Iranian Journal of Mathematical Chemistry, Vol. 1, No. 2, September 2010, pp. 67−72 **IJMC**

Some Lower Bounds for Estrada Index

BO ZHOU[1] AND ZHIBIN DU[2]

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 $\lambda_1, \lambda_2, ..., \lambda_n$ 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 $\lambda_1, \lambda_2, \ldots, \lambda_n$ 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.

[1]- zhoubo@scnu.edu.cn
[2] - zhibindu@126.com

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

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

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

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,

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

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. ■

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

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

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

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

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

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

with equality if and only if $n-n_0$ is even, G consists of copies of complete bipartite graphs K_{r_j,t_j}, $j=1,2,\ldots,(n-n_0)/2$, 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 $n \geq 3$, $n_0 = 0$ (see [21]) and $m = n$, we have

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

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).

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