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LOWER BOUNDS FOR THE ESTRADA INDEX OF GRAPHS*

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Abstract. Let G be a graph with n vertices and $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues. The Estrada index of G is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$. In this paper, new lower bounds for the Estrada index are established.

Key words. Estrada index, Lower bound, Graph spectrum, Zagreb index.

AMS subject classifications. 15A18, 05C50.

1. Introduction. Throughout this paper, let G be an undirected simple graph with n vertices and m edges. We say that G is an (n, m)-graph. Let the spectrum of G be $\lambda_1, \lambda_2, \ldots, \lambda_n$ arranged in a non-increasing order. The properties of graph spectrum can be found in [1]. The Estrada index [3] is a spectrum-based graph invariant promoted by Estrada [4, 5, 6, 7, 8, 9] and defined by

$$EE = EE(G) = \sum_{i=1}^{n} e^{\lambda_i}. \tag{1.1}$$

The Estrada index was used to study the folding degree of proteins and other long-chain molecules [4, 5, 6, 9]. It also has numerous applications in the vast field of complex networks [7, 8, 13, 14, 17]. A number of properties especially lower and upper bounds [3, 10, 11, 12, 15, 16, 18, 19, 20] for the Estrada index are known. In this paper, we establish further lower bounds improving some results in [3, 12].

2. Preliminaries. We begin by some notation that will be used in the following proofs of results.

For $1 \leq i \leq n$, let d_i be the degree of vertex v_i in G. The first Zagreb index [2] of the graph G is defined as $Zg(G) = \sum_{i=1}^{n} d_i^2$. For $k = 0, 1, 2, \ldots$, let $M_k = M_k(G)$ be the kth spectral moment of a graph G,

$$M_k = \sum_{i=1}^{n} \lambda_i^k.$$

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From (1.1) we have

$$EE(G) = \sum_{k\geq 0} \frac{M_k(G)}{k!}. \tag{2.1}$$

Recall that M_k is the number of close walks of length k in the graph [1]. The first few spectral moments of an (n,m)-graph G are well known: $M_0 = n$, $M_1 = 0$, $M_2 = 2m$ and $M_3 = 6t$, where $t = t(G)$ is the number of triangles in G. Denote by K_n the complete graph on n vertices.

Lemma 2.1 ([19]). *Let G be a graph with m edges. For $k \geq 4$,*

$$M_{k+2} \geq M_k,$$

with equality for all even $k \geq 4$ if and only if G consists of m copies of K_2 and possibly isolated vertices, and with equality for all odd $k \geq 5$ if and only if G is a bipartite graph.

The following is an immediate result of Lemma 2.1.

Corollary 2.2. *Let G be an (n,m)-graph. For $k \geq 4$, we have*

$$\sum_{i=1}^{n} (2\lambda_i)^{k+2} \geq 4 \sum_{i=1}^{n} (2\lambda_i)^k,$$

with equality for all even $k \geq 4$ if and only if G consists of m copies of K_2 and possibly isolated vertices, and with equality for all odd $k \geq 5$ if and only if G is a bipartite graph.

3. Results. In this section, we present our lower bounds for the Estrada index and compare them to some existing bounds.

Theorem 3.1. *Let G be an (n,m)-graph. Then we have*

$$EE(G) \geq \sqrt{n^2 + 4m + 8t + \left(\frac{e^2+e^{-2}}{2} - 3\right) M_4 + \left(\frac{e^2-e^{-2}}{2} - \frac{10}{3}\right) M_5}\,, \tag{3.1}$$

with equality if and only if $n = 2$ or $m = 0$.

As a simple example, for $G = K_2$, it follows from the above result that $EE(K_2) = e + e^{-1}$ since $n = M_4 = 2$, $m = 1$ and $t = M_5 = 0$. This is confirmed by directly applying definition (1.1).

Proof. From the definition of (1.1), we have

$$EE^2 = \sum_{i=1}^{n} e^{2\lambda_i} + 2\sum_{i<j} e^{\lambda_i} e^{\lambda_j}. \tag{3.2}$$

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By the arithmetic and geometric mean inequality and the fact that $M_1 = 0$,

$$\begin{aligned} 2\sum_{i<j} e^{\lambda_i} e^{\lambda_j} &\geq n(n-1)\left(\prod_{i<j} e^{\lambda_i} e^{\lambda_j}\right)^{\frac{2}{n(n-1)}} \\ &= n(n-1)\left[\left(\prod_{i=1}^{n} e^{\lambda_i}\right)^{n-1}\right]^{\frac{2}{n(n-1)}} \\ &= n(n-1)\left(e^{M_1}\right)^{\frac{2}{n}} = n(n-1), \end{aligned} \tag{3.3}$$

where the equality holds if and only if $\lambda_i + \lambda_j$ are equal for all $i < j$. This condition is tantamount to the fact that $\lambda_1 = \cdots = \lambda_n$ or $n = 2$. Therefore, the equality in (3.3) holds if and only if $m = 0$ or $n = 2$.

In view of the properties of M_0, M_1, M_2 and M_3, we obtain

$$\begin{aligned} \sum_{i=1}^{n} e^{2\lambda_i} &= \sum_{i=1}^{n}\sum_{k\geq 0} \frac{(2\lambda_i)^k}{k!} \\ &= n + 4m + 8t + \sum_{i=1}^{n}\sum_{k\geq 4} \frac{(2\lambda_i)^k}{k!} \\ &= n + 4m + 8t + \sum_{k\geq 2} \frac{\sum_{i=1}^{n}(2\lambda_i)^{2k}}{(2k)!} + \sum_{k\geq 2} \frac{\sum_{i=1}^{n}(2\lambda_i)^{2k+1}}{(2k+1)!}. \end{aligned} \tag{3.4}$$

Invoking Corollary 2.2, we get

$$\begin{aligned} \sum_{i=1}^{n} e^{2\lambda_i} &\geq n + 4m + 8t + \sum_{k\geq 2} \frac{4^{k-2}\sum_{i=1}^{n}(2\lambda_i)^4}{(2k)!} + \sum_{k\geq 2} \frac{4^{k-2}\sum_{i=1}^{n}(2\lambda_i)^5}{(2k+1)!} \\ &= n + 4m + 8t + \left(\frac{e^2+e^{-2}}{2} - 3\right) M_4 + \left(\frac{e^2-e^{-2}}{2} - \frac{10}{3}\right) M_5, \end{aligned} \tag{3.5}$$

with equality holding if and only if G consists of m copies of K_2 and possibly isolated vertices.

Combining with (3.3) and (3.5), we obtain the desired lower bound (3.1), with equality if and only if $n = 2$ or $m = 0$. ∎

Corollary 3.2. *Let G be an (n, m)-graph. Then we have*

$$EE(G) \geq \sqrt{n^2 + 4m + (e^2 + e^{-2} - 6)(Zg(G) - m) + [15(e^2 - e^{-2}) - 92]\, t}, \tag{3.6}$$

with equality if and only if $n = 2$ or $m = 0$.

Proof. Recall that we have [1]

$$M_4 = 2Zg(G) - 2m + 8q,$$

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where q is the number of quadrangles in G, and

$$M_5 = 30t + 10p + 10r,$$

where p is the number of pentagons, and r is the number of subgraphs consisting of a triangle with a pendent vertex attached. When $n = 2$ or $m = 0$, we have $p = q = r = 0$. The result then follows directly from Theorem 3.1. □

When $n = 2$ or $m = 0$, we clearly have $t = 0$. Thus, we have the following corollary.

Corollary 3.3. *Let G be an (n, m)-graph. Then we have*

$$EE(G) \geq \sqrt{n^2 + 4m + (e^2 + e^{-2} - 6)(Zg(G) - m)}, \tag{3.7}$$

with equality if and only if $n = 2$ or $m = 0$.

For an (n, m)-graph G, it is proved in [3] that

$$EE(G) \geq \sqrt{n^2 + 4m + 8t}. \tag{3.8}$$

Our bound in (3.1) is obviously better than the bound in (3.8). Recently, the lower bound is improved to [12]

$$EE(G) \geq \sqrt{n^2 + 5\frac{1}{3}m + 8t}. \tag{3.9}$$

By noting that $M_4 \geq 2m$ and $M_5 \geq 0$, we have

$$\left(\frac{e^2 + e^{-2}}{2} - 3\right) M_4 > \frac{4}{3}m,$$

and hence, our bound in (3.1) is better than the one in (3.9).

In [18] it is shown that if $n \geq 2$,

$$EE(G) \geq e^{\lambda_1} + (n-1)e^{-\frac{\lambda_1}{n-1}}. \tag{3.10}$$

Clearly, the bounds in (3.1) and (3.10) are incomparable in general.

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