Some Lower Bounds for Estrada Index

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ABSTRACT

For a graph G with n vertices, its Estrada index is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$ where $\lambda_1, \lambda_2, ..., \lambda_n$ are the eigenvalues of G. A lot of properties especially lower and upper bounds for the Estrada index are known. We now establish further lower bounds for the Estrada index.

Keywords: Estrada index, eigenvalues (of graph), spectral moments, lower bounds.

1 **INTRODUCTION**

Let G be a simple graph with n vertices. Let $\lambda_1, \lambda_2, \dots, \lambda_n$ be the eigenvalues of G arranged in a non-increasing order [1]. The Estrada index of the graph G is defined as

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

This graph invariant was proposed as a structure-descriptor, used in the modeling of certain features of the 3D structure of organic molecules [2], in particular of the degree of proteins and other long-chains biopolymers [3,4]. It has also found applications in a large variety of other problems, see, e.g., [5-7]. Lower and upper bounds have been established for the Estrada index, see [8–14]. Some other properties for the Estrada index may be found in [15–19]. Here we present some easily computed lower bounds for the Estrada index.

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2 PRELIMINARIES

Let G be a graph with n vertices. For k = 0, 1, 2, ..., denote by $M_k = M_k(G)$ the k-th spectral moment of the graph G, i.e., $M_k = \sum_{i=1}^n \lambda_i^k$. Note that $M_1 = 0$. Then

$$EE(G) = \sum_{i=1}^{n} \sum_{k\geq 0} \frac{\lambda_i^k}{k!} = \sum_{k\geq 0} \frac{M_k}{k!} = n + \sum_{k\geq 2} \frac{M_k}{k!}.$$

The first Zagreb index [20] of the graph G is defined as $Zg(G) = \sum_{u \in V(G)} d_u^2$, where d_u is the degree of vertex u and V(G) is the vertex set of G. Let t(G) be the number of triangles in G. Recall that M_k is equal to the number of closed walks of length k in the graph [1].

Lemma 1. Let G be a graph with m edges. Then for $k \ge 4$, $M_{k+2} \ge M_k$ with equality for all even $k \ge 4$ if and only if G consists of m copies of complete graph on two vertices and possibly isolated vertices, and with equality for all odd $k \ge 5$ if and only if G is a bipartite graph.

Proof (i) For even $k \ge 4$, by repeating the first edge twice for a closed walk of length k, we get a closed walk of length k+2, and then $M_{k+2} \ge M_k$ with equality for all even $k \ge 4$ if and only if G consists of m copies of complete graph on two vertices and possibly isolated vertices.

(ii) For odd $k \ge 5$, by similar considering as above, it is easily seen that $M_{k+2} \ge M_k$ with equality for all odd $k \ge 5$ if and only if G is bipartite.

3 RESULTS

We now establish several lower bounds for the Estrada index and compare them with the known bounds in the literature.

Proposition 2. Let G be a graph with n vertices and m edges. Then

$$EE(G) \ge n + m + t(G) + \frac{1}{2}(e + e^{-1} - 3)M_4 + \frac{1}{2}\left(e - e^{-1} - \frac{7}{3}\right)M_5$$
(1)

$$EE(G) \ge n + m + t(G) + (e + e^{-1} - 3)[Zg(G) - m] + 15\left(e - e^{-1} - \frac{7}{3}\right)t(G)$$
(2)

with either equality if and only if G consists of m copies of complete graph on two vertices and possibly isolated vertices.

Proof. Note that $M_2 = 2m$, $M_3 = 6t(G)$. By Lemma 1,

$$\begin{split} EE(G) &= n + m + t(G) + \sum_{k \ge 2} \frac{M_{2k}}{(2k)!} + \sum_{k \ge 2} \frac{M_{2k+1}}{(2k+1)!} \\ &\ge n + m + t(G) + \sum_{k \ge 2} \frac{M_4}{(2k)!} + \sum_{k \ge 2} \frac{M_5}{(2k+1)!} \\ &= n + m + t(G) + M_4 \left(\frac{e + e^{-1}}{2} - 1 - \frac{1}{2!}\right) + M_5 \left(\frac{e - e^{-1}}{2} - 1 - \frac{1}{3!}\right) \\ &= n + m + t(G) + \frac{1}{2}(e + e^{-1} - 3)M_4 + \frac{1}{2}\left(e - e^{-1} - \frac{7}{3}\right)M_5 \end{split}$$

with equality if and only if $M_k = M_4$ for all even $k \ge 4$ and $M_k = M_5$ for all odd $k \ge 5$, which by Lemma 1, is equivalent to the fact that G consists of m copies of complete graph on two vertices and possibly isolated vertices.

For a fixed vertex u, there are at least d_u^2 closed walks of length four starting from u and $d_u(d_u-1)$ closed walks of length four starting from a neighbor of u such that vertices in such walks are only u and its neighbors, and then $M_4 \ge 2Zg(G) - 2m$. (Actually, $M_4 = 2Zg(G) - 2m + 8q$ where q is the number of quadrangles in G, see [21]). Note also that $M_5 \ge 30t(G)$ because there are ten closed walks of length five starting from a fixed vertex on a fixed triangle such that the vertices of the walks are only the vertices of the triangle. (Actually, $M_5 = 30t(G) + 10p + 10r$ where p is the number of pentagons, and r is the number of subgraphs consisting of a triangle with a pendent vertex attached [21]. Now the second inequality follows.

Corollary 3. Let G be a graph with n vertices and m edges. Then

$$EE(G) \ge n + m + (e + e^{-1} - 3)[Zg(G) - m]$$
 (3)

with equality if and only if G consists of m copies of complete graphs on two vertices and possibly isolated vertices.

Recently, Das and Lee [14] showed that for a connected graph with *n* vertices and $m \ge 1.8n + 4$ edges, $EE(G) > EE(P_n)$. This may be improved slightly using Corollary 3. Recall that [14] $EE(P_n) < 2.746n + 3.569$. If $m \ge 1.4n + 2$, then by Corollary 3 and the Cauchy-Schwarz inequality, we have

$$EE(G) \ge n + m + (e + e^{-1} - 3)\left(\frac{4m^2}{n} - m\right) > 2.746n + 3.569 > EE(P_n).$$

Remark 4. For a graph G with $n \ge 2$ vertices, it was shown in [12] that

$$EE(G) \ge e^{\lambda_1} + (n-1)e^{-\frac{\lambda_1}{n-1}}$$
 (4)

with equality if and only if G is the empty graph or the complete graph. Obviously, (3) and (4) are incomparable.

Remark 5. Let G be a graph with n vertices, m edges and nullity (number of zero eigenvalues) $n_0 < n$. Note that $n_0 = n$ if and only if G is an empty graph. Gutman [11] showed that

$$EE(G) \ge n_0 + \frac{n - n_0}{2} (e^a + e^{-a})$$
 (5)

with equality if and only if $n - n_0$ is even, *G* consists of copies of complete bipartite graphs K_{r_j,t_j} , $j = 1, 2, ..., (n - n_0)/2$, such that all $r_j t_j$ are equal, and the remaining vertices if exist are isolated vertices, where $a = \sqrt{2m/(n - n_0)}$. A different proof may be found in [12]. For odd cycle C_n with $n \ge 3$, $n_0 = 0$ (see [21]) and m = n, we have

$$n + m + (e + e^{-1} - 3)[Zg(G) - m] - \left[n_0 + \frac{n - n_0}{2}(e^a + e^{-a})\right]$$
$$= n\left[2 + 3(e + e^{-1} - 3) - \frac{e^{\sqrt{2}} + e^{-\sqrt{2}}}{2}\right] > 0.$$

Then for odd cycle C_n with $n \ge 3$, the bound in (3) is better than the one in (5), and thus it is easily seen that (3) and (5) are incomparable in general.

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