

# Bounds of distance Estrada index of graphs

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## Abstract

Let  $\lambda_1, \lambda_2, \dots, \lambda_n$  be the eigenvalues of the distance matrix of a connected graph  $G$ . The distance Estrada index of  $G$  is defined as  $DEE(G) = \sum_{i=1}^n e^{\lambda_i}$ . In this note, we present new lower and upper bounds for  $DEE(G)$ . In addition, a Nordhaus-Gaddum type inequality for  $DEE(G)$  is given.

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## 1 Introduction

Let  $G = (V(G), E(G))$  be a simple connected graph with vertex set  $V(G) = \{v_1, v_2, \dots, v_n\}$  and edge set  $E(G)$ . The adjacency matrix of  $G$  is  $A(G) = (a_{ij}) \in \mathbb{R}^{n \times n}$  (or  $A$  for short), where  $a_{ij} = 1$  if two vertices  $v_i$  and  $v_j$  are adjacent in  $G$  and  $a_{ij} = 0$  otherwise. The eigenvalues of  $A$  are real, and can be ordered as  $\lambda_1(A) \geq \lambda_2(A) \geq \dots \geq \lambda_n(A)$ . The distance matrix of  $G$  is a symmetric matrix  $D(G) = (d_{ij}) \in \mathbb{R}^{n \times n}$  (or  $D$  for short) in which  $d_{ij}$  denotes the length of shortest path between two vertices  $v_i$  and  $v_j$ . Since  $D$  is real symmetric, its eigenvalues (called distance eigenvalues or distance spectra) can also be arranged in non-increasing order as  $\lambda_1(D) \geq \lambda_2(D) \geq \dots \geq \lambda_n(D)$ . We refer the reader to [1] for a comprehensive survey on distance eigenvalues.

The Estrada index of graph  $G$ , put forward by Estrada [7], is defined as

$$EE(G) = \sum_{i=1}^n e^{\lambda_i(A)}.$$

This graph-spectrum-based invariant has found a number of applications in chemistry, physics, and complex networks. For example, it is used as a measure for the degree of folding of long chain polymeric molecules [8]. It also characterizes the centrality [9] as well as robustness [17] of complex

networks. For various mathematical properties of the Estrada index, see e.g. [4, 5, 12, 18].

Quite recently, in full analogy with the Estrada index, the distance Estrada index of a connected graph  $G$  was introduced in [11] as

$$DEE(G) = \sum_{i=1}^n e^{\lambda_i(D)}. \quad (1)$$

Let  $K_n$  be the complete graph on  $n$  vertices. Some upper and lower bounds for  $DEE(G)$  were established as follows.

**Theorem 1.** [11] *Let  $G$  be a connected graph with  $n$  vertices and  $m$  edges, and  $\rho = \rho(G)$  the diameter of  $G$ . Then*

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

*Equality holds on both sides of (2) if and only if  $G = K_1$ .*

**Theorem 2.** [3] *Let  $G$  be a connected graph with  $n \geq 2$  vertices and  $m$  edges. Then*

$$DEE(G) \geq e^{2(n-1) - \frac{2m}{n}} + e^{-2(n-1) + \frac{2m}{n}} + n - 2 \quad (3)$$

*with equality if and only if  $G = K_2$ .*

Some results relating  $DEE(G)$  to the Winer index and graph energy can be found in [3, 11]. Moreover, the distance Estrada index for strongly quotient graphs and Erdős-Rényi random graphs were discussed in [2] and [19], respectively. In this note, we establish some new bounds for  $DEE(G)$  involving diameter, maximum degree, and second maximum degree. Our bounds improve some results in [3, 11]. Furthermore, a Nordhaus-Gaddum type inequality for  $DEE(G)$  is presented.

## 2 Some lemmas

We list some useful lemmas for distance spectra in this section.

**Lemma 1.** [16] *Let  $G$  be a connected graph with  $n$  vertices and  $m$  edges. Then  $\sum_{i=1}^n \lambda_i(D) = 0$  and  $\sum_{i=1}^n \lambda_i^2(D) = 2 \sum_{i < j} d_{ij}^2$ .*

The next result relies on a special relation between the adjacency and distance matrices of graphs having diameter 2. It has been applied in deriving  $DEE(G)$  in dense random graph settings [19].

**Lemma 2.** [6, 14] *Let  $G$  be an  $r$ -regular graph on  $n$  vertices with diameter at most 2 and adjacency eigenvalues  $\lambda_1(A) = r, \lambda_2(A), \lambda_3(A), \dots, \lambda_n(A)$ . Then the distance eigenvalues of  $G$  are  $2n - 2 - r, -2 - \lambda_2(A), -2 - \lambda_3(A), \dots, -2 - \lambda_n(A)$ .*

**Lemma 3.** [23] *Let  $G$  be a connected graph on  $n$  vertices with maximum degree  $\Delta_1$  and second maximum degree  $\Delta_2$ . Then*

$$\lambda_1(D) \geq \sqrt{(2n - 2 - \Delta_1)(2n - 2 - \Delta_2)}$$

*with equality if and only if  $G$  is a regular graph with diameter at most 2.*

More details on extremal values for the largest distance eigenvalue of a graph can be found in e.g. [13, 22, 23]. Let  $K_{n_1, n_2, \dots, n_s}$  denote the complete  $s$ -partite graph. The following result characterizes the least distance eigenvalue.

**Lemma 4.** [21] *Let  $G$  be a graph on  $n$  vertices. For  $n \geq 2$ ,  $\lambda_n(D) = -1$  if and only if  $G = K_n$ . For  $n \geq 3$ ,  $\lambda_n(D) = -2$  if and only if  $G = K_{n_1, n_2, \dots, n_s}$  for some  $s \in [2, n - 1]$  with  $\sum_{i=1}^s n_i = n$ . Moreover, for  $n \geq 3$ , if  $G \neq K_n$  and  $G \neq K_{n_1, n_2, \dots, n_s}$  for some  $s \in [2, n - 1]$  with  $\sum_{i=1}^s n_i = n$ , then  $\lambda_n(D) < -2.383$ .*

### 3 Bounds for distance Estrada index

**Theorem 3.** *Let  $G$  be a connected graph on  $n \geq 2$  vertices with maximum degree  $\Delta_1$  and second maximum degree  $\Delta_2$ . Then*

$$DEE(G) \geq e^{\sqrt{(2n-2-\Delta_1)(2n-2-\Delta_2)}} + (n-1)e^{-\sqrt{(2-\frac{\Delta_1}{n-1})(2-\frac{\Delta_2}{n-1})}} \quad (4)$$

*with equality if and only if  $G = K_n$ .*

**Proof.** Using Lemma 1 and the arithmetic-geometric inequality, we obtain

$$\begin{aligned} DEE(G) &= e^{\lambda_1(D)} + \sum_{i=2}^n e^{\lambda_i(D)} \\ &\geq e^{\lambda_1(D)} + (n-1) \left( e^{\sum_{i=2}^n \lambda_i(D)} \right)^{\frac{1}{n-1}} \\ &= e^{\lambda_1(D)} + (n-1) e^{-\frac{\lambda_1(D)}{n-1}}, \end{aligned}$$

with equality if and only if  $\lambda_2(D) = \lambda_3(D) = \dots = \lambda_n(D)$ .

For  $x \geq 0$ , define  $f(x) = e^x + (n-1)e^{-\frac{x}{n-1}}$ . It is easy to see that  $f'(x) = e^x - e^{-\frac{x}{n-1}} \geq 0$  for any  $x \geq 0$ . By Lemma 3, we have  $\lambda_1(D) \geq \sqrt{(2n-2-\Delta_1)(2n-2-\Delta_2)} \geq 0$ . Therefore,

$$DEE(G) \geq f(\lambda_1(D)) \geq f(\sqrt{(2n-2-\Delta_1)(2n-2-\Delta_2)}),$$

and (4) follows.

To see the sharpness of (4), note that the complete graph  $K_n$  has distance spectrum  $\{n-1, -1, -1, \dots, -1\}$ . Hence, if  $G = K_n$ , we obtain  $DEE(G) = e^{n-1} + (n-1)e^{-1}$ , and the equality holds in (4).

Conversely, if the equality holds in (4) then  $G$  must be a regular graph, say,  $r$ -regular, with diameter at most 2 by Lemma 3. Employing Lemma 2 and the fact that  $\lambda_2(D) = \lambda_3(D) = \dots = \lambda_n(D)$ , we conclude that  $\lambda_1(A) = r$ ,  $\lambda_2(A) = \lambda_3(A) = \dots = \lambda_n(A)$ . Since the trace of  $A$  is zero, we know that  $\lambda_1(A) > \lambda_2(A)$ . It is well known that a connected graph with two distinct adjacency eigenvalues must be complete, which completes the proof.  $\square$

It is evident that our bound is better than the lower bound in (2). Notice that our bound is incomparable to the bound in (3). Nevertheless, there are more graphs which attain our bound.

In 1956, Nordhaus and Gaddum [15] presented lower and upper bounds on the sum of the chromatic number of a graph and its complement, in terms of the order of the graph. Here, we give a Nordhaus-Gaddum type result for the distance Estrada index.

**Theorem 4.** *Let  $G$  be a connected graph on  $n \geq 2$  vertices with a connected complement  $\overline{G}$ . Then*

$$DEE(G) + DEE(\overline{G}) > 2e^{\frac{3(n-1)}{2}} + 2e^{-\frac{3(n-1)}{2}} + 2n - 4. \quad (5)$$

**Proof.** Define a function  $g(n, m) = e^{2(n-1) - \frac{2m}{n}} + e^{-2(n-1) + \frac{2m}{n}} + n$ .

Suppose that  $|E(G)| = m$ . Hence,  $|E(\overline{G})| = \binom{n}{2} - m$ . Since  $\overline{G}$  is connected, it follows from Theorem 2 that

$$\begin{aligned} DEE(G) + DEE(\overline{G}) &> g(n, m) + g\left(n, \binom{n}{2} - m\right) - 4 \\ &= e^{2(n-1) - \frac{2m}{n}} + e^{-2(n-1) + \frac{2m}{n}} + e^{2(n-1) - \frac{n(n-1) - 2m}{n}} \\ &\quad + e^{-2(n-1) + \frac{n(n-1) - 2m}{n}} + 2n - 4. \end{aligned}$$

We have  $e^{x_1} + e^{x_2} \geq 2e^{\frac{x_1+x_2}{2}}$  since  $e^x$  is convex. Therefore, we obtain

$$DEE(G) + DEE(\overline{G}) > 2e^{\frac{3(n-1)}{2}} + 2e^{-\frac{3(n-1)}{2}} + 2n - 4$$

as desired.  $\square$

**Theorem 5.** *Let  $G$  be a connected graph with  $n \geq 2$  vertices, and  $\rho = \rho(G)$  the diameter of  $G$ . Then*

$$DEE(G) < n - 1 + e^{\sqrt{n(n-1)\rho^2 - 1}}. \quad (6)$$

**Proof.** Denote by  $n_+$  the number of positive eigenvalues of  $D$ . We obtain

$$\begin{aligned}
 DEE(G) &= \sum_{i=1}^n e^{\lambda_i(D)} < n - n_+ + \sum_{i=1}^{n_+} e^{\lambda_i(D)} \\
 &= n - n_+ + \sum_{i=1}^{n_+} \sum_{k \geq 0} \frac{\lambda_i^k(D)}{k!} \\
 &= n + \sum_{k \geq 1} \frac{1}{k!} \sum_{i=1}^{n_+} \lambda_i^k(D) \\
 &= n + \sum_{k \geq 1} \frac{1}{k!} \sum_{i=1}^{n_+} (\lambda_i^2(D))^{\frac{k}{2}} \\
 &\leq n + \sum_{k \geq 1} \frac{1}{k!} \left( \sum_{i=1}^{n_+} \lambda_i^2(D) \right)^{\frac{k}{2}}, \quad (7)
 \end{aligned}$$

where the first inequality holds due to the strict monotonicity of  $e^x$ .

In view of Lemma 1 and (7), we deduce

$$DEE(G) < n + \sum_{k \geq 1} \frac{1}{k!} \left( 2 \sum_{i < j} d_{ij}^2 - \sum_{i=n_++1}^n \lambda_i^2(D) \right)^{\frac{k}{2}}.$$

Since  $G$  is a connected graph on  $n \geq 2$  vertices, Lemma 4 implies that  $\lambda_n(D) \leq -1$ . Accordingly,

$$\begin{aligned}
 DEE(G) &< n + \sum_{k \geq 1} \frac{1}{k!} \left( 2 \sum_{i < j} d_{ij}^2 - 1 \right)^{\frac{k}{2}} \\
 &\leq n + \sum_{k \geq 1} \frac{1}{k!} (n(n-1)\rho^2 - 1)^{\frac{k}{2}} \\
 &= n - 1 + e^{\sqrt{n(n-1)\rho^2 - 1}},
 \end{aligned}$$

where the second inequality holds since  $d_{ij} \leq \rho$ , and the last equality is because of the power-series expansion of  $e^x$ . The proof is complete.  $\square$

Obviously, our upper bound is better than that in (2).

To conclude this note, we mention a result relating  $DEE(G)$  to  $EE(\overline{G})$  for regular graphs, which is a direct corollary of Lemma 2.

**Theorem 6.** *Let  $G$  be an  $r$ -regular graph on  $n$  vertices with diameter at most 2. Then*

$$DEE(G) = e^{2n-r-2} - e^{n-r-2} + e^{-1}EE(\overline{G}). \quad (8)$$

**Proof.** It is well known that (see e.g. [10, p.172]) the adjacency eigenvalues of  $\overline{G}$  are  $\{n - r - 1, -1 - \lambda_2(A(G)), -1 - \lambda_3(A(G)), \dots, -1 - \lambda_n(A(G))\}$ .

Hence,  $EE(\overline{G}) = \sum_{i=1}^n e^{\lambda_i(A(\overline{G}))} = e^{n-r-1} + e(e^{-2-\lambda_2(A(G))}) + \dots + e^{-2-\lambda_n(A(G))}$ . Thanks to Lemma 2, we have

$$\begin{aligned} DEE(G) &= \sum_{i=1}^n e^{\lambda_i(D)} = e^{2n-r-2} + e^{-2-\lambda_2(A(G))} + \dots + e^{-2-\lambda_n(A(G))} \\ &= e^{2n-r-2} + e^{-1}(EE(\overline{G}) - e^{n-r-1}), \end{aligned}$$

which readily implies the desired result.  $\square$

It would be interesting to explore whether the techniques in this note can be applied to evolving graphs [20], where a dynamic notion of distance becomes relevant.

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