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On Distance Spectral Radius and Distance Energy of Graphs

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Abstract

For a connected graph, the distance spectral radius is the largest eigenvalue of its distance matrix, and the distance energy is defined as the sum of the absolute values of the eigenvalues of its distance matrix. We establish lower and upper bounds for the distance spectral radius of graphs and bipartite graphs, lower bounds for the distance energy of graphs, and characterize the extremal graphs. We also discuss upper bounds for the distance energy.

1. INTRODUCTION

Let G be a connected graph with vertex set $\{v_1, v_2, \dots, v_n\}$. The distance between vertices v_i and v_j of G, denoted by d_{ij}, is defined to be the length (i. e., the number of edges) of the shortest path from v_i to v_j. The distance matrix of G, denoted by $\mathbf{D}(G)$, is the $n \times n$ matrix whose (i,j)-entry is equal to d_{ij}, $i,j = 1,2,\dots,n$, (see [1, 2]). Note that $d_{ii} = 0$, $i = 1,2,\dots,n$. The eigenvalues of $\mathbf{D}(G)$ are said to be the D-eigenvalues of G. Since $\mathbf{D}(G)$ is a real symmetric matrix, the D-eigenvalues are real and can be ordered in non-increasing order, $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$. The distance spectral radius of G is the largest D-eigenvalue ρ_1 and denoted by $\rho(G)$.

Balaban et al. [3] proposed the use of $\rho(G)$ as a molecular descriptor, while in [4] it was successfully used to infer the extent of branching and model boiling points of alkanes. In [5], the author gave lower and upper bounds for $\rho(G)$ when G is a tree. In [6], the authors provided lower and upper bounds for $\rho(G)$ when G is a connected graph in terms of the number of vertices, the sum of the squares of the distances between all unordered pairs of vertices and the sum of the distances between a given vertex and all other vertices, and the Nordhaus–Gaddum–type result for $\rho(G)$, see also [7] for more results on $\rho(G)$. A survey on the properties of $\rho(G)$ may be found in [8]. Recently, Das [9] obtained lower and upper bounds for the distance spectral radius of a connected bipartite graph and characterize those graphs for which these bounds are best possible. Note that earlier study of the eigenvalues of the distance matrix may be found in [10–14].

The distance energy of a connected graph G is defined in [15] as

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

Lower and upper bounds for distance energy have been obtained in [15–19]. For more recent results on DE see [20–23].

In this paper, we establish lower and upper bounds for the distance spectral radius of graphs and bipartite graphs, lower bounds for the distance energy of graphs, and characterize the extremal graphs. We also discuss upper bounds for the distance energy.

2. PRELIMINARIES

Let K_n be the complete graph with n vertices. Let P_n be the path with n vertices. Let $K_{p,q}$ be the complete bipartite graph with p vertices in one partite set and q vertices in the other partite set. Let d_i be the degree of vertex v_i of the graph G. A graph is semi–regular if it is bipartite and all vertices in the same partite set have the same degree.

Let G be a connected graph. Let $v_r v_s$ be an edge of G such that $G - v_r v_s$ is also connected. Then $d_{ij}(G) \leq d_{ij}(G - v_r v_s)$ for all $i, j \in V(G)$. Moreover, $1 = d_{rs}(G) < d_{rs}(G - v_r v_s)$ and thus by the Perron–Frobenius theorem, we conclude that

$$\rho(G) < \rho(G - v_r v_s)\,. \tag{1}$$

Similarly, for two nonadjacent vertices v_r and v_s,

$$\rho(G + v_r v_s) < \rho(G)\,. \tag{2}$$

Let G be a graph with n vertices. Let $\mathbf{A}(G)$ be the adjacency matrix of the graph G. The eigenvalues λ_i, $i = 1, 2, \ldots, n$, of G are the eigenvalues of its adjacency matrix $\mathbf{A}(G)$, and they can be ordered as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ [1]. If G is r-regular, then $\lambda_1 = r$. Let $\overline{G}$ be the complement of G. Denote by $\mathbf{J}_n$ the all 1's $n \times n$ matrix and by $\mathbf{I}_n$ the identity matrix of order n. If the diameter of G is at most two, then $\mathbf{D}(G) = 2\,\mathbf{J}_n - 2\,\mathbf{I}_n - \mathbf{A}(G) = \mathbf{J}_n - \mathbf{I}_n + \mathbf{A}(\overline{G})$ (see [24]).

For an r-regular graph G, the eigenvectors of $\mathbf{A}(G)$ associated to any eigenvalue not equal to r are orthogonal to the all 1's vector. If G is an r-regular graph of diameter two, then $\mathbf{D}(G) = 2\,\mathbf{J}_n - 2\,\mathbf{I}_n - \mathbf{A}(G)$, and thus the D-eigenvalues of G are $2n - r - 2$, $-\lambda_n - 2$, $\ldots$, $-\lambda_2 - 2$, arranged in a non-increasing manner.

3. BOUNDS FOR ρ OF GENERAL GRAPHS

In this section, we present lower and upper bound for $\rho(G)$ of a connected graph G.

Theorem 1. *Let G be a connected graph with n vertices, maximum degree Δ_1 and second maximum degree Δ_2. Then*

$$\rho(G) \geq \sqrt{(2n-2-\Delta_1)(2n-2-\Delta_2)}$$

with equality if and only if G is a regular graph with diameter less than or equal to 2.

Proof. Let $x = (x_1, x_2, \ldots, x_n)^T$ be a Perron eigenvector of $D(G)$ corresponding to the largest eigenvalue $\rho(G)$, such that

$$x_i = \min_{k \in V(G)} x_k \quad \text{and} \quad x_j = \min_{\substack{k \in V(G) \\ k \neq i}} x_k .$$

From the eigenvalue equation $\rho(G) \cdot x = D(G) \cdot x$, written for the component x_i we have

$$\begin{aligned} \rho(G) x_i &= \sum_{k=1}^{n} d_{ik} \cdot x_k \\ &\geq d_i x_j + (n-1-d_i) 2 x_j = (2n-2-d_i) x_j . \end{aligned}$$

Analogously for the component x_j we have

$$\begin{aligned} \rho(G) x_j &= \sum_{k=1}^{n} d_{jk} \cdot x_k \\ &\geq d_j x_i + (n-1-d_j) 2 x_i = (2n-2-d_j) x_i . \end{aligned}$$

Combining these two inequalities, it follows

$$\rho(G) \geq \sqrt{(2n-2-d_i)(2n-2-d_j)} \geq \sqrt{(2n-2-\Delta_1)(2n-2-\Delta_2)} .$$

The equality holds if and only if the diameter of G is less than or equal to 2, and all coordinates x_i are equal. For $d = 1$, we get a complete graph K_n. For $d = 2$, we get $\rho(G) x_i = d_i x_i + 2(n-1-d_i) x_i$, and then $\rho(G) = 2n-2-d_i$, which means that G is a regular graph. Conversely, it is easily seen that $\rho(G) = 2n-2-\Delta_1$ if G is a regular graph with diameter less than or equal to 2. ■

Theorem 2. *Let G be a connected graph with n vertices, minimum degree δ_1 and second minimum degree δ_2. Let d be the diameter of G. Then*

$$\rho(G) \leq \sqrt{\left[dn - \frac{d(d-1)}{2} - 1 - \delta_1(d-1)\right]\left[dn - \frac{d(d-1)}{2} - 1 - \delta_2(d-1)\right]}$$

with equality if and only if G is a regular graph with diameter less than or equal to 2.

Proof. Let $x = (x_1, x_2, \ldots, x_n)^T$ be a Perron eigenvector of $D(G)$ corresponding to the largest eigenvalue $\rho(G)$, such that

$$x_i = \max_{k \in V(G)} x_k \quad \text{and} \quad x_j = \max_{\substack{k \in V(G)\\ k \neq i}} x_k \,.$$

From the eigenvalue equation $\rho(G) \cdot x = D(G) \cdot x$, written for the component x_i we have

$$\begin{aligned}
\rho(G)x_i &= \sum_{k=1}^{n} d_{ik} \cdot x_k \\
&\leq d_i x_j + 2x_j + 3x_j + \cdots + (d-1)x_j \\
&\quad + d\,[n - 1 - d_i - (d-2)]\, x_j \\
&= \left[dn - \frac{d(d-1)}{2} - 1 - d_i(d-1)\right] x_j \,.
\end{aligned}$$

Analogously for the component x_j we have

$$\begin{aligned}
\rho(G)x_j &= \sum_{k=1}^{n} d_{jk} \cdot x_k \\
&\leq d_j x_i + 2x_i + 3x_i + \cdots + (d-1)x_i \\
&\quad + d\,[n - 1 - d_j - (d-2)]\, x_i \\
&= \left[dn - \frac{d(d-1)}{2} - 1 - d_j(d-1)\right] x_i \,.
\end{aligned}$$

Combining these two inequalities, it follows that

$$\rho(G) \leq \sqrt{\left[dn - \frac{d(d-1)}{2} - 1 - d_i(d-1)\right]\left[dn - \frac{d(d-1)}{2} - 1 - d_j(d-1)\right]}$$

$$\leq \sqrt{\left[dn - \frac{d(d-1)}{2} - 1 - \delta_1(d-1)\right]\left[dn - \frac{d(d-1)}{2} - 1 - \delta_2(d-1)\right]}\,.$$

The equality holds if and only if all coordinates of Perron's eigenvector are equal, and hence, $D(G)$ has equal row sums. If the diameter of G is greater than or equal to 3, that means that for every vertex i, there is exactly one vertex j that is of distance two from i, and then the diameter of G must be smaller than 4. If the diameter of G is 3 and equality holds, then for a center vertex s (with the eccentricity two), from $\rho(G) \cdot x = D(G) \cdot x$, written for the component x_s, we have

$$\rho(G)x_s = d_s x_s + (n-1-d_s)2x_s = \left[3n - \frac{3(3-1)}{2} - 1 - d_s(3-1)\right] x_s$$

and then $d_s = n-2$, which implies that $G \cong P_4$. But the coordinates of Perron's eigenvector of $D(P_4)$ can not be all equal. Therefore, in the case of equality we have that G is a regular graph with diameter $d \leq 2$. ■

4. BOUNDS FOR ρ OF BIPARTITE GRAPHS

The inequality (1) shows that the maximum distance spectral radius will be attained for trees. Subhi and Powers in [12] proved that for $n \geq 3$ the path P_n has the maximum distance spectral radius among trees with n vertices. Stevanović and Ilić in [14] generalized this result, and proved that among trees with n vertices and fixed maximum degree Δ, the broom graph $B_{n,\Delta}$ (formed by attaching $\Delta - 1$ pendent vertices to an end vertex of the path $P_{n-\Delta+1}$) has the maximum ρ-value.

The inequality (2) tells us that the complete bipartite graph $K_{p,q}$ has the minimum distance spectral radius among connected bipartite graphs with p vertices in one partite set and q vertices in the other partite set. Following [24], the distance spectrum of the complete bipartite graph $K_{p,q}$ consists of simple eigenvalues $p+q-2 \pm \sqrt{p^2 - pq + q^2}$, and an eigenvalue -2 with multiplicity $p+q-2$. Let G be a connected bipartite graph with bipartition $V(G) = A \cup B$, $|A| = p$, $|B| = q$, $p+q = n$. Then $\rho(G) \geq n-2+\sqrt{n^2 - 3pq}$ with equality if and only if $G \cong K_{p,q}$. This was shown by Das [9] using a different reasoning. Note that $\rho(K_{p,q}) = p+q-2+\sqrt{(p+q)^2-3pq}$ attains minimum if and only if $|p-q| \leq 1$. Therefore, we have:

Theorem 3. *Among connected bipartite graphs with n vertices, $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$ has minimum, while P_n has maximum distance spectral radius.*

Here we present a stronger lower bound for $\rho(G)$ for a bipartite graph G, involving the maximum degrees in both partite sets.

Theorem 4. *Let G be a connected bipartite graph with bipartition $V(G) = A \cup B$, $|A| = p$, $|B| = q$, $p+q=n$. Let Δ_A and Δ_B be maximum degrees among vertices from A and B, respectively. Then*

$$\rho(G) \geq n-2+\sqrt{n^2-4pq+(3q-2\Delta_A)(3p-2\Delta_B)}$$

with equality if and only if G is a complete bipartite graph $K_{p,q}$ or G is a semi–regular graph with every vertex eccentricity equal to 3.

Proof. Let $A = \{1, 2, \ldots, p\}$ and $B = \{p+1, p+2, \ldots, p+q\}$. Let $x = (x_1, x_2, \ldots, x_n)^T$ be a Perron eigenvector of $D(G)$ corresponding to the largest eigenvalue $\rho(G)$, such that

$$x_i = \min_{k \in A} x_k \quad \text{and} \quad x_j = \min_{k \in B} x_k \,.$$

From the eigenvalue equation $\rho(G) \cdot x = D(G) \cdot x$, written for the component x_i we have

$$\begin{aligned} \rho(G)x_i &= \sum_{k=1}^{p} d_{ik} \cdot x_k + \sum_{k=p+1}^{p+q} d_{ik} \cdot x_k \\ &\geq 2(p-1)x_i + d_i x_j + 3(q-d_i)x_j \\ &\geq 2(p-1)x_i + (3q-2\Delta_A)x_j \,. \end{aligned}$$

Analogously for the component x_j we have

$$\rho(G)x_j = \sum_{k=1}^{p} d_{jk} \cdot x_k + \sum_{k=p+1}^{p+q} d_{jk} \cdot x_k$$

$$\begin{aligned} &\geq d_j x_i + 3(p-d_j)x_i + 2(q-1)x_j \\ &\geq (3p-2\Delta_B)x_i + 2(q-1)x_j\,. \end{aligned}$$

Combining these two inequalities, it follows

$$(\rho(G)-2(p-1))(\rho(G)-2(q-1))x_ix_j \geq (3q-2\Delta_A)(3p-2\Delta_B)x_ix_j\,.$$

Since $x_k > 0$ for $1 \leq k \leq p+q$,

$$\rho^2(G) - 2(p+q-2)\rho(G) + 4(p-1)(q-1) - (3q-2\Delta_A)(3p-2\Delta_B) \geq 0\,.$$

From this inequality, we get the result.

For the case of equality, we have $x_i = x_k$ for $k = 1,2,\ldots,p$ and $x_j = x_k$ for $k = p+1, p+2, \ldots, p+q$. This means that eigenvector x has at most two different coordinates, the degrees of vertices in A are equal to Δ_A, and the degrees of vertices in B are equal to Δ_B, implying that G is a semi–regular graph. If G is not a complete bipartite graph, it follows from $p\Delta_A = q\Delta_B$ that $\Delta_A < q$ and $\Delta_B < p$ and the eccentricity of every vertex must be equal to 3. ■

It is evident that the lower bound in previous theorem improves the bound in [9] mentioned above.

Let G be a connected bipartite graph with n vertices, diameter d and bipartition $V(G) = A \cup B$, $|A| = p$, $|B| = q$, $p+q = n$. Das in [9] proved that

$$\rho(G) \leq \frac{1}{2}\left[d(n-2) + \sqrt{d^2n^2 - 4pq(2d-1)}\right]$$

for even d, and

$$\begin{aligned} \rho(G) \leq\ & \frac{1}{2}(d-1)(n-2) \\ & + \frac{1}{2}\sqrt{(d-1)^2n^2 + 4\delta^2(d-1)^2 - 4pq(2d-1) - 4d(d-1)\delta n} \end{aligned}$$

for odd d. Here we improve this result.

Theorem 5. *Let G be a connected bipartite graph with n vertices, diameter d and bipartition $V(G) = A \cup B$, $|A| = p$, $|B| = q$, $p+q = n$. Let δ_A and δ_B be the minimum degrees among vertices from A and B, respectively. Then*

$$\begin{aligned}\rho(G) &\leq \frac{d}{2}\left(n-1-\frac{d}{2}\right)\\ &\quad + \frac{1}{2}\sqrt{d^2n^2 + 4\delta_A\delta_B(d-2)^2 - 4pq(2d-1) - 4(d-1)(d-2)(p\delta_A + q\delta_B)}\end{aligned}$$

for even d, and

$$\begin{aligned}\rho(G) &\leq \frac{2(d-1)n + 1 - d^2}{4}\\ &\quad + \frac{1}{2}\sqrt{(d-1)^2n^2 + 4\delta_A\delta_B(d-1)^2 + 4pq(2d-1) - 4d(d-1)(p\delta_A + q\delta_B)}\end{aligned}$$

for odd d.

Proof. Let $A = \{1, 2, \ldots, p\}$ and $B = \{p+1, p+2, \ldots, p+q\}$. Let $x = (x_1, x_2, \ldots, x_n)^T$ be a Perron eigenvector of $D(G)$ corresponding to the largest eigenvalue $\rho(G)$, such that

$$x_i = \max_{k \in A} x_k \quad \text{and} \quad x_j = \max_{k \in B} x_k\,.$$

Suppose d is even. From the eigenvalue equation $\rho(G) \cdot x = D(G) \cdot x$, written for the component x_i we have

$$\begin{aligned}\rho(G)x_i &= \sum_{k=1}^{p} d_{ik} \cdot x_k + \sum_{k=p+1}^{p+q} d_{ik} \cdot x_k\\ &\leq x_i \cdot [2 + 4 + \cdots + (d-2)] + x_i \cdot d\left[p - 1 - \left(\frac{d}{2} - 1\right)\right]\\ &\quad + x_j \cdot [1 \cdot \delta_A + 3 + \cdots + (d-3)]\\ &\quad + x_j \cdot (d-1)\left[q - \left(\frac{d}{2} - 1\right) - (\delta_A - 1)\right]\\ &= \left(-\frac{d^2}{4} - \frac{d}{4} + dp\right) x_i + \left[(d-1)q - (d-2)\delta_A - \frac{d^2}{4} + \frac{3d}{2} - 2\right] x_j\end{aligned}$$

or equivalently

$$\left(\rho(G) + \frac{d^2}{4} + \frac{d}{2} - dp\right) x_i \leq \left[(d-1)q - (d-2)\delta_A - \frac{d^2}{4} + \frac{3d}{2} - 2\right] x_j\,.$$

Note that for d being an even number, $-\frac{d^2}{4}+\frac{3d}{2}-2 \le 0$. We get

$$\left(\rho(G)+\frac{d^2}{4}+\frac{d}{2}-dp\right)x_i \;\le\; \left[(d-1)q-(d-2)\delta_A\right]x_j\,.$$

Analogously for the component x_j we have

$$\left(\rho(G)+\frac{d^2}{4}+\frac{d}{2}-dq\right)x_j \;\le\; \left[(d-1)p-(d-2)\delta_B\right]x_i\,.$$

Combining these two inequalities, it follows

$$\begin{aligned}0 \;\ge\; & \rho^2(G)+\left[\frac{d^2}{2}+d-d(p+q)\right]\rho(G)+\frac{d^2}{16}(2+d-4p)(2+d-4q)\\ & -\left[(d-1)q-(d-2)\delta_A\right]\left[(d-1)p-(d-2)\delta_B\right]\,.\end{aligned}$$

By analyzing the quadratic inequality and using $p+q=n$, we get

$$\begin{aligned}\rho(G) \;\le\; & \frac{d}{2}\left(n-1-\frac{d}{2}\right)\\ & +\frac{1}{2}\sqrt{d^2n^2+4\delta_A\delta_B(d-2)^2-4pq(2d-1)-4(d-1)(d-2)(p\delta_A+q\delta_B)}\end{aligned}$$

as desired for even d.

Now suppose that d is odd. From the eigenvalue equation $\rho(G)\cdot x = D(G)\cdot x$, written for component x_i we have

$$\begin{aligned}\rho(G)x_i \;&=\; \sum_{k=1}^{p} d_{ik}x_k+\sum_{k=p+1}^{p+q} d_{ik}x_k\\ &\le\; x_i\cdot[2+4+\ldots+(d-3)]+x_i\cdot(d-1)\left(p-1-\frac{d-3}{2}\right)\\ &\quad +x_j\cdot[1\cdot\delta_A+3+\ldots+(d-2)]+x_j\cdot d\left(q-\frac{d-3}{2}-\delta_A\right)\\ &=\; \left[-\frac{d^2}{4}+\frac{1}{4}+(d-1)p\right]x_i+\left[dq-(d-1)\delta_A-\frac{d^2}{4}+d-\frac{3}{4}\right]x_j\end{aligned}$$

or equivalently

$$\left[\rho(G)+\frac{d^2}{4}-\frac{1}{4}-(d-1)p\right]x_i \;\le\; \left[dq-(d-1)\delta_A-\frac{d^2}{4}+d-\frac{3}{4}\right]x_j\,.$$

Note that for d being an odd number, $-\frac{d^2}{4}+d-\frac{3}{4}\leq 0$. We get

$$\left[\rho(G)+\frac{d^2}{4}-\frac{1}{4}-(d-1)p\right]x_i \;\leq\; [dq-(d-1)\delta_A]\,x_j\,.$$

Analogously for the component x_j we have

$$\left[\rho(G)+\frac{d^2}{4}-\frac{1}{4}-(d-1)q\right]x_j \;\leq\; [dp-(d-1)\delta_B]\,x_i\,.$$

Then the result for odd d follows easily. ■

If the upper bound with even d is attained in Theorem 5 for $d=4$, then we have equal values of eigencomponents in both partite sets, from which G is semi–regular, for every vertex v there is a unique vertex at distance 2 and thus all vertices have degree at most 2, which is impossible. Thus the upper bound is attained for even d in Theorem 5 if and only if $d=2$, $\delta_A=q, \delta_B=p$ and $G\cong K_{p,q}$. The upper bound is attained for odd d in Theorem 5 if and only if $d=1$, $p=q=\Delta_A=\Delta_B=1$ and $G\cong K_{1,1}$, or $d=3$, G is semi–regular, any two vertices from the same partite set are at distance 2 and all vertex eccentricities are equal to 3.

Under the conditions of Theorem 5, let δ be the minimum degree. Then $\delta=\min\{\delta_A,\delta_B\}$ and by Theorem 5, for even d we have

$$\begin{aligned}\rho(G) \;\leq\; & \frac{d}{2}\left(n-1-\frac{d}{2}\right)\\ & +\frac{1}{2}\sqrt{d^2n^2+4\delta^2(d-2)^2-4pq(2d-1)-4\delta(d-1)(d-2)n}\end{aligned}$$

while for odd n we have

$$\begin{aligned}\rho(G) \;\leq\; & \frac{2(d-1)n+1-d^2}{4}\\ & +\frac{1}{2}\sqrt{(d-1)^2n^2+4\delta^2(d-1)^2+4pq(2d-1)-4\delta d(d-1)n}\,.\end{aligned}$$

These two upper bounds for $\rho(G)$ improve the upper bounds for $\rho(G)$ in [9] mentioned above for even d and for odd d, respectively.

5. LOWER BOUNDS FOR DE

Let G be a connected graph with $n \geq 2$ vertices. Note that $\rho(G) > 0$. Then

$$DE(G) \geq 2\rho(G)$$

with equality if and only if G has exactly one positive D-eigenvalue. Thus, the lower bounds for $\rho(G)$ may be converted to lower bounds for DE.

Let G be a connected graph with $n \geq 2$ vertices. Let D_i be the i-th row sum of $\mathbf{D}(G)$, i. e., $D_i = \sum_{j=1}^{n} d_{ij}$, where $i = 1, 2, \ldots, n$. It was shown in [6] that

$$\rho(G) \geq \sqrt{\frac{1}{n} \sum_{i=1}^{n} D_i^2} \tag{3}$$

with equality if and only if $\mathbf{D}(G)$ has equal row sums. (In the view of matrix theory, by considering the powers of $\mathbf{D}(G)$, this lower bound could be further improved.) Thus, we have:

Theorem 6. *Let G be a connected graph with $n \geq 2$ vertices. Then*

$$DE(G) \geq 2\sqrt{\frac{1}{n} \sum_{i=1}^{n} D_i^2}$$

with equality if and only if G has exactly one positive D-eigenvalue and $\mathbf{D}(G)$ has equal row sums.

Recall that trees [24], connected unicyclic graphs [25], complete bipartite graphs [24] and K_n have exactly one positive D-eigenvalue. A complete characterization of such graphs seems to be not known.

The Wiener index [26, 27] of a connected graph G is defined as $W(G) = \sum_{i<j} d_{ij} = \frac{1}{2} \sum_{i=1}^{n} D_i$. From (3) and using the Cauchy–Schwarz inequality, as in [6], we get

$$\rho(G) \geq \frac{2W(G)}{n}$$

with equality if and only if $\mathbf{D}(G)$ has equal row sums. Thus, for m being the number of edges of G,

$$\rho(G) \geq 2(n-1) - \frac{2m}{n}$$

with equality if and only if $G \cong K_n$ or G is a regular graph of diameter two. It follows

Theorem 7. *Let G be a connected graph with $n \geq 2$ vertices and m edges. Then*

$$DE(G) \geq \frac{4W(G)}{n}$$

with equality if and only if $\mathbf{D}(G)$ has equal row sums and G has exactly one positive D-eigenvalue. Moreover,

$$DE(G) \geq 4(n-1) - \frac{4m}{n}$$

with equality if and only if either $G \cong K_n$ or G is a regular graph of diameter two with exactly one positive D-eigenvalue.

Ramane et al. [18] conjectured that among the n-vertex connected graphs, the complete graph K_n is the unique graph with the smallest distance energy (equal to $2(n-1)$). For a connected graph G with n vertices and m edges, $2m \leq n(n-1)$ with equality if and only if $G \cong K_n$. By Theorem 7, this conjecture is true. A direct reasoning is as follows: Note that K_n for $n \geq 2$ has exactly one positive D-eigenvalue. From (2), we have $\rho_1 \geq n-1$, and then $DE(G) \geq 2\rho_1 \geq 2(n-1)$ with equalities if and only if $G \cong K_n$.

Let G be a graph. The line graph $L(G)$ of G has the edges of G as vertices, and vertices of $L(G)$ are adjacent if the corresponding edges of G have a vertex in common. The cocktail party graph $CP(a)$ is the graph obtained by deleting a disjoint edges from the complete graph K_{2a}. Thus, $CP(a)$ is a regular graph of degree $2a-2$.

Let G be a graph with vertex set $\{v_1, v_2, \ldots, v_n\}$, and let $a_1, a_2, \ldots, a_n$ be nonnegative integers. The generalized line graph $L(G; a_1, a_2 \ldots, a_n)$ consists of the disjoint union of the line graph $L(G)$ and the cocktail party graphs $CP(a_1), CP(a_2), \ldots, CP(a_n)$, together with all edges joining a vertex $\{v_i, v_j\}$ of $L(G)$ with each vertex of $CP(a_i)$ and $CP(a_j)$.

A regular graph G of diameter two has exactly one positive D-eigenvalue if and only if $\lambda_n \geq -2$. For a generalized line graph, its least eigenvalue is at least -2. An exceptional graph is a connected graph, other than a generalized line graph, with least eigenvalue at least -2. From [28], a graph G is a regular graph of diameter two with $\lambda_n \geq -2$ if and only if G is a cocktail party graph, or G is a regular line graph of diameter two (equivalently, G is the line graph with diameter two of a regular graph or of a semi–regular graph), or G is a regular exceptional graph of diameter two. A list of all 187 regular exceptional graphs is given in Table A3 of [28]. These graphs are listed in such a way that it is not possible to see what their diameters are. Of these, exactly 7 graphs are strongly regular, and thus have diameter two. However, it may be that there are other, not strongly regular graphs with diameter two. We do not attempt to count them.

Corollary 1. *Let G be a connected graph with $n \geq 2$ vertices and m edges. Then*

$$DE(G) \geq 4(n-1) - \frac{4m}{n}$$

with equality if and only if $G \cong K_n$, or G is the cocktail party graph, or G is a regular line graph of diameter two, or G is a regular exceptional graph of diameter two.

By discussion above and Theorem 1, we have

Corollary 2. *Let G be a connected graph with n vertices, maximum degree Δ_1 and second maximum degree Δ_2. Then*

$$DE(G) \geq 2\sqrt{(2n-2-\Delta_1)(2n-2-\Delta_2)}$$

with equality if and only if $G \cong K_n$, or G is the cocktail party graph, or G is a regular line graph of diameter two, or G is a regular exceptional graph of diameter two.

For the graph G, the first Zagreb index of G is defined as $M_1(G) = \sum_{i=1}^{n} d_i^2$ [29–32].

Let G be a triangle– and quadrangle–free connected graph with $n \geq 2$ vertices and m edges. Then from [6] it follows

$$\rho(G) \geq 3(n-1) - \frac{2m}{n} - \frac{M_1(G)}{n}$$

with equality if and only if $\mathbf{D}(G)$ has equal row sums and the diameter of G is at most three, and thus

$$DE(G) \geq 2\left[3(n-1) - \frac{2m}{n} - \frac{M_1(G)}{n}\right]$$

with equality if and only if G has exactly one positive D-eigenvalue, $\mathbf{D}(G)$ has equal row sums and the diameter of G is at most three.

Let G be a connected bipartite graph with p vertices in one partite set and q vertices in the other partite set. Recall that $\rho(G) \geq p+q-2+\sqrt{p^2+q^2-pq}$ with equality if and only if $G \cong K_{p,q}$ and that $K_{p,q}$ has exactly one positive D-eigenvalue. This implies:

Theorem 8. *Let G be a connected bipartite graph with p vertices in one partite set and q vertices in the other partite set. Then*

$$DE(G) \geq 2\left(p+q-2+\sqrt{p^2+q^2-pq}\right)$$

with equality if and only if $G \cong K_{p,q}$.

From this theorem, we have: if G is a connected bipartite graph with $n \geq 2$ vertices, then

$$DE(G) \geq 2\left(n-2+\sqrt{n^2-3\left\lfloor\frac{n}{2}\right\rfloor\left\lceil\frac{n}{2}\right\rceil}\right)$$

with equality if and only if $G \cong K_{\lfloor n/2\rfloor,\lceil n/2\rceil}$.

Let G be a connected bipartite graph with bipartition $V(G) = A \cup B$, $|A| = p$, $|B| = q$, $p+q=n$. Let Δ_A and Δ_B be maximum degrees among vertices from A and B, respectively. By Theorem 4 and the discussion above, we have:

$$DE(G) \geq 2(n-2) + 2\sqrt{n^2-4pq+(3q-2\Delta_A)(3p-2\Delta_B)}$$

with equality if and only if G is a complete bipartite graph $K_{p,q}$ or G is a semi–regular graph with every vertex eccentricity equal to 3 and exactly one positive D-eigenvalue.

Theorem 9. *Let G be a connected graph with n vertices. If $\overline{G}$ is also connected, then*

$$DE(G) + DE(\overline{G}) \geq 6(n-1)$$

with equality if and only if G and $\overline{G}$ both have exactly one positive D-eigenvalue and are both regular graphs of diameter two.

Proof. By Theorem 7,

$$DE(G) + DE(\overline{G}) \geq 8(n-1) - \frac{2n(n-1)}{n} = 6(n-1)$$

with equality if and only if G and $\overline{G}$ both have exactly one positive D-eigenvalue and are both regular graphs of diameter two. ■

6. UPPER BOUNDS FOR DE

In the following we discuss upper bounds for the distance energy of graphs of diameter at most two.

Let G be a simple graph with n vertices. The energy of the graph G is defined as [33, 34]

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

The singular eigenvalues of a (complex) matrix $\mathbf{X}$ are the square roots of the eigenvalues of the matrix $\mathbf{X}\mathbf{X}^*$, where $\mathbf{X}^*$ denotes the conjugate transpose of the matrix $\mathbf{X}$. For an $n \times n$ matrix $\mathbf{X}$, its singular values are denoted by $s_i(\mathbf{X})$, $i = 1, 2, \ldots, n$. Then

$$E(G) = \sum_{i=1}^{n} s_i(\mathbf{A}(G))$$

$$DE(G) = \sum_{i=1}^{n} s_i(\mathbf{D}(G)) \,.$$

Lemma 1. [35] *Let $\mathbf{X}$ and $\mathbf{Y}$ be $n \times n$ matrices. Then* $\sum\limits_{i=1}^{n} s_i(\mathbf{X}+\mathbf{Y}) \leq \sum\limits_{i=1}^{n} s_i(\mathbf{X}) + \sum\limits_{i=1}^{n} s_i(\mathbf{Y})$.

Theorem 10. *Let G be a connected graph with n vertices and diameter at most two. Then*

$$DE(G) \leq 2(n-1) + E(\overline{G}) \,.$$

Proof. Note that

$$\mathbf{D}(G) = \mathbf{J}_n - \mathbf{I}_n + \mathbf{A}(\overline{G})\,.$$

Let $\mathbf{X} = \mathbf{J}_n - \mathbf{I}_n$ and $\mathbf{Y} = \mathbf{A}(\overline{G})$ in Lemma 1, we have

$$DE(G) \leq 2(n-1) + E(\overline{G})$$

as desired. ■

In [36], it was shown that for a graph with n vertices, its energy is bounded from above by $\frac{n}{2}(\sqrt{n}+1)$. Thus, for the connected graph G with n vertices and diameter at most two,

$$DE(G) \leq \frac{n}{2}(\sqrt{n}+1) + 2(n-1)\,.$$

For $n \geq 26$, this is better than the bound given in [15]:

$$DE(G) \leq \sqrt{2n(2n^2 - 2n - 3m)}$$

where m is the number of edges of G, because for $n \geq 26$,

$$\frac{n}{2}(\sqrt{n}+1) + 2(n-1) < n\sqrt{n-1} \leq \sqrt{2n(2n^2-2n-3m)}\,.$$

In [15], it was shown that for a graph G with n vertices, m edges and diameter two,

$$DE(G) \leq \frac{1}{n}(2n^2 - 2n - 2m) + \frac{1}{n}\sqrt{(n-1)[(2n+m)(2n^2-4m) - 4n^2]}\,.$$

This upper bound for $K_{1,n-1}$ is equal to $2n - 4 + \frac{2}{n} + \frac{1}{n}\sqrt{6n^4 - 24n^3 + 34n^2 - 20n + 4}$, while the bound in the previous theorem is $DE(K_{1,n-1}) \leq 2(n-1) + 2(n-2) = 4n - 6$. The latter is better than the former for $n \geq 5$.

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