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BOUNDS ON DEGREE SQUARE SUM DISTANCE SQUARE ENERGY OF GRAPHS

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Abstract. The degree square sum distance square matrix DSSDS(G) of a graph G is a square matrix whose $(i,j)^{th}$ entry is $(d_i^2+d_j^2)d_{ij}^2$ whenever $i \neq j$, and otherwise zero,where d_i is the degree of i^{th} vertex of G and $d_{ij} = d(v_i, v_j)$ is distance between v_i and v_j. In this paper, we define degree square sum distance square energy $E_{DSSDS}(G)$ as sum of absolute eigenvalues of $DSSDS(G)$. Also we obtain some bounds on degree square sum distance square eigenvalue and energy.

1. Introduction

The energy of the graph was introduced by I.Gutman in 1978 [**6**] which is having direct connection with total π -electron energy of a molecule in the quantum chemistry as calculated with the Huckel molecular orbital method. Recently several results on energy related with matrices dealing with degree of vertices and distance between vertices have been studied such as distance energy[**8, 12**], degree sum energy [**7**], degree exponent energy [**14, 13**], degree exponent sum energy [**10, 3**], degree square sum energy[**2, 1, 4**] etc.

In continuation with this, in order to upgrade, we now introduce concept of degree square sum distance square energy of connected graph. The purpose of this paper is to compute bounds on largest eigenvalue and energy of the new matrix associated with graph, called degree square sum distance square matrix denoted by DSSDS(G).

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2. Degree Square Sum Distance Square Energy

Let G be a connected graph of order n with vertex set $V(G) = (v_1, v_2, ..., v_n)$.We denote by $d(v_i)$ as the degree of a vertex v_i which is the number of edges incident on it and the distance between two vertices v_i and v_j as d_{ij},the length of the shortest path joining them. Motivated from previous research, we now define the degree square sum distance square matrix of a connected graph G as,
$DSSDS(G) = [dssd_{ij}s]$ where,

$$dssd_{ij}s = (d(v_i)^2 + d(v_j)^2)d_{ij}^2 \text{ if } i \neq j \\ = 0 \text{ if } i = j \tag{2.1}$$

Properties: The following hold for $DSSDS(G)$,

1. $DSSDS(G)$ is real symmetric.
2. The eigenvalues of $DSSDS(G)$ are real.
3. The sum of the eigenvalues of $DSSDS(G)$ is zero, since trace

$$DSSDS(G)] = 0.$$

4. If $\alpha_1, \alpha_2, \ldots, \alpha_n$ are the eigenvalues of $DSSDS(G)$ then, they can be arranged in a non-increasing order as $\alpha_1 \geqslant \alpha_2 \geqslant \ldots \geqslant \alpha_n$.

Analogous to the energy of a graph defined by I. Gutman [**6**] with respect to adjacency matrix, we define the degree square sum distance square energy of a graph as,

$$E_{DSSDS}(G) = \sum_{i=1}^{n} |\alpha_i|.$$

Example 2.1. For the graph $K_4 - e$ with suitable labeling we have

Degrees	DSSDS Matrix	Eigenvalues and Energy
$deg(v_1) = 2$ $deg(v_2) = 2$ $deg(v_3) = 3$ and $deg(v_4) = 3$	$\begin{pmatrix} 0 & 13 & 13 & 10 \\ 13 & 0 & 8 & 20 \\ 13 & 8 & 0 & 20 \\ 10 & 20 & 20 & 0 \end{pmatrix}.$	$\alpha_1 = 51.9258$, $\alpha_2 = -32$ $\alpha_3 = -18$ and $\alpha_4 = -1.9258$. $E_{DSSDS}(K_4 - e) = 103.8516$.

3. Bounds on Degree Square Sum Distance Square Energy

Lemma 3.1. *Let G be a graph of order n. Then we have*

$$\sum_{i=1}^{n} \alpha_i = 0 \quad and \quad \sum_{i=1}^{n} \alpha_i^2 = 2M,$$

where is $M = \sum_{i=1, i<j}^{n} ((d_i^2 + d_j^2) d_{ij}^2)^2$.

LEMMA 3.2 ([**9**]). *Let $a_1, a_2, .., a_n$ be non negative numbers. Then*

$$n\left[\frac{1}{n}\sum_{i=1}^{n} a_i - (\prod_{i=1}^{n} a_i)^{1/n}\right] \leqslant$$

$$n\sum_{i=1}^{n} a_i - (\sum_{i=1}^{n}\sqrt{a_i})^2 \leqslant n(n-1)\left[\frac{1}{n}\sum_{i=1}^{n} a_i - (\prod_{i=1}^{n} a_i)^{1/n}\right].$$

LEMMA 3.3 ([**5**]). *Let a_i and b_i , $1 \leqslant i \leqslant n$, be non-negative real numbers. Then*

$$\sum_{i=1}^{n} b_i^2 + rR\sum_{i=1}^{n}\alpha_i^2 \leqslant (r+R)(\sum_{i=1}^{n} a_i b_i),$$

where r and R are real constants, such that for each i, $1 \leqslant i \leqslant n$, $ra_i \leqslant b_i \leqslant Ra_i$ holds.

LEMMA 3.4 ([**11**]). *Let a_i and b_i , $1 \leqslant i \leqslant n$ non negative real numbers. Then*

$$\sum_{i}^{n} a_i^2 \sum_{i}^{n} b_i^2 - (\sum_{i=1}^{n} a_i b_i)^2 \leqslant \frac{n^2}{4}\left(M_1M_2 - m_1m_2\right)^2$$

where

$M_1 = max_{1\leqslant i\leqslant n} a_i$, $M_2 = min_{1\leqslant i\leqslant n} b_i$, $m_1 = max_{1\leqslant i\leqslant n} a_i$ *and* $m_2 = min_{1\leqslant i\leqslant n} b_i$.

LEMMA 3.5. *The CauchySchwartz inequality: Let a_i and b_i , $1 \leqslant i \leqslant n$ be any real numbers, then*

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \leqslant \left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right).$$

THEOREM 3.1. *If α_1 is the index (largest degree square sum distance square eigenvalue) of a connected graph G of order n, then $\alpha_1 \leqslant \sqrt{\frac{2M(n-1)}{n}}$, where M is defined above.*

PROOF. The trace of $DSSDS(G)$ being zero we have

$$\sum_{i=1}^{n}\alpha_i = 0 \text{ i.e, } \sum_{i=2}^{n}\alpha_i = -\alpha_1.$$

Further $\sum_{i=1}^{n}\alpha_i^2$=trace$DSSDS(G)^2 = 2M$, where M is as defined above. With $a_i = 1$ and $b_i = \alpha_i$ $i = 2, 3, \ldots, n$ and substituting in Lemma 3.5 we get

$$(\sum_{i=2}^{n}\alpha_i)^2 \leqslant (n-1)\sum_{i=2}^{n}\alpha_i^2 \leqslant (n-1)(2M - \alpha_1^2).$$

Therefore $(-\alpha_1)^2 \leqslant (n-1)(2M - \alpha_1^2)$. Hence bound for the index α_1 follows. □

THEOREM 3.2. *Let G be a graph of order $n \geqslant 2$ and M is the quantity defined above. Then*

$$\sqrt{2M} \leqslant E_{DSSDS}(G) \leqslant \sqrt{2Mn}.$$

Proof. With $a_i = 1$, $b_i = |\alpha_i|$ using Lemma 3.5 we get

$$(\sum_{i=1}^{n} |\alpha_i|)^2 \leqslant n \sum_{i=1}^{n} (\alpha_i)^2 \text{ that is, } E_{DSSDS}(G)^2 \leqslant 2nM.$$

Hence $E_{DSSDS}(G) \leqslant \sqrt{2Mn}$. Now for the other part

$$E_{DSSDS}(G)^2 = (\sum_{i=1}^{n} |\alpha_i|)^2 \geqslant \sum_{i=1}^{n} |\alpha_i|^2 = 2M$$

so that, $E_{DSSDS}(G) \geqslant \sqrt{2M}$. Combining these two, inequality follows. □

Theorem 3.3. *Let G be a connected graph of order n and Δ be the absolute value of the determinant of $DSSDS(G)$. Then*

$$\sqrt{2M + n(n-1)\Delta^{2/n}} \leqslant E_{DSSDS}(G) \leqslant \sqrt{2(n-1)M + n\Delta^{2/n}},$$

where M is defined as above.

Proof. Let $a_i = \alpha_i^2$, $i = 1, 2, ..., n$. Then from Lemma 3.1 and Lemma 3.2 we obtain

$$n\left[\frac{1}{n}\sum_{i=1}^{n} \alpha_i^2 - (\prod_{i=1}^{n} \alpha_i^2)^{1/n}\right] \leqslant n\sum_{i=1}^{n} \alpha_i^2 - (\sum_{i=1}^{n} \alpha_i)^2 \leqslant n(n-1)\left[\frac{1}{n}\sum_{i=1}^{n} \alpha_i^2 - (\prod_{i=1}^{n} \alpha_i^2)^{1/n}\right]$$

That is

$$2M - n\Delta^{2/n} \leqslant 2nM - [E_{DSSDS}(G)]^2 \leqslant 2(n-1)M - n(n-1)\Delta^{2/n}.$$

Thus

$$2M + n(n-1)\Delta^{2/n} \leqslant [E_{DSSDS}(G)]^2 \leqslant 2(n-1)M + n\Delta^{2/n}.$$

We get the desired result. □

Theorem 3.4. *If G is any graph of order n and Δ is the absolute value of the determinant of $DSSDS(G)$ then*

$$\sqrt{2M + n(n-1)\Delta^{\frac{2}{n}}} \leqslant E_{DSSDS}(G) \leqslant \sqrt{2Mn},$$

where M is defined as above.

Proof. For lower bound consider,

$$[E_{DSSDS}(G)]^2 = (\sum_{i=1}^{n} |\alpha_i|)^2 = \sum_{i=1}^{n} (\alpha_i)^2 + 2\sum_{i<j} |\alpha_i||\alpha_j| = 2M + \sum_{1\neq j} |\alpha_i||\alpha_j|.$$

Since Arithmetic Mean (AM) $\geqslant$ Geometric Mean (GM) we have,

$$\frac{1}{n(n-1)}\sum_{i\neq j} |\alpha_i||\alpha_j| \geqslant \left(\prod_{i\neq j} |\alpha_i||\alpha_j|\right)^{\frac{1}{n(n-1)}}$$

$$= \prod_{i=1}^{n} \left(|\alpha_i|^{2n-2}\right)^{\frac{1}{n(n-1)}} = \left(\prod_{i=1}^{n} |\alpha_i|^{\frac{2}{n}}\right) = \Delta^{\frac{2}{n}}$$

therefore we have

$$\sum_{i\neq j}|\alpha_i||\alpha_j| \geqslant n(n-1)\Delta^{\frac{2}{n}}$$

Combining we get

$$[E_{DSSDS}(G)]^2 \geqslant 2M + n(n-1)\Delta^{\frac{2}{n}},$$

i.e,

$$E_{DSSDS}(G) \geqslant \sqrt{2M + n(n-1)\Delta^{\frac{2}{n}}}.$$

For upper bound define

$$\begin{aligned} X &= \textstyle\sum_{i=1}^{n}\sum_{j=1}^{n}(|\alpha_i|+|\alpha_j|)^2 \\ &= \textstyle\sum_{i=1}^{n}\sum_{j=1}^{n}(|\alpha_i|^2+|\alpha_j|^2) + 2(\sum_{i,j=1,i\neq j}^{n}|\alpha_i||\alpha_j|) \\ &= n\textstyle\sum_{i=1}^{n}(\alpha_i)^2 + n\sum_{i=1}^{n}(\alpha_j)^2 - 2(\sum_{i=1}^{n}|\alpha_i||\alpha_j|) \\ &= 2nM + 2nM - 2[E_{DSSDS}(G)]^2 = 4nM - 2[E_{DSSDS}(G)]^2. \end{aligned}$$

Since $X \geqslant 0$, we get $E_{DSSDS}(G) \leqslant \sqrt{2Mn}$. Combining lower bound and upper bound, we arrive at the desired result. □

THEOREM 3.5. *Let G be a graph of order n. Then*

$$E_{DSSDS}(G) \geqslant \sqrt{2Mn - \frac{n^2}{4}(\alpha_p-\alpha_q)^2},$$

where α_p, α_q are maximum and minimum absolute value of α_i's, and M as defined above.

PROOF. Suppose $\alpha_1, \alpha_2, ..., \alpha_n$ are the eigenvalues of $DSSDS(G)$. We assume that $a_i = 1$ and $b_i = |\alpha_i|$, by Lemma 3.4 we have

$$\sum_{i=1}^{n}1\sum_{i=1}^{n}|\alpha_i|^2 - (\sum_{i=1}^{n}|\alpha_i|)^2 \leqslant \frac{n^2}{4}(\alpha_p-\alpha_q)^2$$

$$2Mn - (E_{DSSDS(G)})^2 \leqslant \frac{n^2}{4}(\alpha_p-\alpha_q)^2.$$

Now

$$2Mn > \frac{n^2}{4}(\alpha_p-\alpha_q)^2$$

and

$$n\sum_{i=1}^{n}\alpha_i^2 > \frac{n^2}{4}(\alpha_p-\alpha_q)^2.$$

Then

$$\alpha_1^2+\alpha_2^2+\ldots+\alpha_p^2+\alpha_q^2 > \frac{n}{4}(\alpha_p-\alpha_q)^2 \text{ giving } \alpha_1^2+\alpha_2^2+\ldots > \frac{n}{4}(-2\alpha_p\alpha_q)$$

which is true. Hence

$$E_{DSSDS}(G) \geqslant \sqrt{2Mn - \frac{n^2}{4}(\alpha_p-\alpha_q)^2}.$$

□

Theorem 3.6. *Let G be a graph of order n. Let $\alpha_1 \geqslant \alpha_2 \geqslant \ldots \geqslant \alpha_n$ be a non-increasing arrangement of $DSSDS(G)$. Then*

$$E_{DSSDS}(G) \geqslant \frac{\alpha_p.\alpha_q n + 2M}{\alpha_p + \alpha_q},$$

where α_p, α_q are maximum and minimum absolute value of $DSSDS(G)$, and M as defined above.

Proof. Suppose $\alpha_1, \alpha_2, ..., \alpha_n$, are the eigenvalues of $DSSDS(G)$. We assume that $b_i = |\alpha_i|$, $a_i = 1$, $r = \alpha_q$, and $R = \alpha_p$, then by using Lemma 3.3 we have,

$$\sum_{i=1}^{n} |\alpha_i^2| + \alpha_p\alpha_q \sum_{i=1}^{n} 1 \leqslant (\alpha_p + \alpha_q) \sum_{i=1}^{n} |\alpha_i|$$

also we have, $E_{DSSDS}(G) \leqslant \sqrt{2Mn}$. Since $E_{DSSDS}(G) = \sum_{i=1}^{n} |\alpha_i|, \sum_{i=1}^{n} |\alpha_i^2| = 2M$. Hene the theorem. □

Theorem 3.7. *Suppose zero is not an eigenvalue of $DSSDS(G)$. Then*

$$E_{DSSDS}(G) \geqslant \frac{2\sqrt{2Mn}\sqrt{\alpha_p\alpha_q}}{\alpha_p + \alpha_q},$$

where α_p,α_q are maximum and minimum absolute value of $\alpha_i^\prime s$, and M as defined above.

Proof. The AM-GM inequality implies.

$$\frac{\alpha_p\alpha_q n + 2M}{\alpha_p + \alpha_q} \geqslant \frac{2\sqrt{2Mn\alpha_p\alpha_q}}{\alpha_p + \alpha_q}$$

Then the theorem follows as a direct consequence of Theorem 3.6. □

For the graph $K_4 - e$, $M = 2024$, $n = 4$, $\Delta = 57600$, $\alpha_p = 51.9258$ $\alpha_q = 1.9258$ and $E_{DSSDS}(K_4 - e) = 103.8516$, we have the following

Sl.No.	Lower bound	Upper bound
Theorem 3.1.	....	55.0999
Theorem 3.2.	63.62389488	127.24778
Theorem 3.3.	83.23460819	114.4727142
Theorem 3.4.	83.23460819	127.24778
Theorem 3.5.	78.68926229	.....
Theorem 3.6.	47.258379	.....
Theorem 3.7.	82.59726401	......

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