

New Lower Bounds for Estrada Index

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Abstract

Let G be an n -vertex graph. If $\lambda_1, \lambda_2, \dots, \lambda_n$ are the adjacency eigenvalues of G , then the Estrada index and the energy of G are defined as $EE(G) = \sum_{i=1}^n e^{\lambda_i}$ and $E(G) = \sum_{i=1}^n |\lambda_i|$, respectively. Some new lower bounds for $EE(G)$ are obtained in terms of $E(G)$. We also prove that if G has m edges and t triangles, then $EE(G) \geq \sqrt{n^2 + 2mn + 2nt}$. The new lower bounds improve previous lower bounds on EE .

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1 Introduction

Throughout this paper we consider simple graphs, that is finite and undirected graphs without loops and multiple edges. If G is a graph with vertex set $\{1, \dots, n\}$, the *adjacency matrix* of G is an $n \times n$ matrix $A = [a_{ij}]$, where $a_{ij} = 1$ if there is an edge between the vertices i and j , and $a_{ij} = 0$ otherwise. Since A is a real symmetric matrix, its eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ are real numbers. These are referred to as the eigenvalues of G . In what follows we assume that $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$. The multiset of eigenvalues of A is called the *spectrum* of G . For details of the theory of graph spectra see [2, 3]. We denote the complete graph on n vertices by K_n , the complete bipartite graph whose parts are of orders a, b by $K_{a,b}$.

The *energy* of G is defined as [13]

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

For details on graph energy see the [surveys](#) [14, 16, 19], the recent papers [17, 20] and the references cited therein.

The *Estrada index* of G , is defined recently by Ernesto Estrada [6, 7, 8] as

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

The Estrada index has found a variety of applications. Initially it was used to quantify the degree of folding of long-chain molecules, especially proteins [6, 7, 8]; for this purpose the EE-values of pertinently constructed weighted graphs were employed. Another, fully unrelated, application of EE (of simple graphs) was proposed by Estrada and Rodríguez-Velázquez [10, 11]. They showed that EE provides a measure of the centrality of complex (communication, social, metabolic, etc.) networks. In addition to this, in [12] a connection between EE and the concept of extended atomic branching was considered. An application of the Estrada index in statistical thermodynamic has also been reported [9].

Properties of the Estrada index were studied in a number of recent works [4, 15, 18]; for a review see [5].

In this paper we find a lower bound for the Estrada index of a graph in terms of the number of vertices, edges and triangles and another two lower bounds in terms of energy. These bounds improve previous bound given in [1, 4].

2 A lower bound in terms of number of vertices, edges and triangles

In this section we give a lower bound for Estrada index of a graph in terms of the number of vertices, edges and triangles which is a significant improvement of the following bound.

Theorem 1. ([4]) *Let G be graph with n vertices, m edges and t triangles. Then*

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

Equality holds if and only if G is the empty graph \overline{K}_n .

Recall that ([2]) for a graph with eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$, with m edges and t triangles,

$$\sum_{i=1}^n \lambda_i = 0, \tag{1}$$

$$\sum_{i=1}^n \lambda_i^2 = 2m, \tag{2}$$

$$\sum_{i=1}^n \lambda_i^3 = 6t. \tag{3}$$

Lemma 1. *For any real x , one has $e^x \geq 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!}$. Equality holds if and only if $x = 0$.*

Proof. By the Taylor's theorem, for any $x \neq 0$, there is a real $\eta \neq 0$ between x and 0 such that $e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + e^{\eta} \frac{x^4}{4!}$. This proves the lemma. \square

Theorem 2. Let G be graph with n vertices, m edges and t triangles. Then

$$EE(G) \geq \sqrt{n^2 + 2mn + 2nt}.$$

Equality holds if and only if G is the empty graph \overline{K}_n .

Proof. Suppose that $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of G . Using Lemma 1 we have

$$\begin{aligned} EE(G)^2 &= \sum_{i=1}^n \sum_{j=1}^n e^{\lambda_i + \lambda_j} \\ &\geq \sum_{i=1}^n \sum_{j=1}^n \left(1 + \lambda_i + \lambda_j + \frac{(\lambda_i + \lambda_j)^2}{2} + \frac{(\lambda_i + \lambda_j)^3}{6} \right) \\ &= \sum_{i=1}^n \sum_{j=1}^n (1 + \lambda_i + \lambda_j + \lambda_i^2/2 + \lambda_j^2/2 + \lambda_i \lambda_j + \lambda_i^3/6 + \lambda_j^3/6 + \lambda_i^2 \lambda_j/2 + \lambda_i \lambda_j^2/2). \end{aligned}$$

Now, by (1),

$$\begin{aligned} \sum_{i=1}^n \sum_{j=1}^n (\lambda_i + \lambda_j) &= n \sum_{i=1}^n \lambda_i + n \sum_{j=1}^n \lambda_j = 0, \\ \sum_{i=1}^n \sum_{j=1}^n \lambda_i \lambda_j &= \left(\sum_{i=1}^n \lambda_i \right)^2 = 0, \\ \sum_{i=1}^n \sum_{j=1}^n (\lambda_i^2 \lambda_j/2 + \lambda_i \lambda_j^2/2) &= \frac{1}{2} \sum_{i=1}^n \lambda_i^2 \cdot \sum_{j=1}^n \lambda_j + \frac{1}{2} \sum_{i=1}^n \lambda_i \cdot \sum_{j=1}^n \lambda_j^2 = 0. \end{aligned}$$

By (2),

$$\sum_{i=1}^n \sum_{j=1}^n (\lambda_i^2/2 + \lambda_j^2/2) = \frac{n}{2} \sum_{i=1}^n \lambda_i^2 + \frac{n}{2} \sum_{j=1}^n \lambda_j^2 = 2mn.$$

Similarly by (3),

$$\sum_{i=1}^n \sum_{j=1}^n (\lambda_i^3/6 + \lambda_j^3/6) = 2nt.$$

Combining the above relations, we get

$$EE(G)^2 \geq n^2 + 2mn + 2nt.$$

So the inequality of the theorem is proved. By Lemma 1 equality holds if and only if for all i, j , $\lambda_i + \lambda_j = 0$ and this happens if and only if all λ_i are zero that is G is \overline{K}_n . \square

3 Lower bounds in terms of energy

Recently, in [1] the following were proved.

Theorem 3. ([1]) Let p , η , and q be, respectively, the number of positive, zero, and negative adjacency eigenvalues of G . Then

$$EE(G) \geq \eta + pe^{E(G)/(2p)} + qe^{-E(G)/(2q)}.$$

Equality holds if and only if G is either

- (i) a union of complete bipartite graphs $K_{a_1, b_1} \cup \dots \cup K_{a_p, b_p}$ with (possibly) some isolated vertices, such that $a_1 b_1 = a_2 b_2 = \dots = a_p b_p$, or
- (ii) a union of copies of **the complete k -partite graph $K_{t, \dots, t}$** , for some fixed positive integers k, t , with (possibly) some isolated vertices.

Theorem 4. ([1]) If G is a bipartite graph, then $EE(G) \geq \eta + r \cosh\left(\frac{E(G)}{r}\right)$, where r is rank of the adjacency matrix of G . Equality holds if and only if G is a union of complete bipartite graphs $K_{a_1, b_1} \cup \dots \cup K_{a_p, b_p}$ with (possibly) some isolated vertices, such that $a_1 b_1 = a_2 b_2 = \dots = a_p b_p$.

We improve these lower bounds as follows.

Theorem 5. Let G be a graph with largest eigenvalue λ_1 and let p, η, q be, respectively, the number of positive, zero, and negative eigenvalues of G . Then

$$EE(G) \geq e^{\lambda_1} + \eta + (p-1)e^{\frac{E(G)-2\lambda_1}{2(p-1)}} + qe^{-\frac{E(G)}{2q}}. \quad (4)$$

Equality holds if and only if G is a graph such that all negative eigenvalues and all positive eigenvalues but the largest are equal, i.e. the spectrum of G is of the form $\{[\lambda_1], [\theta_1]^{p-1}, [0]^\eta, [\theta_2]^q\}$, with $\lambda_1 \geq \theta_1 > 0 > \theta_2$, where the exponents show the multiplicities.

Proof. Let $\lambda_1 \geq \dots \geq \lambda_p$ be the positive, and $\lambda_{n-q+1}, \dots, \lambda_n$ be the negative eigenvalues of G . As the sum of eigenvalues of a graph is zero, one has

$$E(G) = 2 \sum_{i=1}^p \lambda_i = -2 \sum_{i=n-q+1}^n \lambda_i.$$

By the arithmetic-geometric mean inequality, we have

$$\sum_{i=2}^p e^{\lambda_i} \geq (p-1)e^{(\lambda_2 + \dots + \lambda_p)/(p-1)} = (p-1)e^{\frac{E(G)/2 - \lambda_1}{p-1}}. \quad (5)$$

Similarly,

$$\sum_{i=n-q+1}^n e^{\lambda_i} \geq qe^{-E(G)/(2q)}. \quad (6)$$

For the zero eigenvalues, we also have

$$\sum_{i=p+1}^{n-q} e^{\lambda_i} = \eta.$$

So we obtain

$$EE(G) \geq e^{\lambda_1} + \eta + (p-1)e^{\frac{E(G)/2 - \lambda_1}{p-1}} + qe^{-\frac{E(G)}{2q}}.$$

The equality holds in (4) if and only if equalities hold in both (5) and (6). **By the equality case in the arithmetic-geometric mean inequality, equality occurs in (5) iff $e^{\lambda_2} = \dots = e^{\lambda_p}$ and similarly equality occurs in (6) iff $e^{\lambda_{n-q+1}} = \dots = e^{\lambda_n}$.** Hence, the equality holds in (4) if and only if $\lambda_2 = \dots = \lambda_p$ and $\lambda_{n-q+1} = \dots = \lambda_n$. This means all negative eigenvalues and all positive eigenvalues but the largest are equal which completes the proof. \square

Theorem 5 can be improved for bipartite graphs to the following.

Theorem 6. *If G is a bipartite graph, then*

$$EE(G) \geq \eta + 2 \cosh(\lambda_1) + (r - 2) \cosh\left(\frac{E(G) - 2\lambda_1}{r - 2}\right), \quad (7)$$

where r is rank of the adjacency matrix of G and λ_1 is the largest eigenvalue of G . Equality holds if and only if the spectrum of G is of the form $\{[\pm\lambda_1], [\pm\lambda_2]^{p-1}, [0]^\eta\}$, with $\lambda_1 \geq \lambda_2 > 0$.

Proof. Since G is bipartite, its eigenvalues are symmetric with respect to zero, i.e. $\lambda_i = -\lambda_{n-i+1}$ for $i = 1, \dots, \lfloor n/2 \rfloor$. With a similar argument as the proof of Theorem 5, we find that

$$\begin{aligned} EE(G) &= \eta + e^{\lambda_1} + e^{-\lambda_1} + \sum_{i=2}^p e^{\lambda_i} + \sum_{i=2}^p e^{-\lambda_i} \\ &\geq \eta + e^{\lambda_1} + e^{-\lambda_1} + (p-1)e^{\frac{E(G)/2-\lambda_1}{p-1}} + (p-1)e^{-\frac{E(G)/2-\lambda_1}{p-1}}. \end{aligned}$$

Since the rank of adjacency matrix of G is equal to $2p$, (7) follows.

By the equality case in the arithmetic-geometric mean inequality, equality holds in (7) if and only if $e^{\lambda_2} = \dots = e^{\lambda_p}$ and $e^{-\lambda_2} = \dots = e^{-\lambda_p}$. The proof is now complete. \square

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