Some Lower Bounds for Estrada Index

BO ZOU\textsuperscript{1} AND ZHIBIN DU

Department of Mathematics, South China Normal University, Guangzhou 510631, China

(Received July 20, 2010)

ABSTRACT

For a graph $G$ with $n$ vertices, its Estrada index is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$ where $\lambda_1, \lambda_2, \ldots, \lambda_n$ 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.

\textbf{Keywords:} Estrada index, eigenvalues (of graph), spectral moments, lower bounds.

1 INTRODUCTION

Let $G$ be a simple graph with $n$ vertices. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ 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.

\textsuperscript{1} Corresponding author (Email: zhoubo@scnu.edu.cn).
2 Preliminaries

Let $G$ be a graph with $n$ vertices. For $k = 0, 1, 2, \ldots$, 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 $k \geq 4$, $M_{k+2} \geq M_k$ with equality for all even $k \geq 4$ if and only if $G$ consists of $m$ copies of complete graph on two vertices and possibly isolated vertices, and with equality for all odd $k \geq 5$ if and only if $G$ is a bipartite graph.

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

(ii) For odd $k \geq 5$, by similar considering as above, it is easily seen that $M_{k+2} \geq M_k$ with equality for all odd $k \geq 5$ 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

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

(1)
Some Lower Bounds for Estrada Index

\[ EE(G) \geq n + m + t(G) + (e + e^{-1} - 3)[Zg(G) - m] + 15 \left( e - e^{-1} - \frac{7}{3} \right) t(G) \]  \hspace{1cm} (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,

\[ EE(G) = n + m + t(G) + \sum_{k \geq 2} \frac{M_{2k}}{(2k)!} + \sum_{k \geq 2} \frac{M_{2k+1}}{(2k+1)!} \]

\[ \geq n + m + t(G) + \sum_{k \geq 2} \frac{M_4}{(2k)!} + \sum_{k \geq 2} \frac{M_5}{(2k+1)!} \]

\[ = n + m + t(G) + \frac{1}{2} \left( e + e^{-1} - 1 - \frac{1}{2!} \right) M_4 + \frac{1}{2} \left( e - e^{-1} - \frac{7}{3} \right) M_5 \]

with equality if and only if \( M_k = M_4 \) for all even \( k \geq 4 \) and \( M_k = M_5 \) for all odd \( k \geq 5 \), 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 \( M_4 \geq 2Zg(G) - 2m \). (Actually, \( M_4 = 2Zg(G) - 2m + 8q \) where \( q \) is the number of quadrangles in \( G \), see [21]).

Note also that \( M_5 \geq 30t(G) \) 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. \( \blacksquare \)

**Corollary 3.** Let \( G \) be a graph with \( n \) vertices and \( m \) edges. Then

\[ EE(G) \geq n + m + (e + e^{-1} - 3)[Zg(G) - m] \]  \hspace{1cm} (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 $m \geq 1.8n + 4$ 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 $m \geq 1.4n + 2$, then by Corollary 3 and the Cauchy-Schwarz inequality, we have

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

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

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

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

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

with equality if and only if $n-n_0$ is even, $G$ consists of copies of complete bipartite graphs $K_{r_j,t_j}, j = 1,2,\ldots,(n-n_0)/2$, such that all $r_jt_j$ 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 $n \geq 3$, $n_0 = 0$ (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 $n \geq 3$, 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.
ACKNOWLEDGEMENTS: This work was supported by the Guangdong Provincial Natural Science Foundation of China (Grant No. 8151063101000026).

REFERENCES


