Computer Science Journal of Moldova, vol.**29**, no.2(86), 2021

Bounds for Degree-Sum adjacency eigenvalues of a graph in terms of Zagreb indices

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Abstract

For a graph G the degree sum adjacency matrix $DS_A(G)$ is defined as a matrix, in which every element is sum of the degrees of the vertices if and only if the corresponding vertices are adjacent, otherwise it is zero. In this paper we obtain the bounds for the spectral radius and partial sum of the eigenvalues of the DS_A matrix. We also find the bounds for the DS_A energy of a graph in terms of its Zagreb indices.

Keywords: Adjacency eigenvalues, degree sum adjacency matrix, Zagreb index, Eigenvalues, Energy.

MSC 2010: 05C05.

1 Introduction

Association of Graph theory with Chemistry has resulted in introducing more molecular structure descriptors, in particular Topostructural descriptors (Wiener index, Hosoya Z index, Zagreb indices, Mohar indices, and many more). In [6] Gutman and Trinajstić observed that the total π-electron energy depended on the molecular structure. So some expressions were deduced for the π-electron energy containing these two terms:

$$M_1 = \sum_{vertices} (d_u)^2$$

and

$$M_2 = \sum_{edges} d_u \cdot d_v.$$

It was observed that both the terms reflect the extent of branching of a molecular structure and hence were responsible for decreasing the total π-electron energy with increasing branches. Later M_1 and M_2 were renamed as first Zagreb index and second Zagreb index respectively [12]. Numerous results are obtained by mathematicians on M_1 and M_2 [1], [7], [9], [15], [16].

The degree sum matrix for a graph was defined by [13] and the characteristic polynomial of the degree sum matrix for a graph in terms of its adjacency polynomial was also obtained. In the first part of this paper, we discuss the bounds for the DS_A-spectral radius and bounds for the partial sum of the DS_A-eigenvalues in terms of the Zagreb indices. In the later part, we obtain the bounds for the energy of a degree sum adjacency matrix in terms of the Zagreb indices.

The degree sum adjacency matrix $DS_A(G)$ of a graph G is defined as

$$DS_A(G) = [ds_{ij}] = \begin{cases} d_i + d_j, & \text{if there is an edge between } v_i \text{ and } v_j; \\ 0, & \text{otherwise.} \end{cases}$$

The characteristic polynomial of $DS_A(G)$ is defined as

$$P_{DS_A(G)} = \beta^n + a_1\beta^{n-1} + a_2\beta^{n-2} + \cdots + a_n.$$

As $DS_A(G)$ matrix is a real and symmetric, its eigenvalues are real and can be arranged as $\beta_1 \geq \beta_2 \geq \cdots \geq \beta_n$. The largest DS_A eigenvalue is known as the DS_A spectral radius of a graph G.

The first and the second Zagreb indices introduced in the year 1972 by I. Gutman [6] are

$$Zg_1 = Zg_1(G) = M_1(G) = \sum_{i=1}^{n} d_i^2 = \sum_{edge\ e=ij} (d_i + d_j).$$

$$Zg_2 = Zg_2(G) = M_2(G) = \sum_{edge\ e=ij} d_i d_j.$$

Lemma 1. *Let G be a simple n-ordered graph, with every vertex v_i having the degree d_i, $i = 1, 2, \ldots, n$. Let $DS_A(G)$ be the degree sum adjacency matrix of G, then*

$$\sum_{i=1}^{n} \beta_i = 0; \tag{1}$$

$$\sum_{i=1}^{n} \beta_i^2 = 2 \sum_{1 \le i < j \le n} (d_i + d_j)^2. \tag{2}$$

Lemma 2. *Let G be a simple n-ordered graph, with every vertex v_i having the degree d_i, $i = 1, 2, \ldots, n$. Let $DS_A(G)$ be the degree sum adjacency matrix of G with $\beta_1, \beta_2, \ldots, \beta_n$ as its eigenvalues. Let $Zg_1(G)$ and $Zg_2(G)$ be the Zagreb indices. Then,*

$$\begin{aligned}
\sum_{i=1}^{n} \beta_i^2 &= 2 \sum_{1 \le i < j \le n} (d_i + d_j)^2 = 2 \sum_{1 \le i < j \le n} (d_i^2 + d_j^2 + 2 d_i d_j) \\
&= 2 \left[\sum_{i=1}^{n} d_i (d_i)^2 + 2 \sum_{edge\ e = ij} d_i d_j \right] \\
&= 2 \left[\sum_{edge\ e = ij} (d_i + d_j) + \sum_{i=1}^{n} d_i^2 (d_i - 1) + 2 \sum_{edge\ e = ij} d_i d_j \right] \\
&= 2 \left[Zg_1(G) + \sum_{i=1}^{n} d_i^2 (d_i - 1) + 2 Zg_2(G) \right].
\end{aligned} \tag{3}$$

Lemma 3. *If $(c_1, c_2, \ldots, c_n)$ and $(d_1, d_2, \ldots, d_n)$ be n vectors, then by Cauchy-Schwartz inequality [14]:*

$$\left(\sum_{i=1}^{n} c_i d_i \right)^2 \le \left(\sum_{i=1}^{n} c_i^2 \right) \left(\sum_{i=1}^{n} d_i^2 \right). \tag{4}$$

Lemma 4. *Let G be a graph having n vertices and m edges, with adjacency eigenvalues as $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n$. Let H be another graph* *with n vertices having $d_1, d_2, \ldots, d_n$ as its vertex degrees and let the degree sum adjacency eigenvalues of H be $\beta_1 \geq \beta_2 \geq \cdots \geq \beta_n$. Then*

$$\sum_{i=1}^{n} (\lambda_i \beta_i) \leq \sqrt{4m[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)]}. \tag{5}$$

Proof. By using Lemma 2 and Lemma 3 we have,

$$\begin{aligned}
\sum_{i=1}^{n} (\lambda_i \beta_i)^2 &\leq \left(\sum_{i=1}^{n} \lambda^2\right)\left(\sum_{i=1}^{n} \beta^2\right) \\
&= 2m(2[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)]) \\
&= 4m[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)] \\
\sum_{i=1}^{n} \lambda_i \beta_i &\leq \sqrt{4m[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)]}.
\end{aligned}$$

□

2 Bounds for spectra of $DS_A(G)$

There are various bounds obtained for largest eigenvalue of an adjacency matrix in literature. In [5], [11] various bounds on the other eigenvalues of signless Laplacian and adjacency matrices are given.
If G is a simple graph of order n having e edges with adjacency eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$, then for $1 \leq p \leq n$,

$$\sqrt{\frac{(n-p)2e}{np}} \geq \lambda_p \geq -\sqrt{\frac{(p-1)2e}{n(n-p+1)}}. \tag{6}$$

For a adjacency matrix we have $\sum_{i=1}^{n} \lambda_i^2 = 2e$. Here, in degree sum adjacency matrix, the term $2[Zg_1(G)+2Zg_2(G)+\sum_{i=1}^{n} d_i^2(d_i-1)]$ plays the same role. So the direct consequence of Eq.(6) will be Eq.(7).

Theorem 1. *For a graph G, with degree sum adjacency eigenvalues $\beta_1 \geq \beta_2 \geq \cdots \geq \beta_n$ and for $1 \leq p \leq n$*

$$\sqrt{\frac{(n-p)2M}{np}} \geq \beta_p \geq -\sqrt{\frac{(p-1)2M}{n(n-p+1)}}, \tag{7}$$

where $M = [Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)]$.

Theorem 2. *Let G be a simple n-ordered graph. Let β_1 be the spectral radius of $DS_A(G)$ and $Zg_1(G)$ be the first Zagreb index. Then*

$$\beta_1 \geq \frac{2}{n} Zg_1(G). \tag{8}$$

Proof. Let G be a simple connected graph with n vertices with every vertex v_i having the degree d_i respectively. By the definition of $DS_A(G)$ we observe that the sum of all the entries of $DS_A(G)$ is $\sum_{i \neq j} ds_{ij} = \sum_{i \neq j}(d_i + d_j)$. Let $x = [1, 1, \ldots, 1]$ be the all one vector. Then by Rayleigh principle we have:

$$\begin{aligned}
\beta_1 &\geq \frac{x DS_A x^T}{x x^T} = \frac{1}{n} \sum_{i \neq j} (d_i + d_j) \\
&= \frac{1}{n} 2 \sum_{i<j} (d_i + d_j) \\
&\geq \frac{2}{n} Zg_1(G).
\end{aligned}$$

If G is a r-regular graph, then $Zg_1(G) = nr^2$.

$$\beta_1 = \frac{2}{n} nr^2 = 2r^2.$$

Hence the equality holds for regular graph. $\square$

Theorem 3. *Let G be a graph with n vertices and m edges, with $d_1, d_2, \ldots, d_n$ as its vertex degrees and the degree sum adjacency eigenvalues be $\beta_1 \geq \beta_2 \geq \cdots \geq \beta_n$. Then*

$$\beta_1 \leq \sqrt{\frac{2p}{p-1}[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)]} + \frac{1}{p-1} \sum_{i=2}^{p} \beta_{n-p+i}. \tag{9}$$

Proof. Let $\beta_1, \beta_2, \ldots, \beta_{n-p+1}, \beta_{n-p+2}, \ldots, \beta_n$ be the degree sum adjacency eigenvalues of G. Let $H = K_p \cup \overline{K_{n-p}}$. The adjacency eigenvalues of H are

$$\lambda_i = \begin{cases} p-1, & 1 \text{ time;} \\ 0, & (n-p) \text{ times;} \\ -1, & (p-1) \text{ times;} \end{cases}$$

and the number of edges of H is $m = \dfrac{p(p-1)}{2}$. Using Lemma 4 we get

$$\sum_{i=1}^{n}(\lambda_i\beta_i) \leq \sqrt{4m[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i-1)]} \ ;$$

$$(p-1)\beta_1 + (0)\sum_{i=2}^{n-p-1}\beta_i - \sum_{i=n-p+2}^{n}\beta_i$$

$$\leq \sqrt{4\frac{p(p-1)}{2}[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i-1)]} \ ;$$

$$(p-1)\beta_1 \leq \sqrt{2p(p-1)[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i-1)]} + \sum_{i=n-p+2}^{n}\beta_i \ ;$$

$$\beta_1 \leq \sqrt{\frac{2p}{(p-1)}[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i-1)]} + \frac{1}{p-1}\sum_{i=2}^{p}\beta_{n-p+i} \ .$$

□

Corollary 1. *Let G be a graph on n vertices and m edges, with $d_1, d_2, \ldots, d_n$ as its vertex degrees. Then,*

$$\beta_1 \leq \sqrt{\frac{2(n-1)}{n}[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i-1)]}. \qquad (10)$$

Proof. Putting $p = n$ in (9) and using Eq.(1) we get,

$$\beta_1 \leq \sqrt{\frac{2n}{(n-1)}[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)] + \frac{1}{n-1}\sum_{i=2}^{n}\beta_i} ;$$

$$\beta_1 \leq \sqrt{\frac{2n}{(n-1)}[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)] + \frac{1}{n-1}(-\beta_1)} ;$$

$$\beta_1 \leq \sqrt{\frac{2(n-1)}{n}[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)]}.$$

□

Remark 1. *The equality in (10) is satisfied for complete graphs. As* $Zg_1(G) = nr^2 = n(n-1)^2$, $\sum_{i=1}^{n} d_i^2(d_i - 1) = n(n-2)(n-1)^2$, $Zg_2(G) = mr^2 = \frac{n(n-1)^3}{2}$, *substituting this in (10) we get*

$$\beta_1 = 2(n-1)^2.$$

Corollary 2. *The spectral radius of* $DS_A(G)$ *is bounded by*

$$\frac{2}{n}Zg_1(G) \leq \beta_1 \leq \sqrt{\frac{2(n-1)}{n}[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)]}. \tag{11}$$

Proof. Combining Eq.(8) and Eq.(10), we get the bounds for the DS_A spectral radius of graph G. □

Remark 2. *The equality in (11) holds for complete graphs.*

Theorem 4. *Let* G *be an* n*-ordered graph with vertex degrees* $d_1, d_2, \ldots,$ d_n *and its degree sum adjacency eigenvalues as* $\beta_1 \geq \beta_2 \geq \cdots \geq \beta_n$*. Then,*

$$\sum_{i=1}^{k}\beta_i \leq \sqrt{\frac{2k(p-1)}{p}[Zg_1(G)+2Zg_2(G)+\sum_{i=1}^{n}d_i^2(d_i-1)]}\ ,$$
$$1 \leq k \leq n. \tag{12}$$

Proof. Let $\beta_1, \beta_2, \ldots, \beta_k, \beta_{k+1}, \ldots, \beta_n$ be the degree sum adjacency eigenvalues of G. Let H be the union of k copies of complete graph K_p, that is $H = \cup_k K_p$, where $kp = n$. The adjacency eigenvalues of H are

$$\lambda_i = \begin{cases} p-1, & k \ \text{ times;} \\ -1, & (n-k) \ \text{ times.} \end{cases}$$

Then the number of vertices of H is $n = pk$, and therefore its edges are $\frac{kp(p-1)}{2}$. Using Lemma 4,

$$\begin{aligned}
(p-1)\sum_{i=1}^{k}\beta_i - \sum_{i=k+1}^{n}\beta_i &\leq \sqrt{\frac{4kp(p-1)}{p}[Zg_1(G)+2Zg_2(G)+\sum_{i=1}^{n}d_i^2(d_i-1)]}; \\
p\sum_{i=1}^{k}\beta_i - \sum_{i=1}^{n}\beta_i &\leq \sqrt{2kp(p-1)[Zg_1(G)+2Zg_2(G)+\sum_{i=1}^{n}d_i^2(d_i-1)]}; \\
p\sum_{i=1}^{k}\beta_i &\leq \sqrt{2kp(p-1)[Zg_1(G)+2Zg_2(G)+\sum_{i=1}^{n}d_i^2(d_i-1)]}; \\
\sum_{i=1}^{k}\beta_i &\leq \sqrt{\frac{2k(p-1)}{p}[Zg_1(G)+2Zg_2(G)+\sum_{i=1}^{n}d_i^2(d_i-1)]}.
\end{aligned}$$

Thus we have obtained the bound for the sum of k, DS_A eigenvalues of a graph G. If $k = 1$, we observe that the Eq.(12) get reduced to Eq.(10). □

Theorem 5. *Let G be a graph on n vertices and m edges, with $d_1, d_2, \ldots, d_n$ as its vertex degrees and degree sum adjacency eigenvalues $\beta_1 \geq \beta_2 \geq \cdots \geq \beta_n$. Then,*

$$\sum_{i=1}^{k}(\beta_i - \beta_{n-k+i}) \leq \sqrt{4k[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)]}. \quad (13)$$

Proof. Let $\beta_1, \beta_2, \ldots, \beta_k, \beta_{k+1}, \ldots, \beta_{n-k}, \beta_{n-k+1}, \ldots, \beta_n$ be the degree sum adjacency eigenvalues of G. Let H be the union of k copies of $K_{p,q}$ a complete bipartite graph, that is $H = \cup_k K_{p,q}$, where $kp = n$. The adjacency eigenvalues of H are

$$\lambda_i = \begin{cases} \sqrt{pq}, & k \text{ times;} \\ 0, & (n-2k) \text{ times;} \\ -\sqrt{pq}, & k \text{ times.} \end{cases}$$

The number of edges of H is kpq. Using Lemma 4, we get:

$$\sqrt{pq}\sum_{i=1}^{k}\beta_i + 0\sum_{i=k+1}^{n-k}\beta_i - \sqrt{pq}\sum_{i=k+1}^{n}\beta_i$$
$$\leq \sqrt{4kpq[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)]} \ ;$$
$$\sqrt{pq}\sum_{i=1}^{k}\beta_i - \sum_{i=1}^{k}\beta_{n-k+i}$$
$$\leq \sqrt{4kpq[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)]} \ ;$$
$$\sum_{i=1}^{k}(\beta_i - \beta_{n-k+i})$$
$$\leq \sqrt{4k[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)]}.$$

□

3 Bounds for Energy of a DS_A matrix

The Energy of a Degree Sum adjacency matrix $DS_AE(G)$ can be defined as the sum of the absolute DS_A eigenvalues of a graph G, analogous to the various energy concepts like energy of an adjacency matrix [8] and distance matrix [3]. This energy is also referred to as Zagreb energy in [10]:

$$DS_AE(G) = \sum_{i=1}^{n} |\beta_i|. \qquad (14)$$

Hyper-Zagreb index was recently introduced in [4], which is defined as $HM(G) = \sum_{edge\ e=ij}(d_i+d_j)^2$. So using Lemma (2), we can express hyper-Zagreb index in terms of first two Zagreb indices.

$$HM = [Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)]. \qquad (15)$$

In [10], authors have expressed bounds for Zagreb energy in terms of hyper-zagreb index. So using Eq.(15) we state that bounds for Zargeb energy can also be expressed in terms of first and second Zagreb indices.

$$\sqrt{2[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)]} \leq DS_AE(G)$$
$$\leq \sqrt{2n[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)]};$$

$$DS_AE(G)$$
$$\geq \sqrt{2[Zg_1(G) + 2Zg_2(G) + \sum_{i=1}^{n} d_i^2(d_i - 1)] + n(n-1)|det(DS_A(G))|^{2/n}}.$$

Theorem 6. *Let G be an r-regular graph with n vertices. Then*

$$DS_AE(G) \geq 4r^2. \qquad (16)$$

Proof. Let G be an r regular graph with n vertices and $2r^2, 2r\lambda_2, 2r\lambda_3, \ldots, 2r\lambda_n$ be its DS_A eigenvalues in terms of its adjacency eigenvalues. Then

$$\begin{aligned} DS_AE(G) &= |2r^2| + \sum_{i=2}^{n} |2r\lambda_i| \\ &\geq 2r^2 + \left|\sum_{i=2}^{n} 2r(-r)\right| \\ &\geq 2r^2 + \left|-2r^2\right| \\ &\geq 4r^2. \end{aligned}$$

□

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Received June 25, 2020
Accepted March 16, 2021

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