Hacettepe Journal of Mathematics and Statistics
Volume 38 (3) (2009), 277 – 283

ON THE DISTANCE ESTRADA INDEX OF GRAPHS

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Received 24 : 02 : 2009 : Accepted 25 : 09 : 2009

Abstract

The D-eigenvalues $\mu_1, \mu_2, \dots, \mu_n$ of a connected graph G are the eigenvalues of its distance matrix D. In this paper we define and investigate the distance Estrada index of the graph G as $\mathrm{DEE} = \mathrm{DEE}(G) = \sum_{i=1}^{n} \mathrm{e}^{\mu_i}$ and obtain bounds for $\mathrm{DEE}(G)$ and some relation between $\mathrm{DEE}(G)$ and the distance energy.

Keywords: Distance energy, Distance Estrada index, Bound.

2000 AMS Classification: 05 C 12, 05 C 90.

1. Introduction

Let $G = (V, E)$ be a simple graph with n vertices and m edges. Such a graph will be referred to as an (n, m)-graph.

Let the graph G be connected on the vertex set $V = \{v_1, v_2, \dots, v_n\}$. The distance matrix $D = D(G)$ of G is defined so that its (i, j)-entry is equal to $d_G(v_i, v_j)$, denoted by d_{ij}, the distance (i.e., the length of the shortest path [1]) between the vertices v_i and v_j of G. The diameter of the graph G is the maximum distance between any two vertices of G. Let Δ be the diameter of G, and $A(G)$ the $(0, 1)$-adjacency matrix of G. The eigenvalues of $D(G)$ are called the D-eigenvalues of G, and the eigenvalues of the adjacency matrix of G are said to be the eigenvalues of G [2]. Since $D(G)$ and $A(G)$ are real symmetric matrices, their eigenvalues are real numbers. So we can order them so that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ are the eigenvalues and D-eigenvalues of G, respectively.

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†Material based on part of the master thesis of the second author.

The energy of the graph G is defined in [11-13] as:

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

The Estrada index of the graph G is defined in [5-10] as:

$$\text{(2)} \qquad \mathrm{EE} = \mathrm{EE}(G) = \sum_{i=1}^{n} \mathrm{e}^{\lambda_i}$$

Denoting by $M_k = M_k(G)$ the k-th moment of the graph G,

$$M_k = M_k(G) = \sum_{i=1}^{n} (\lambda_i)^k,$$

and recalling the power-series expansion of e^x, we have

$$\text{(3)} \qquad \mathrm{EE} = \sum_{k=0}^{\infty} \frac{M_k}{k!}.$$

It is well known that [8] $M_k(G)$ is equal to the number of closed walks of length k of the graph G.

The Estrada index of graphs has an important role in Chemistry and Physics. There exists a vast literature that studies the Estrada index of graphs. We refer the reader to [3-10] for surveys and more information.

Recently, J. A. de la Peña *et al.* [3] established lower and upper bounds for EE in terms of the number of vertices and edges. They also obtained some inequalities between EE and the energy of G. Their results are the following.

1.1. Theorem. [3] *Let G be an (n, m)-graph. Then the Estrada index of G is bounded as follows:*

$$\text{(4)} \qquad \sqrt{n^2 + 4m} \leq \mathrm{EE}(G) \leq n - 1 + \mathrm{e}^{\sqrt{2m}}.$$

Equality on both sides of (4) *is attained if and only if* $G \simeq \overline{K}_n$.

1.2. Theorem. [3] *Let G be an (n, m)-graph. Then*

$$\text{(5)} \qquad \mathrm{EE}(G) - \mathrm{E}(G) \leq n - 1 - \sqrt{2m} + \mathrm{e}^{\sqrt{2m}}$$

or

$$\text{(6)} \qquad \mathrm{EE}(G) \leq n - 1 + \mathrm{e}^{\mathrm{E}(G)}.$$

Equality in (5) *or* (6) *is attained if and only if* $G \simeq \overline{K}_n$.

The distance energy of the graph G is defined in [14] as:

$$\text{(7)} \qquad \mathrm{E}_D = \mathrm{E}_D(G) = \sum_{i=1}^{n} |\mu_i| \,.$$

Now we define the distance Estrada index of the graph G and obtain bounds for $\mathrm{DEE}(G)$ and some relations between $\mathrm{DEE}(G)$ and the distance energy.

2. The distance Estrada index of graphs

2.1. Definition. If G is an (n,m)-graph, then the *distance Estrada index of* G, denoted by DEE(G), is equal to

$$\text{DEE} = \text{DEE}(G) = \sum_{i=1}^{n} e^{\mu_i}, \tag{8}$$

where $\mu_1 \geq \mu_2 \geq \cdots \mu_n$ are the $D-$eigenvalues of G.

Let

$$N_k = \sum_{i=1}^{n} (\mu_i)^k.$$

Then

$$\text{DEE}(G) = \sum_{k=0}^{\infty} \frac{N_k}{k!}. \tag{9}$$

2.2. Lemma. [15] *Let G be a connected (n,m)-graph and $\mu_1, \mu_2, \cdots, \mu_n$ its D-eigenvalues. Then*

$$\sum_{i=1}^{n} \mu_i = 0$$

and

$$\sum_{i=1}^{n} \mu_i^2 = 2\sum_{i<j} (d_{ij})^2.$$

2.3. Lemma. *Let G be a connected (n,m)-graph and Δ the diameter of G. Then*

$$m \leq \sum_{i<j} (d_{ij})^2 \leq \frac{n(n-1)}{2}\Delta^2. \tag{10}$$

Equality holds on both sides of (10) *if and only if* $G \simeq K_n$.

Proof. Since $d_{ij} \geq 1$ $(i \neq j)$ and $d_{ij} \leq \Delta$, we obtain

$$\sum_{i<j} (d_{ij})^2 \geq \frac{n(n-1)}{2} \geq m$$

and

$$\sum_{i<j} (d_{ij})^2 \leq \frac{n(n-1)}{2}\Delta^2.$$

Also, equality holds on both sides of (10) if and if $G \simeq K_n$. Hence we get the result. □

2.4. Theorem. *Let G be a connected (n,m)-graph and Δ the diameter of G. Then the distance Estrada index is bounded as follows*

$$\sqrt{n^2+4m} \leq \text{DEE}(G) \leq n-1+e^{\Delta\sqrt{n(n-1)}}. \tag{11}$$

Equality holds on both sides of (11) *if and only if* $G \simeq K_1$.

Proof. **Lower bound:** Directly from Eq. (8) we get

$$\text{DEE}^2(G) = \sum_{i=1}^{n} e^{2\mu_i} + 2\sum_{i<j} e^{\mu_i} e^{\mu_j}. \tag{12}$$

By the arithmetic geometric mean inequality, we get

$$
\begin{aligned}
2\sum_{i<j} \mathrm{e}^{\mu_i}\mathrm{e}^{\mu_j} &\geq n(n-1)\left(\prod_{i<j}\mathrm{e}^{\mu_i}\mathrm{e}^{\mu_j}\right)^{\frac{2}{n(n-1)}} \\
&= n(n-1)\left[\left(\prod_{i=1}^{n}\mathrm{e}^{\mu_i}\right)^{n-1}\right]^{\frac{2}{n(n-1)}} \\
&= n(n-1)(\mathrm{e}^{N_1})^{\frac{2}{n}} \\
&= n(n-1).
\end{aligned}
\tag{13}
$$

By means of a power-series expansion and $N_0 = n$; $N_1 = 0$ and $N_2 = 2\sum_{i<j}(d_{ij})^2$, we obtain

$$\sum_{i=1}^{n} \mathrm{e}^{2\mu_i} = \sum_{i=1}^{n}\sum_{k\geq 0}\frac{(2\mu_i)^k}{k!} = n + 4\sum_{i<j}(d_{ij})^2 + \sum_{i=1}^{n}\sum_{k\geq 3}\frac{(2\mu_i)^k}{k!}.$$

Since we want to get as good a lower bound as possible, it looks reasonable to replace $\sum_{k\geq 3}\frac{(2\mu_i)^k}{k!}$ by $4\sum_{k\geq 3}\frac{(\mu_i)^k}{k!}$. However, we use a multiplier $t \in [0,4]$ instead of $4 = 2^2$, so as to arrive at

$$
\begin{aligned}
\sum_{i=1}^{n}\mathrm{e}^{2\mu_i} &\geq n + 4\sum_{i<j}(d_{ij})^2 + t\sum_{i=1}^{n}\sum_{k\geq 3}\frac{(\mu_i)^k}{k!} \\
&= n + 4\sum_{i<j}(d_{ij})^2 - tn - t\sum_{i<j}(d_{ij})^2 + t\sum_{i=1}^{n}\sum_{k\geq 0}\frac{(\mu_i)^k}{k!} \\
&= n(1-t) + (4-t)\sum_{i<j}(d_{ij})^2 + t\mathrm{DEE}(G).
\end{aligned}
$$

By Lemma 2.3, we get

$$\sum_{i=1}^{n}\mathrm{e}^{2\mu_i} \geq n(1-t) + (4-t)m + t\mathrm{DEE}(G). \tag{14}$$

By substituting (13) and (14) back into (12), and solving for DEE(G), we get

$$\mathrm{DEE}(G) \geq \frac{t}{2} + \sqrt{\left(n - \frac{t}{2}\right)^2 + (4-t)m}.$$

It is easy to see that for $n \geq 2$ and $m \geq 1$ the function

$$f(x) := \frac{x}{2} + \sqrt{\left(n - \frac{x}{2}\right)^2 + (4-x)m}$$

monotonically decreases in the interval $[0,4]$. As a result, the best lower bound for DEE(G) is attained for $t = 0$. This gives us the first part of the theorem.

Upper bound. Starting from the following inequality, we get

$$\begin{aligned}
\mathrm{DEE}(G) &= n + \sum_{i=1}^{n}\sum_{k\geq 1}\frac{(\mu_i)^k}{k!}\\
&= n + \sum_{i=1}^{n}\sum_{k\geq 1}\frac{|\mu_i|^k}{k!}\\
&= n + \sum_{k\geq 1}\frac{1}{k!}\sum_{i=1}^{n}(\mu_i^2)^{\frac{k}{2}}\\
&\leq n + \sum_{k\geq 1}\frac{1}{k!}\left[\sum_{i=1}^{n}(\mu_i^2)\right]^{\frac{k}{2}}\\
&= n + \sum_{k\geq 1}\frac{1}{k!}\left[2\sum_{i<j}(d_{ij})^2\right]^{\frac{k}{2}}\\
&= n - 1 + \sum_{k\geq 0}\frac{\left(\sqrt{2\sum_{i<j}(d_{ij})^2}\right)^k}{k!}\\
&= n - 1 + \mathrm{e}^{\sqrt{2\sum_{i<j}(d_{ij})^2}}.
\end{aligned}$$

By Lemma 2.3, we obtain

$$\mathrm{DEE}(G) \leq n - 1 + \mathrm{e}^{\Delta\sqrt{n(n-1)}}.$$

Hence we get the right-hand side of inequality of (11).

From the derivation of (11) it is clear that equality holds if and only if the graph G has all zero D-eigenvalues. Since G is a connected graph, this only happens in the case of $G \simeq K_1$.

Hence we get the proof of theorem. □

3. Bounds for the distance Estrada index involving the distance energy

3.1. Theorem. *Let G be a connected (n, m)-graph and Δ the diameter of G. Then*

$$\mathrm{DEE}(G) - \mathrm{E}_D(G) \leq n - 1 - \Delta\sqrt{n(n-1)} + \mathrm{e}^{\Delta\sqrt{n(n-1)}}, \tag{15}$$

or

$$\mathrm{DEE}(G) \leq n - 1 + \mathrm{e}^{\mathrm{E}_D(G)}. \tag{16}$$

Equality holds in (16) *or* (17) *if and only if $G \simeq K_1$.*

Proof. From the proof of Theorem 2.4., we have

$$\mathrm{DEE}(G) = n + \sum_{i=1}^{n}\sum_{k\geq 1}\frac{(\mu_i)^k}{k!} \leq n + \sum_{i=1}^{n}\sum_{k\geq 1}\frac{|\mu_i|^k}{k!}.$$

Taking into account the definition of the distance energy (7), we get

$$\mathrm{DEE}(G) \leq n + \mathrm{E}_D(G) + \sum_{i=1}^{n}\sum_{k\geq 2}\frac{|\mu_i|^k}{k!},$$

which leads (as in Theorem 2.4) to

$$\begin{aligned}\mathrm{DEE}(G) - \mathrm{E}_D(G) &\leq n + \sum_{i=1}^{n} \sum_{k \geq 2} \frac{|\mu_i|^k}{k!} \\ &\leq n - 1 - \sqrt{2\sum_{i<j}(d_{ij})^2} + \mathrm{e}^{\sqrt{2\sum_{i<j}(d_{ij})^2}}.\end{aligned} \tag{17}$$

One can easily see that the function

$$f(x) := \mathrm{e}^x - x$$

monotonically increases in the interval $[0, +\infty]$. Therefore the best upper bound for $\mathrm{DEE}(G) - \mathrm{E}_D(G)$ is obtained for $\sum_{i<j}(d_{ij})^2 = \frac{n(n-1)}{2}\Delta^2$ by Lemma 2.3. Then we get

$$\mathrm{DEE}(G) - \mathrm{E}_D(G) \leq n - 1 - \Delta\sqrt{n(n-1)} + \mathrm{e}^{\Delta\sqrt{n(n-1)}}.$$

Another route to connect $\mathrm{DEE}(G)$ and $\mathrm{E}_D(G)$ as follows:

$$\begin{aligned}\mathrm{DEE}(G) &\leq n + \sum_{i=1}^{n} \sum_{k \geq 1} \frac{|\mu_i|^k}{k!} \\ &\leq n + \sum_{k \geq 1} \frac{1}{k!}\left(\sum_{i=1}^{n} |\mu_i|^k\right) \\ &= n + \sum_{k \geq 1} \frac{(\mathrm{E}_D(G))^k}{k!} \\ &= n - 1 + \sum_{k \geq 0} \frac{(\mathrm{E}_D(G))^k}{k!},\end{aligned}$$

implying

$$\mathrm{DEE}(G) \leq n - 1 + \mathrm{e}^{\mathrm{E}_D(G)}.$$

Also, equality holds in (16) or (17) if and only if $G \simeq K_1$. □

Acknowledgement. This work is supported by the Coordinating Office of Selçuk University Scientific Research Projects.

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