right)^2}.$$

□

Corollary 2.13. *If G is a number weighted graph of order $n\,(\geq 3)$ with positive edge weights, then*

$$E_{Z_w^{(1)}}(G) \geq \sqrt{2n\mathcal{W}_1 - \frac{n^2}{4}\left(\lambda_{w,1}^{(1)} - \lambda_{w,n}^{(1)}\right)^2}, \tag{2.11}$$

where $\lambda_{w,1}^{(1)}$ and $\lambda_{w,n}^{(1)}$ are maximum and minimum of the absolute value of $\lambda_{w,i}^{(1)}$s, respectively.

Proof. Setting $t = 1$ in (2.10), proof is obvious. □

Corollary 2.14. *If G is an unweighted graph of order $n\,(\geq 3)$, then*

$$E_{Z^{(1)}}(G) \geq \sqrt{2nHM - \frac{n^2}{4}\left(\lambda_1^{(1)} - \lambda_n^{(1)}\right)^2},$$

where $\lambda_1^{(1)}$ and $\lambda_n^{(1)}$ are maximum and minimum of the absolute value of $\lambda_i^{(1)}$s, respectively.

Proof. For an unweighted graph, $t = 1$, $w_{ij} = 1$ and for all i, j and $i \sim j$, $w_i = d_i$. Thus from (2.10) and (2.3), we have

$$\begin{aligned} E_{Z^{(1)}}(G) &\geq \sqrt{2n\mathcal{W}_1 - \frac{n^2}{4}\left(\lambda_1^{(1)} - \lambda_n^{(1)}\right)^2} \\ &= \sqrt{2nHM - \frac{n^2}{4}\left(\lambda_1^{(1)} - \lambda_n^{(1)}\right)^2}, \end{aligned}$$

completes proof. □

In molecular graphs, the atoms of the molecule represent the vertices and the chemical bonds joining the atoms represent the edges. Now, we give an example for a number weighted molecular graph and calculate the weighted first Zagreb energy. In addition, the presented bounds are calculated for this graph (see Table 1).

Example 2.15. Consider the edge weighted molecular graph of methane (CH_4) molecule and assume that each edge has bond length weight (in nanometer). The bond length of $C - H$ is 0.11. So, all of the edge weights are 0.11. Thus

$$Z_w^{(1)} = \begin{bmatrix} 0 & 0.55 & 0.55 & 0.55 & 0.55 \\ 0.55 & 0 & 0 & 0 & 0 \\ 0.55 & 0 & 0 & 0 & 0 \\ 0.55 & 0 & 0 & 0 & 0 \\ 0.55 & 0 & 0 & 0 & 0 \end{bmatrix}$$

with eigenvalues -1.1 (once) , 0 (3 times), 1.1(once). Hence $E_{Z_w^{(1)}} = 2.2$. Moreover,

$$\mathcal{W}_1 = \sum_{\substack{j:\ j\sim i \\ i,j\in\{1,2,3,4,5\}}} \left(w_i + w_j\right)^2 = 4\,(0.55)^2 = 1.21.$$

lower bounds in Eq. (2.8)-(2.11)	$E_{Z_w^{(1)}}$	upper bounds in Eq. (2.8)-(2.6)
1.5 – 2.1	2.2	3.4 – 3.3

Table 1. Bounds for number weighted first Zagreb energy

3. Bounds for Weighted Second Zagreb Energy

In this section, we obtain some bounds for the second Zagreb energy of matrix weighted graphs, number weighted and unweighted graphs. Assume that all of the matrix weighted graphs have $t \times t$ positive definite matrix edge weights and recall $\mathcal{W}_2 = \sum_{\substack{j:\ j\sim i \\ i,j\in\{1,2,\dots,n\}}} \left(w_i w_j\right)^2$.

Theorem 3.1. *If G is a matrix weighted graph of order n (≥ 3), then*

$$E_{Z_w^{(2)}}(G) \le \left|\lambda_{w,1}^{(2)}\right| + \sqrt{(nt-1)\left(2\mathcal{W}_2 - \left(\lambda_{w,1}^{(2)}\right)^2\right)} \tag{3.1}$$

where $\lambda_{w,1}^{(2)}$ *is the largest eigenvalue of* $Z_w^{(2)}(G)$.

Proof. Consider $E_{Z_w^{(2)}}$ and setting $x_i = 1$ and $y_i = \left|\lambda_{w,i}^{(2)}\right|$ $(1 \le i \le nt)$, applying Cauchy-Schwarz inequality and using (2.2) yields

$$\begin{aligned}
\left(E_{Z_w^{(2)}} - \left|\lambda_{w,1}^{(2)}\right|\right)^2 &= \left(\sum_{i=2}^{nt} \left|\lambda_{w,i}^{(2)}\right|.1\right)^2 \le \sum_{i=2}^{nt}\left(\lambda_{w,i}^{(2)}\right)^2 \sum_{i=2}^{nt} 1^2 \\
&= (nt-1)\sum_{i=2}^{nt}\left(\lambda_{w,i}^{(2)}\right)^2 \\
&= (nt-1)\left(\sum_{i=1}^{nt}\left(\lambda_{w,i}^{(2)}\right)^2 - \left(\lambda_{w,1}^{(2)}\right)^2\right) \\
&= (nt-1)\left(2\sum_{\substack{j:\ j\sim i \\ i,j\in\{1,2,\dots,n\}}}\left(w_i w_j\right)^2 - \left(\lambda_{w,1}^{(2)}\right)^2\right),
\end{aligned}$$

the result. □

Corollary 3.2. *If G is a number weighted graph of order n (≥ 3) with positive edge weights, then*

$$E_{Z_w^{(2)}}(G) \le \left|\lambda_{w,1}^{(2)}\right| + \sqrt{(n-1)\left(2\mathcal{W}_2 - \left(\lambda_{w,1}^{(2)}\right)^2\right)}, \tag{3.2}$$

where $\lambda_{w,1}^{(2)}$ *is the largest eigenvalue of* $Z_w^{(2)}(G)$.

Proof. Proof is obvious from setting $t = 1$ in (3.1). □

Corollary 3.3. *If G is an unweighted graph of order n (≥ 3) , then*

$$E_{Z^{(2)}}(G) \le \left|\lambda_1^{(2)}\right| + \sqrt{(n-1)\left(2M_2^{(2)} - \left(\lambda_1^{(2)}\right)^2\right)},$$

where $\lambda_1^{(2)}$ *is the largest eigenvalue of* $Z^{(2)}(G)$.

Proof. Consider (3.1) for an unweighted graph with $t = 1$. Proof is obvious from Remark 2.2, since for an unweighted graph $\mathcal{W}_2 = M_2^{(2)}$. □

Theorem 3.4. *If G is a matrix weighted graph of order n (≥ 3), then*

$$\sqrt{2\mathcal{W}_2} \leq E_{Z_w^{(2)}}(G) \leq \sqrt{(2nt)\mathcal{W}_2}. \tag{3.3}$$

Proof. Consider $E_{Z_w^{(2)}}(G)$. Setting $x_i = 1$, $y_i = \left|\lambda_{w,i}^{(2)}\right|$ $(1 \leq i \leq nt)$ and applying Cauchy-Schwarz inequality, then

$$\left(E_{Z_w^{(2)}}\right)^2 = \left(\sum_{i=1}^{nt} 1.\left|\lambda_{w,i}^{(2)}\right|\right)^2 \leq \sum_{i=1}^{nt} 1^2 \sum_{i=1}^{nt}\left(\lambda_{w,i}^{(2)}\right)^2 = nt\sum_{i=1}^{nt}\left(\lambda_{w,i}^{(2)}\right)^2.$$

From (2.2), we get the upper bound as

$$\left(E_{Z_w^{(2)}}\right)^2 \leq 2nt \sum_{\substack{j:\ j\sim i\\ i,j\in\{1,2,\ldots,n\}}} \left(w_i w_j\right)^2 = 2nt\mathcal{W}_2.$$

On the other hand, using (2.2)

$$\begin{aligned}\left(E_{Z_w^{(2)}}\right)^2 &= \left(\sum_{i=1}^{nt}\left|\lambda_{w,i}^{(2)}\right|\right)^2 \geq \sum_{i=1}^{nt}\left(\lambda_{w,i}^{(2)}\right)^2\\ &= 2\sum_{\substack{j:\ j\sim i\\ i,j\in\{1,2,\ldots,n\}}}\left(w_i w_j\right)^2 = 2\mathcal{W}_2,\end{aligned}$$

completes proof. □

Corollary 3.5. *If G is a number weighted graph of order n (≥ 3) with positive edge weights, then*

$$\sqrt{2\mathcal{W}_2} \leq E_{Z_w^{(2)}}(G) \leq \sqrt{2n\mathcal{W}_2}. \tag{3.4}$$

Proof. Proof can be seen by $t = 1$ in (3.3). □

Corollary 3.6. *If G is an unweighted graph of order n (≥ 3), then*

$$\sqrt{2M_2^{(2)}} \leq E_{Z^{(2)}}(G) \leq \sqrt{2nM_2^{(2)}},$$

where $M_2^{(2)}$ is the general Randić index of G with $\alpha = 2$.

Proof. Consider (3.3) for an unweighted graph with $t = 1$. Proof can be seen from Remark 2.2 since $\mathcal{W}_2 = M_2^{(2)}$ for unweighted case. □

Theorem 3.7. *If G is a matrix weighted graph of order n (≥ 3) and zero is not an eigenvalue of $Z_w^{(2)}(G)$, then*

$$E_{Z_w^{(2)}}(G) \geq \frac{2\sqrt{\lambda_{w,1}^{(2)}\lambda_{w,nt}^{(2)}}\sqrt{2nt\mathcal{W}_2}}{\lambda_{w,1}^{(2)} + \lambda_{w,nt}^{(2)}}, \tag{3.5}$$

where $\lambda_{w,1}^{(2)}$ and $\lambda_{w,nt}^{(2)}$ are maximum and minimum of the absolute value of $\lambda_{w,i}^{(2)}$s, respectively.

Proof. By choosing $x_i = \left|\lambda_{w,i}^{(2)}\right|$ and $y_i = 1$ $(1 \leq i \leq nt)$ and applying Pólya-Szegő inequality yields

$$\sum_{i=1}^{nt}\left|\lambda_{w,i}^{(2)}\right|^2 \sum_{i=1}^{nt} 1^2 \leq \frac{1}{4}\left(\sqrt{\frac{\lambda_{w,nt}^{(2)}}{\lambda_{w,1}^{(2)}}} + \sqrt{\frac{\lambda_{w,1}^{(2)}}{\lambda_{w,nt}^{(2)}}}\right)^2\left(\sum_{i=1}^{nt}\left|\lambda_{w,i}^{(2)}\right|\right)^2.$$

From (2.2), we have

$$2nt\sum_{\substack{j:\ j\sim i\\ i,j\in\{1,2,\ldots,n\}}}\left(w_i w_j\right)^2 \leq \frac{1}{4}\frac{\left(\lambda_{w,1}^{(2)} + \lambda_{w,nt}^{(2)}\right)^2}{\lambda_{w,1}^{(2)}\lambda_{w,nt}^{(2)}}\left(E_{Z_w^{(2)}}\right)^2.$$

So, proof is obvious since $\mathcal{W}_2 = \sum_{\substack{j:\ j\sim i\\ i,j\in\{1,2,\ldots,n\}}}\left(w_i w_j\right)^2$. □

Corollary 3.8. *If G is a number weighted graph of order $n\,(\geq 3)$ with positive edge weights and zero is not an eigenvalue of $Z_w^{(2)}(G)$, then*

$$E_{Z_w^{(2)}}(G) \geq \frac{2\sqrt{\lambda_{w,1}^{(2)}\lambda_{w,n}^{(2)}}\sqrt{2n\mathcal{W}_2}}{\lambda_{w,1}^{(2)}+\lambda_{w,n}^{(2)}},$$

where $\lambda_{w,1}^{(2)}$ and $\lambda_{w,n}^{(2)}$ are maximum and minimum of the absolute value of $\lambda_{w,i}^{(2)}$s, respectively.

Proof. Taking $t = 1$ in (3.5) completes proof. □

Corollary 3.9. *If G is an unweighted graph of order $n\,(\geq 3)$ and zero is not an eigenvalue of $Z^{(2)}(G)$, then*

$$E_{Z^{(2)}}(G) \geq \frac{2\sqrt{2nM_2^{(2)}\lambda_1^{(2)}\lambda_n^{(2)}}}{\lambda_1^{(2)}+\lambda_n^{(2)}},$$

where $\lambda_1^{(2)}$ and $\lambda_n^{(2)}$ are maximum and minimum of the absolute value of $\lambda_i^{(2)}$s, respectively.

Proof. Consider (3.5) for an unweighted graph with $t = 1$. Proof is obvious from Remark 2.2 since $\mathcal{W}_2 = M_2^{(2)}$ for unweighted case. □

Theorem 3.10. *If G is a matrix weighted graph of order $n\,(\geq 3)$, then*

$$E_{Z_w^{(2)}}(G) \geq \sqrt{2nt\mathcal{W}_2 - \frac{n^2t^2}{4}\left(\lambda_{w,1}^{(2)} - \lambda_{w,nt}^{(2)}\right)^2}, \tag{3.6}$$

where $\lambda_{w,1}^{(2)}$ and $\lambda_{w,nt}^{(2)}$ are maximum and minimum of the absolute value of $\lambda_{w,i}^{(2)}$s, respectively.

Proof. If we choose $x_i = \left|\lambda_{w,i}^{(2)}\right|$ and $y_i = 1$ $(1 \leq i \leq nt)$ and apply Ozeki inequality, then

$$\sum_{i=1}^{nt}\left|\lambda_{w,i}^{(2)}\right|^2\sum_{i=1}^{nt}1^2 - \left(\sum_{i=1}^{nt}\left|\lambda_{w,i}^{(2)}\right|\right)^2 \leq \frac{n^2t^2}{4}\left(\lambda_{w,1}^{(2)} - \lambda_{w,nt}^{(2)}\right)^2.$$

From (2.2), we have

$$2nt\sum_{\substack{j:\ j\sim i \\ i,j\in\{1,2,\ldots,n\}}}\left(w_iw_j\right)^2 - \left(E_{Z_w^{(2)}}\right)^2 \leq \frac{n^2t^2}{4}\left(\lambda_{w,1}^{(2)} - \lambda_{w,nt}^{(2)}\right)^2.$$

Now, proof is obvious. □

Corollary 3.11. *If G is a number weighted graph of order $n\,(\geq 3)$ with positive edge weights, then*

$$E_{Z_w^{(2)}}(G) \geq \sqrt{2n\mathcal{W}_2 - \frac{n^2}{4}\left(\lambda_{w,1}^{(2)} - \lambda_{w,n}^{(2)}\right)^2}, \tag{3.7}$$

where $\lambda_{w,1}^{(2)}$ and $\lambda_{w,n}^{(2)}$ are maximum and minimum of the absolute value of $\lambda_{w,i}^{(2)}$s, respectively.

Proof. Setting $t = 1$ in (3.6), proof can be seen. □

Corollary 3.12. *If G is an unweighted graph of order $n\,(\geq 3)$, then*

$$E_{Z^{(2)}}(G) \geq \sqrt{2nM_2^{(2)} - \frac{n^2}{4}\left(\lambda_1^{(2)} - \lambda_n^{(2)}\right)^2},$$

where $\lambda_1^{(2)}$ and $\lambda_n^{(2)}$ are maximum and minimum of the absolute value of $\lambda_i^{(2)}$s, respectively.

Proof. Consider (3.6) with (2.4) for an unweighted graph, we obtain

$$\begin{aligned} E_{Z^{(2)}}(G) &\geq \sqrt{2n\mathcal{W}_2 - \frac{n^2}{4}\left(\lambda_1^{(2)} - \lambda_n^{(2)}\right)^2} \\ &= \sqrt{2nM_2^{(2)} - \frac{n^2}{4}\left(\lambda_1^{(2)} - \lambda_n^{(2)}\right)^2}, \end{aligned}$$

which completes proof. □

Finally, we calculate the number weighted second Zagreb energy of a molecular graph and compute the bounds presented in this section (see Table 2).

Example 3.13. Consider the edge weighted molecular graph of methane (CH_4) molecule with bond length weight (in nanometer). The bond length of $C-H$ is 0.11. So, all of the edge weights are 0.11. Thus

$$Z_w^{(2)} = \begin{bmatrix} 0 & 0.0484 & 0.0484 & 0.0484 & 0.0484 \\ 0.0484 & 0 & 0 & 0 & 0 \\ 0.0484 & 0 & 0 & 0 & 0 \\ 0.0484 & 0 & 0 & 0 & 0 \\ 0.0484 & 0 & 0 & 0 & 0 \end{bmatrix}$$

with eigenvalues -0.0968 (once) , 0 (3 times), 0.0968 (once). Hence $E_{Z_w^{(2)}} = 0.1936$. Further, $\mathcal{W}_2 = \sum_{\substack{j:\ j\sim i \\ i,j\in\{1,2,3,4,5\}}} \left(w_i w_j\right)^2 = 4\,(0.0484)^2 = 0.0093$.

lower bounds in Eq. (3.4)-(3.7)	$E_{Z_w^{(2)}}$	upper bounds in Eq. (3.2)-(3.4)
0.1368 − 0.1874	0.1936	0.2904 − 0.3061

Table 2. Bounds for number weighted second Zagreb energy

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Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this article.

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