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Research Article

New bounds on distance Estrada index of graphs

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Abstract: For a connected graph G with vertex set $\{v_1, \ldots, v_n\}$, the distance matrix of G, denoted by $D(G)$, is an $n \times n$ matrix with zero main diagonal, such that its (i, j)-entry is $d(v_i, v_j)$, where $i \neq j$ and $d(v_i, v_j)$ is the distance between v_i and v_j. Let $\theta_1, \ldots, \theta_n$ be the eigenvalues of $D(G)$. The distance Estrada index of G is defined as $DEE(G) = \sum_{i=1}^{n} e^{\theta_i}$. In this paper we find some new sharp bounds for the distance Estrada index of graphs. Our results improve the previous bounds on the distance Estrada index of graphs.

Keywords: distance matrix, distance Estrada index.

AMS Subject classification: 05C09, 05C50, 05C92, 15A18.

1. Introduction

In this paper we consider only simple graphs (finite and undirected, without loops and multiple edges). Let $G = (V(G), E(G))$ be a simple graph. The *order* of G denotes the number of vertices of G. For two vertices u and v by $e = uv$ we mean the edge e between the vertices u and v. By $u \sim v$ we mean that u and v are adjacent (similarly, by $u \nsim v$ we mean that u and v are not adjacent). The *degree* of a vertex v of G, denoted by $deg_G(v)$, is the number of edges incident with v. A r-regular graph is a graph such that every vertex of that has degree r. The *distance* between two vertices u and v denoted by $d(u, v)$ is the length of a shortest path between u and v. The *diameter* of G denoted by $diam(G)$ is the maximum of $d(u, v)$ among all pairs of vertices of u and v of G. A graph is called *connected* if there is at least one path between any two vertices of that. The *complement* of G, denoted by $\overline{G}$, is the simple graph with vertex set $V(G)$ such that two distinct vertices of $\overline{G}$ are adjacent if and only if they are not adjacent in G. As usual the *edgeless graph* (*empty graph*), the *complete graph*, the *cycle*, and the *path* of order n, are denoted by $\overline{K_n}$, K_n, C_n and P_n, respectively. By $K_{n_1,\ldots,n_t}$ we mean the *complete multipartite graph* with parts size $n_1, \ldots, n_t$. In particular, the *complete bipartite graph* with part sizes m and n is denoted by $K_{m,n}$. For two disjoint graphs G and H, the *disjoint union* of G and H, denoted by $G \cup H$ is the graph with the vertex set $V(G) \cup V(H)$ and the edge set $E(G) \cup E(H)$. The graph rG denotes the disjoint union of r copies of G. The *identity* matrix and the matrix whose all of entries are equal to 1 are denoted by I and J, respectively.

Let G be a simple connected graph with vertex set $\{v_1, \ldots, v_n\}$. The *distance matrix* of G, denoted by $D(G) = [d_{ij}]$, is the $n \times n$ matrix such that

$$d_{ij} := \begin{cases} 0, & \text{if } i = j; \\ d(v_i, v_j), & \text{if } i \neq j. \end{cases}$$

Since the distance matrix is real and symmetric, all of its eigenvalues are real. By distance eigenvalues of G, denoted by $\theta_1(G), \ldots, \theta_n(G)$, we mean the eigenvalues of its distance matrix (see [9–11]).

In chemical graph theory, there are very important invariants. One of them is the *Estrada index*. This index was introduced by Ernesto Estrada. We recall that the Estrada index of a graph G of order n, denoted by $EE(G)$, is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$, where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of G. There are remarkable variety of properties, chemical and non-chemical applications of the Estrada index of graphs. For more details on some of the chemical applications of this index we refer to [3–7]. Using power-series expansion of the function e^x, we note that

$$EE(G) = \sum_{t=0}^{+\infty} \frac{A_t(G)}{t!},$$

where

$$A_t(G) = \sum_{i=1}^{n} \lambda_i^t.$$

It is well known that for every graph G of order n, $A_1(G) = 0$, $A_2(G) = 2m$ and $A_3(G) = 6t$, where m is the number of edges and t is the number of triangles of G, see [2].

Similar to the definition of the Estrada index, in [8] the authors defined the *distance Estrada index* as follows. Let G be a connected graph of order n. The distance Estrada index of G, denoted by $DEE(G)$, is

$$DEE(G) = \sum_{i=1}^{n} e^{\theta_i},$$

where $\theta_1, \ldots, \theta_n$ are the distance eigenvalues of G (the eigenvalues of $D(G)$).

In [1, 8, 14] some properties of the distance Estrada index of graphs have been obtained. In [8] the authors found some bounds for this index in terms of the number of vertices and the number of edges of graphs. In this paper we study the distance Estrada index of graphs and find some sharp bounds for this. We show that our results generalize and improve the previous bounds on the distance Estrada index of graphs that have been obtained in [8] and [14].

2. Distance Estrada index of graphs

In this section, we find some bounds for the Distance Estrada index of graphs in terms of the number of vertices, the number of edges and the diameter of graphs. Our approach is different from the other researchers. We use the next result to obtain our bounds.

Theorem 1. [13] *Let $f(x_1, \ldots, x_n) = e^{x_1} + \cdots + e^{x_n}$. Then the maximum and the minimum value of the function f under the conditions*

$$x_1 + \cdots + x_n = 0 \text{ and } x_1^2 + \cdots + x_n^2 = k > 0, \tag{2.1}$$

are as following. If $k \geq n$, then for every $(x_1, \ldots, x_n)$ satisfying the conditions (2.1),

$$(n-1)e^{\sqrt{\frac{k}{n(n-1)}}} + e^{-\sqrt{\frac{k(n-1)}{n}}} \leq f(x_1, \ldots, x_n) \leq e^{\sqrt{\frac{k(n-1)}{n}}} + (n-1)e^{-\sqrt{\frac{k}{n(n-1)}}}.$$

Moreover in the left hand side the equality holds if and only if $(x_{\sigma(1)}, \ldots, x_{\sigma(n)}) = (-c, d, d, \ldots, d)$ and in the right hand side the equality holds if and only if $(x_{\rho(1)}, \ldots, x_{\rho(n)}) = (c, -d, -d, \ldots, -d)$ for some permutations σ and ρ on $\{1, \ldots, n\}$, where $c = \sqrt{\frac{k(n-1)}{n}}$ and $d = \sqrt{\frac{k}{n(n-1)}}$.

It is not hard to prove the following lemmas.

Lemma 1. *Let A, B and C are positive numbers. Then the following hold:*

(i) *$f(x) = e^{\sqrt{Ax}} + Be^{-\sqrt{Cx}}$ is a strictly increasing function on the interval $[0, \infty)$ if and only if $A \geq B^2C$.*

(ii) *$g(x) = Ae^{\sqrt{Bx}} + e^{-\sqrt{Cx}}$ is a strictly increasing function on the interval $[0, \infty)$ if and only if $A^2B \geq C$.*

Lemma 2. [13] *Let B be a real symmetric matrix of order n such that the main diagonal of B is zero and the other entries are positive. Then the following hold:*

(i) *The eigenvalues of B are $\alpha, \underbrace{\beta, \ldots, \beta}_{n-1}$ where $\alpha > 0$ and $\beta < 0$ if and only if $n \geq 2$ and $B = t(J - I)$ for some positive real number t.*

(ii) *The eigenvalues of B are $\alpha, \underbrace{\beta, \ldots, \beta}_{n-1}$ where $\alpha < 0$ and $\beta > 0$ if and only if $n = 2$ and $B = t(J - I)$ for some positive real number t.*

Lemma 3. [8] *Let G be a connected graph on n vertices $v_1, \ldots, v_n$. Assume that $\theta_1, \ldots, \theta_n$ are the distance eigenvalues of G. Then the following hold:*

$$\theta_1 + \cdots + \theta_n = 0 \tag{2.2}$$

and

$$\theta_1^2 + \cdots + \theta_n^2 = 2 \sum_{1 \leq i < j \leq n} d(v_i, v_j)^2. \tag{2.3}$$

Now we prove one of the main results of this paper. We remark that if G is a graph with one vertex, then $G = K_1$ and so $DEE(G) = e^0 = 1$. Thus in continue we study graphs of order $n \geq 2$.

Theorem 2. *Let G be a connected graph on $n \geq 2$ vertices $v_1, \ldots, v_n$ and with m edges. Let*

$$S' = 2 \sum_{1 \leq i < j \leq n} d(v_i, v_j)^2.$$

Then

$$(n-1)e^{\sqrt{\frac{S'}{n(n-1)}}} + e^{-\sqrt{\frac{S'(n-1)}{n}}} \leq DEE(G) \leq e^{\sqrt{\frac{S'(n-1)}{n}}} + (n-1)e^{-\sqrt{\frac{S'}{n(n-1)}}}. \tag{2.4}$$

Moreover in the left hand side the equality holds if and only if $G = K_2$ and in the right hand side the equality holds if and only if $G = K_n$.

Proof. We note that for every adjacent vertices u and v of G, $d(u, v) = 1$. Hence $S' \geq 2m \geq 2n - 2 \geq n$. By putting $k = S'$ in Theorem 1 and considering Lemma 3, Equation (2.4) is obtained. Now we investigate the equality. By Theorem 1, on the right hand side the equality holds if and only if the distance eigenvalues of G are

$$\sqrt{\frac{S'(n-1)}{n}}, \underbrace{-\sqrt{\frac{S'}{n(n-1)}}, \ldots, -\sqrt{\frac{S'}{n(n-1)}}}_{n-1}.$$

Thus by the first part of Lemma 2 we find that $D(G) = t(J - I)$ for some positive number t. This shows that the entries of $D(G)$ are 0 or t. If $v_i v_j$ is an edge of G, then the (i, j)-entry of $D(G)$ is equal to 1. Hence $t = 1$ and so $D(G) = J - I$. This shows that $G = K_n$. Conversely for $G = K_n$ the upper bound in (2.4) happens. Similarly, by the second part of Lemma 2, one can prove the equality of the left hand side. The proof is complete. $\square$

In [8] the authors find the following bounds for the distance Estrada index of graphs.

Theorem 3. [8] *Let G be a connected graph with n vertices and with m edges and with diameter d. Then*

$$\sqrt{n^2+4m} \leq DEE(G) \leq n-1+e^{d\sqrt{n(n-1)}},$$

and the equality holds in both sides if and only if $G = K_1$.

Shang [14] found the following upper bound for the distance Estrada index of graphs in terms of the Wiener index and the diameter of graphs. We recall that the Wiener index [12] of a connected graph G, denoted by $W(G)$, is

$$\sum_{1\leq i<j\leq n} d(v_i, v_j),$$

where $V(G) = \{v_1, \ldots, v_n\}$.

Theorem 4. [14] *Let G be a connected graph of order n and $d = diam(G)$ and $W = W(G)$. Then*

$$DEE(G) \leq n-1+e^{\sqrt{2dW}},$$

and the equality holds if and only if $G = K_1$.

Here we improve the bounds of Theorem 3. In addition, we show that our bounds are better than the bound of Theorem 4 for some families of graphs.

Theorem 5. *Let G be a connected graph with $n \geq 2$ vertices and m edges and $d = diam(G)$. Then*

$$(n-1)e^{\sqrt{\frac{4n^2-4n-6m}{n(n-1)}}} + e^{-\sqrt{\frac{(4n^2-4n-6m)(n-1)}{n}}} \leq DEE(G)$$
$$\leq e^{\sqrt{\frac{d^2n^2-d^2n-(2d^2-2)m}{n(n-1)}}} + (n-1)e^{-\sqrt{\frac{(d^2n^2-d^2n-(2d^2-2)m)(n-1)}{n}}}.$$

In addition, in the left hand side the equality holds if and only if $G = K_2$ and in the right hand side the equality holds if and only if $G = K_n$.

Proof. Let $V(G) = \{v_1, \ldots, v_n\}$ and

$$S' = S'(G) = 2\sum_{1\leq i<j\leq n} d(v_i, v_j)^2.$$

For every $i \neq j$, $d(v_i, v_j) = 1$ or $2 \leq d(v_i, v_j) \leq d$. Thus

$$m+4(\binom{n}{2}-m) \leq \sum_{1\leq i<j\leq n, v_i\sim v_j} d(v_i, v_j)^2 + \sum_{1\leq i<j\leq n, v_i\not\sim v_j} d(v_i, v_j)^2 \leq m+d^2(\binom{n}{2}-m).$$

Therefore

$$4n^2 - 4n - 6m \leq S' \leq d^2n^2 - d^2n - (2d^2 - 2)m \tag{2.5}$$

and the equality holds (in both sides) if and only if $diam(G) \leq 2$. Let

$$f(x) = e^{\sqrt{\frac{(n-1)x}{n}}} + (n-1)e^{-\sqrt{\frac{x}{n(n-1)}}}$$

and

$$g(x) = (n-1)e^{\sqrt{\frac{x}{n(n-1)}}} + e^{-\sqrt{\frac{(n-1)x}{n}}}.$$

By Theorem 2,

$$g(S') \leq DEE(G) \leq f(S') \tag{2.6}$$

and in the left hand side the equality holds if and only if $G = K_2$ and in the right hand side the equality holds if and only if $G = K_n$.
On the other hand, by Lemma 1, $f(x)$ and $g(x)$ are strictly increasing functions on the interval $[0, \infty)$. Thus by Equation (2.5), $f(S') \leq f(d^2n^2 - d^2n - (2d^2 - 2)m)$ and $g(S') \geq g(4n^2 - 4n - 6m)$ and the equality holds (for both of them) if and only if $diam(G) \leq 2$. Using Equation (2.6) we conclude that

$$g(4n^2 - 4n - 6m) \leq DEE(G) \leq f(d^2n^2 - d^2n - (2d^2 - 2)m)$$

and the equality holds in the left hand side if and only if $G = K_2$ and the equality holds in the right hand side if and only if $G = K_n$. Since

$$f(d^2n^2 - d^2n - (2d^2 - 2)m) = e^{\sqrt{\frac{d^2n^2 - d^2n - (2d^2-2)m}{n(n-1)}}} + (n-1)e^{-\sqrt{\frac{(d^2n^2 - d^2n - (2d^2-2)m)(n-1)}{n}}}$$

and

$$g(4n^2 - 4n - 6m) = (n-1)e^{\sqrt{\frac{4n^2-4n-6m}{n(n-1)}}} + e^{-\sqrt{\frac{(4n^2-4n-6m)(n-1)}{n}}}$$

the proof is complete. $\square$

Now we show that our bounds for the distance Estrada index (the bounds of Theorem 5) are better than the bounds of Theorem 3. Assume that $n \geq 2$. Related to the upper bound note that $d^2n(n-1) < d^2n^2(n-1)^2$. Thus

$$\sqrt{\frac{d^2n^2 - d^2n - (2d^2 - 2)m}{n(n-1)}} < d\sqrt{n(n-1)}.$$

Therefore

$$e^{\sqrt{\frac{d^2n^2-d^2n-(2d^2-2)m}{n(n-1)}}} < e^{d\sqrt{n(n-1)}}. \tag{2.7}$$

On the other hand

$$e^{-\sqrt{\frac{(d^2n^2-d^2n-(2d^2-2)m)(n-1)}{n}}} < 1 \tag{2.8}$$

Now by inequalities (2.7) and (2.8), we obtain that

$$e^{\sqrt{\frac{d^2n^2-d^2n-(2d^2-2)m}{n(n-1)}}} + (n-1)e^{-\sqrt{\frac{(d^2n^2-d^2n-(2d^2-2)m)(n-1)}{n}}} < n-1+e^{d\sqrt{n(n-1)}}.$$

Now we investigate the lower bound. Since $2m \leq n^2-n$, so

$$\frac{4n^2-4n-6m}{n(n-1)} \geq 1.$$

Thus

$$(n-1)e^{\sqrt{\frac{4n^2-4n-6m}{n(n-1)}}} \geq e(n-1). \tag{2.9}$$

On the other hand (for $n \geq 2$),

$$e^2(n-1)^2 > 7(n-1)^2 > 3n^2-2n \geq n^2+4m.$$

This shows that (by inequality (2.9))

$$(n-1)e^{\sqrt{\frac{4n^2-4n-6m}{n(n-1)}}} \geq e(n-1) > \sqrt{n^2+4m} \tag{2.10}$$

and so

$$(n-1)e^{\sqrt{\frac{4n^2-4n-6m}{n(n-1)}}} + e^{-\sqrt{\frac{(4n^2-4n-6m)(n-1)}{n}}} > \sqrt{n^2+4m}.$$

Remark 1. Let G be a connected graph of order n on vertices $v_1, \ldots, v_n$. Let

$$S'(G) = 2\sum_{1\leq i<j\leq n} d(v_i,v_j)^2.$$

Using the technique that we used in the proof of Theorem 5, by considering the lower bounds and upper bounds for $S'(G)$, one can find other bounds for the distance Estrada index of graphs. Let d be the diameter of G. One can see that

$$n(n-1) \leq S'(G) \leq n(n-1)d^2 \leq n(n-1)^3. \tag{2.11}$$

In addition, from the left, the first and the second equality holds if and only if G is the complete graph K_n and in the right hand side the equality holds if and only if G is the complete graph K_1 or K_2. Now by using these bounds for $S'(G)$ and applying Theorem 2, we obtain some bounds for the distance Estrada index of graphs (see the two following results).

Besides the upper bound of Theorem 5, the following upper bound also improves the upper bound of Theorem 3 for the distance Estrada index of graphs.

Theorem 6. *Let G be a connected graph of order n and with diameter d. Then*

$$(n-1)e + e^{1-n} \leq DEE(G) \leq e^{d(n-1)} + (n-1)e^{-d}$$

and the equality holds in both sides if and only if $G = K_n$.

Remark 2. We note that the upper bound of Theorem 6 is better than the upper bound of Theorem 2 for some families of graphs. For example one can check for stars the upper bound of Theorem 6 is better that the upper bound of Theorem 2. We note that for $n \geq 2$, $W(K_{1,n-1}) = (n-1)^2$ and for $n \geq 3$, $diam(K_{1,n-1}) = 2$.

Using Remark 1 we obtain an upper bound for the distance Estrada index of graphs in terms of the number of vertices.

Theorem 7. *Let G be a connected graph of order n. Then*

$$DEE(G) \leq e^{(n-1)^2} + (n-1)e^{1-n}$$

and the equality holds if and only if $G = K_1$ or $G = K_2$.

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