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New Lower Bounds for Estrada Index

Hamidreza Bamdad[1]

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

Keywords Estrada index · Energy · Eigenvalues of graphs

Mathematics Subject Classification 05C50

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 $\{1, \ldots, n\}$, 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 0 otherwise. Since A is a real symmetric matrix, its eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ are real numbers. These are referred to as the eigenvalues of G. In what follows we assume that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. 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 $K_{a,b}$.

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✉ Hamidreza Bamdad
hr_bamdad@pnu.ac.ir

1 Department of Mathematics, Payame Noor University,
P.O. Box 19395-3697, Tehran, Iran

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

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

For details on graph energy see the reviews [14,16,18], the recent papers [17,19] and the references cited therein.

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

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

Although invented in year 2000 [6], the Estrada index has already found a remarkable variety of applications. Initially it was used to quantify the degree of folding of long-chain molecules, especially proteins [6–8]; 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].

Mathematical properties of the Estrada index were studied in a number of recent works [4,15]; 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 two lower bounds 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*

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

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

Recall that ([2]) for a graph with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, 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 theorem, for any $x \neq 0$, there is a real $\eta \neq 0$ between x and 0 such that $e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{\eta^4}{4!}$. This proves the lemma. □

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

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

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

Proof Suppose that $\lambda_1, \lambda_2, \ldots, \lambda_n$ is the spectrum of G. Using Lemma 1 we have

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

Now, by (1),

$$\sum_{i=1}^{n}\sum_{j=1}^{n} (\lambda_i + \lambda_j) = n\sum_{i=1}^{n} \lambda_i + n\sum_{j=1}^{n} \lambda_j = 0,$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n} \lambda_i\lambda_j = (\sum_{i=1}^{n} \lambda_i)^2 = 0,$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n} (\lambda_i^2\lambda_j/2 + \lambda_i\lambda_j^2/2) = \frac{1}{2}\sum_{i=1}^{n} \lambda_i^2 \cdot \sum_{j=1}^{n} \lambda_j + \frac{1}{2}\sum_{i=1}^{n} \lambda_i \cdot \sum_{j=1}^{n} \lambda_j^2 = 0.$$

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

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

So the inequality of the theorem is proved. By Lemma 1 equality holds if and only if all λ_i are zero that is G is $\overline{K}_n$. □

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*

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

Equality holds if and only if G is either

(i) *a union of complete bipartite graphs $K_{a_1,b_1} \cup \cdots \cup K_{a_p,b_p}$ with (possibly) some isolated vertices, such that $a_1b_1 = a_2b_2 = \cdots = a_pb_p$, or*
(ii) *a union of copies of $K_{k\times t}$, for some fixed positive integers k, t, with (possibly) some isolated vertices.*

Theorem 4 ([1]) *If G is a bipartite graph, then $\mathrm{EE}(G) \geq \eta + r\cosh\left(\frac{\mathrm{E}(G)}{r}\right)$, where r is the rank of the adjacency matrix of G. Equality holds if and only if G is a union of complete bipartite graphs $K_{a_1,b_1} \cup \cdots \cup K_{a_p,b_p}$ with (possibly) some isolated vertices, such that $a_1b_1 = a_2b_2 = \cdots = a_pb_p$.*

We improve these lower bounds as follows.

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

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

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

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

By the arithmetic–geometric mean inequality, we have

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

Similarly,

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

For the zero eigenvalues, we also have

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

So we obtain

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

The equality holds in (4) if and only if equality holds in both (5) and (6) and these happen if and only if $\lambda_2 = \cdots = \lambda_p$ and $\lambda_{n-q+1} = \cdots = \lambda_n$. This completes the proof. □

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

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

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

where r is the 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 $i = 1, \ldots, \lfloor n/2 \rfloor$. With a similar argument as the proof of Theorem 5, we find that

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

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

Equality holds in (7) if and only if $\lambda_2 = \cdots = \lambda_p$. The proof is now complete. □

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