MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **60** (2008) 485-492

ISSN 0340 - 6253

ON ESTRADA INDEX

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(Received January 3, 2008)

Abstract

Let G be a graph with n vertices and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues. The Estrada index of G is $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$. We present some lower and upper bounds for $EE(G)$ in terms of graph invariants such as the number of vertices, the number of edges, the spectral moments, the first Zagreb index, the nullity and the largest eigenvalue.

1. INTRODUCTION

Let G be a simple graph with n vertices and m edges. In what follows we say that G is an (n, m)-graph. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of G arranged in non-increasing order [1].

The Estrada index of the graph G is defined as

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

It has found successful applications in a large variety of problems, including those in biochemistry and in complex networks, see [2–7]. Various bounds for the Estrada index can be found in [8–11]. See [12–14] for more recent results.

A similar invariant is energy. The energy of G is defined as [15]

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

Denoting by $M_k = M_k(G)$ the k-th spectral moment of the graph G, i.e.,

$$M_k = \sum_{i=1}^{n} \lambda_i^k \,,$$

we have

$$EE(G) = \sum_{k \geq 0} \frac{M_k}{k!} \,.$$

Recall that for an (n,m)-graph G,

$$M_0 = n\,, \;\; M_1 = 0\,, \;\; M_2 = 2m\,, \;\; M_3 = 6t$$

where t is the number of triangles.

The first Zagreb index of the graph G is defined as [16]

$$Zg = Zg(G) = \sum_{u \in V(G)} d_u^2$$

where d_u denotes the degree (number of first neighbors) of vertex u in G and $V(G)$ is the vertex set of G.

Let K_n be the complete graph with n vertices and $\overline{K_n}$ its (edgeless) complement. Let $K_{a,b}$ be the complete bipartite graph with two partite sets having a and b vertices, respectively.

Now we establish some lower and upper bounds for the Estrada index in terms of graph invariants such as the number of vertices, the number of edges, the spectral moments, the first Zagreb index, the nullity and the largest eigenvalue.

2. LOWER BOUNDS

Theorem 1. *Let G be a graph with n vertices. Then for any integer $k_0 \geq 2$,*

$$EE(G) \geq \sqrt{n^2 + \sum_{k=2}^{k_0} \frac{2^k M_k(G)}{k!}} \tag{1}$$

with equality if and only if $G \cong \overline{K_n}$.

Proof. Note that $M_k(G)$ is equal to the trace of A^k, where A is the $(0,1)$-adjacency matrix of G. Thus

$$\sum_{k \geq k_0+1} \frac{2^k M_k(G)}{k!} \geq 0$$

with equality if and only if G has no non-zero eigenvalues. Then

$$\sum_{i=1}^{n} e^{2\lambda_i} = \sum_{i=1}^{n} \sum_{k \geq 0} \frac{(2\lambda_i)^k}{k!} = \sum_{k \geq 0} \frac{2^k M_k(G)}{k!} \geq \sum_{k=0}^{k_0} \frac{2^k M_k(G)}{k!} \,.$$

By the arithmetic–geometric mean inequality and using the fact that $\sum_{i=1}^{n} \lambda_i = 0$, we have [8]

$$2 \sum_{1 \leq i < j \leq n} e^{\lambda_i} e^{\lambda_j} \geq n(n-1)$$

with equality if and only if all the eigenvalues are equal. Now by the definition of the Estrada index,

$$EE(G)^2 = \sum_{i=1}^{n} e^{2\lambda_i} + 2 \sum_{1 \leq i < j \leq n} e^{\lambda_i} e^{\lambda_j} \geq n(n-1) + \sum_{k=0}^{k_0} \frac{2^k M_k(G)}{k!} \,.$$

Now (1) follows easily. From the derivation of (1) it is evident that equality will be attained if and only if all the eigenvalues are equal to zero, i.e., $G \cong \overline{K_n}$. □

Let G be an (n,m)-graph. Setting $k_0 = 2,\ 3$ in (1), we have [8]

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

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

and either equality is attained if and only if $G \cong \overline{K_n}$.

Theorem 2. *Let G be a graph with $n \geq 2$ vertices and the first Zagreb index Zg. Then*

$$EE(G) \geq e^{\sqrt{\frac{Zg}{n}}} + (n-1) e^{-\frac{1}{n-1}\sqrt{\frac{Zg}{n}}} \tag{2}$$

with equality if and only if $G \cong K_n$ or $G \cong \overline{K_n}$.

Proof. By the arithmetic–geometric mean inequality,

$$\begin{aligned} EE(G) &= e^{\lambda_1} + \sum_{i=2}^{n} e^{\lambda_i} \\ &\geq e^{\lambda_1} + (n-1) \left(\prod_{i=2}^{n} e^{\lambda_i} \right)^{\frac{1}{n-1}} \\ &= e^{\lambda_1} + (n-1) e^{\frac{\sum_{i=2}^{n} \lambda_i}{n-1}} \\ &= e^{\lambda_1} + (n-1) e^{-\frac{\lambda_1}{n-1}} \end{aligned}$$

with equality if and only if $e^{\lambda_2} = \cdots = e^{\lambda_n}$, i.e., $\lambda_2 = \cdots = \lambda_n$.

Note that the function $f(x) = e^x + (n-1)e^{-\frac{x}{n-1}}$ is increasing for $x \geq 0$ and that [17] $\lambda_1 \geq \sqrt{\frac{Zg}{n}}$ with equality if and only if every component is either regular of degree λ_1 or bipartite semiregular such that the product of degrees of any two adjacent vertices is equal to λ_1^2. We have

$$EE(G) \geq f\left(\sqrt{\frac{Zg}{n}}\right) = e^{\sqrt{\frac{Zg}{n}}} + (n-1)e^{-\frac{1}{n-1}\sqrt{\frac{Zg}{n}}}$$

Suppose that equality holds in (2). Then $\lambda_2 = \cdots = \lambda_n$ and $\lambda_1 = \sqrt{\frac{Zg}{n}}$. If $\lambda_1 > \lambda_2$, then G has exactly one positive eigenvalue λ_1 and $n-1$ equal negative eigenvalues, G is connected, regular, and so $\frac{2m}{n} = \lambda_1 = n-1$, which implies that $G \cong K_n$. If $\lambda_1 = \lambda_2$, then $G \cong \overline{K_n}$.

Conversely, it is easy to see that equality holds in (2) if $G \cong K_n$ or $G \cong \overline{K_n}$. □

Remark 1. Let G be an (n,m)-graph with $n \geq 2$. By the interlacing theorem [1], we have $\lambda_2 \geq 0$ if $G \ncong K_n$. Thus, from the proof above, we may have

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

with equality if and only if $G \cong K_n$ or $G \cong \overline{K_n}$. Obviously, we may have better lower bounds for EE than (2) if we use improved lower bounds for $\lambda_1 \geq \sqrt{\frac{Zg}{n}}$. If only the number n of vertices and the number m of edges are known, then since $\lambda_1 \geq \frac{2m}{n}$, we have

$$EE(G) \geq e^{\frac{2m}{n}} + (n-1)e^{-\frac{2m}{n(n-1)}}$$

with equality if and only if $G \cong K_n$ or $G \cong \overline{K_n}$.

Remark 2. Let G be a graph with $n \geq 2$ vertices. Let $\overline{G}$ be the complement of G. Let $\overline{\lambda_1}$ be the largest eigenvalue of $\overline{G}$. Note that $\lambda_1 + \overline{\lambda_1} \geq n-1$. It follows that

$$\begin{aligned} EE(G) + EE(\overline{G}) &\geq e^{\lambda_1} + e^{\overline{\lambda_1}} + (n-1)\left(e^{-\frac{\lambda_1}{n-1}} + e^{-\frac{\overline{\lambda_1}}{n-1}}\right) \\ &\geq 2e^{\frac{\lambda_1+\overline{\lambda_1}}{2}} + 2(n-1)e^{-\frac{\lambda_1+\overline{\lambda_1}}{2(n-1)}} \\ &\geq 2e^{\frac{n-1}{2}} + 2(n-1)e^{-\frac{1}{2}}. \end{aligned}$$

Since $\lambda_1 \neq \overline{\lambda_1}$ for $G \cong K_n$ or $G \cong \overline{K_n}$ with $n \geq 2$, we have $EE(G) + EE(\overline{G}) > 2e^{\frac{n-1}{2}} + 2(n-1)e^{-\frac{1}{2}}$.

The number n_0 of zeros in the spectrum of the graph G is called its nullity. For an (n,m)-graph G, $n_0 \leq n$ with equality if and only if $m = 0$, i.e., $G \cong \overline{K_n}$.

The following lower bound for the Estrada index has been obtained in [11, Theorems 1 and 5]. Here an alternate proof is given.

Theorem 3. [11] *Let G be an (n,m)-graph with nullity $n_0 < n$. Then*

$$EE(G) \geq n_0 + (n-n_0)\cosh\left(\sqrt{\frac{2m}{n-n_0}}\right) \tag{3}$$

with equality if and only if $n-n_0$ is even, G consists of copies of complete bipartite graphs K_{r_i,t_i}, $i=1,2,\ldots,\frac{n-n_0}{2}$, such that all $r_i t_i$ are equal, and $\left[n - \sum_{i=1}^{\frac{n-n_0}{2}} (r_i+t_i)\right]$ isolated vertices.

Proof. It has been known that [11]

$$EE(G) \geq \sum_{i=1}^{n} \cosh(\lambda_i) = \frac{1}{2}\sum_{i=1}^{n}\left(e^{\lambda_i}+e^{-\lambda_i}\right)$$

with equality if and only if G is a bipartite graph.

We will use the following inequality: For positive $a_1,a_2,\ldots,a_n$, and integer $k\geq 0$,

$$\sum_{i=1}^{n} a_i^k \geq n\left(\frac{1}{n}\sum_{i=1}^{n} a_i\right)^k$$

with equality for $k \geq 2$ if and only if all a_i are equal. It is trivial for $k=0,1$, and follows from Hölder's inequality for $k\geq 2$.

Note that $\sum_{i:\lambda_i\neq 0} \lambda_i^2 = 2m$. We have

$$\begin{aligned} EE(G) &\geq n_0 + \frac{1}{2}\sum_{i:\lambda_i\neq 0}\left(e^{\lambda_i}+e^{-\lambda_i}\right) \\ &= n_0 + \sum_{k\geq 0}\frac{1}{(2k)!}\sum_{i:\lambda_i\neq 0}\left(\lambda_i^2\right)^k \\ &\geq n_0 + \sum_{k\geq 0}\frac{1}{(2k)!}(n-n_0)\left(\frac{1}{n-n_0}\sum_{i:\lambda_i\neq 0}\lambda_i^2\right)^k \\ &= n_0 + (n-n_0)\sum_{k\geq 0}\frac{\left(\sqrt{\frac{2m}{n-n_0}}\right)^{2k}}{(2k)!}. \end{aligned}$$

This proves (3).

¿From the derivation of (3) it is evident that equality will be attained in (3) if and only if G is bipartite and all the positive eigenvalues are equal, i.e., G is bipartite and has exactly two distinct eigenvalues or exactly three distinct eigenvalues, by [1, Theorems 6.4 and 6.5, p. 162], this is equivalent to say that G consists of copies of K_{r_i,t_i}, $i=1,2,\ldots,\frac{n-n_0}{2}$, such that all $r_i t_i$ are equal, and $\left[n - \sum_{i=1}^{\frac{n-n_0}{2}} (r_i+t_i)\right]$ isolated vertices. $\square$

3. UPPER BOUNDS

Theorem 4. *Let G be an (n,m)-graph. Then for any integer $k_0 \geq 2$,*

$$EE(G) \leq n-1-\sqrt{2m}+\sum_{k=2}^{k_0}\frac{M_k(G)-\left(\sqrt{2m}\right)^k}{k!}+e^{\sqrt{2m}} \tag{4}$$

with equality if and only if $G \cong \overline{K_n}$.

Proof. Note that $\sum_{i=1}^{n}\lambda_i^2 = 2m$. We have

$$\begin{aligned}
EE(G) &= \sum_{k=0}^{k_0}\frac{M_k(G)}{k!}+\sum_{k\geq k_0+1}\frac{1}{k!}\sum_{i=1}^{n}\lambda_i^k \\
&\leq \sum_{k=0}^{k_0}\frac{M_k(G)}{k!}+\sum_{k\geq k_0+1}\frac{1}{k!}\sum_{i=1}^{n}|\lambda_i|^k \\
&\leq \sum_{k=0}^{k_0}\frac{M_k(G)}{k!}+\sum_{k\geq k_0+1}\frac{1}{k!}\left(\sum_{i=1}^{n}\lambda_i^2\right)^{k/2} \\
&= \sum_{k=0}^{k_0}\frac{M_k(G)}{k!}+\sum_{k\geq k_0+1}\frac{\left(\sqrt{2m}\right)^k}{k!} \\
&= \sum_{k=0}^{k_0}\frac{M_k(G)}{k!}+e^{\sqrt{2m}}-\sum_{k=0}^{k_0}\frac{\left(\sqrt{2m}\right)^k}{k!}\,.
\end{aligned}$$

In the second inequality above, we use an easy inequality: For nonnegative $a_1, a_2, \ldots, a_n$, and integer $k \geq 2$,

$$\sum_{i=1}^{n}a_i^k \leq \left(\sum_{i=1}^{n}a_i^2\right)^{k/2}.$$

Now (4) follows easily. From the derivation of (4) it is evident that equality will be attained in (4) if and only if G has no non-zero eigenvalues, i.e., $G \cong \overline{K_n}$. □

Setting $k_0 = 2,\ 3$ in (4), we have

$$EE(G) \leq n-1-\sqrt{2m}+e^{\sqrt{2m}}$$

$$EE(G) \leq n-1-\left(1+\frac{m}{3}\right)\sqrt{2m}+t+e^{\sqrt{2m}}\,.$$

We can go further.

Theorem 5. *Let G be an (n,m)-graph. Then for any integer $k_0 \geq 2$,*

$$\begin{aligned}
EE(G) \;\leq\; & n-2-\lambda_1-\sqrt{2m-\lambda_1^2} \\
& +\sum_{k=2}^{k_0}\frac{M_k(G)-\lambda_1^k-\left(\sqrt{2m-\lambda_1^2}\right)^k}{k!}+e^{\lambda_1}+e^{\sqrt{2m-\lambda_1^2}}
\end{aligned} \tag{5}$$

with equality if and only if $G \cong \overline{K_n}$.

Proof. Note that $\sum_{i=1}^{n} \lambda_i^2 = 2m$. We have

$$\begin{aligned}
EE(G) - e^{\lambda_1} &= \sum_{k=0}^{k_0} \frac{M_k(G) - \lambda_1^k}{k!} + \sum_{k \geq k_0+1} \frac{1}{k!} \sum_{i=2}^{n} \lambda_i^k \\
&\leq \sum_{k=0}^{k_0} \frac{M_k(G) - \lambda_1^k}{k!} + \sum_{k \geq k_0+1} \frac{1}{k!} \sum_{i=2}^{n} |\lambda_i|^k \\
&\leq \sum_{k=0}^{k_0} \frac{M_k(G) - \lambda_1^k}{k!} + \sum_{k \geq k_0+1} \frac{1}{k!} \left(\sum_{i=2}^{n} \lambda_i^2 \right)^{k/2} \\
&= \sum_{k=0}^{k_0} \frac{M_k(G) - \lambda_1^k}{k!} + \sum_{k \geq k_0+1} \frac{\left(\sqrt{2m - \lambda_1^2} \right)^k}{k!} \\
&= \sum_{k=0}^{k_0} \frac{M_k(G) - \lambda_1^k}{k!} + e^{\sqrt{2m-\lambda_1^2}} - \sum_{k=0}^{k_0} \frac{\left(\sqrt{2m - \lambda_1^2} \right)^k}{k!} .
\end{aligned}$$

Now the result follows easily. □

Setting $k_0 = 2,\, 3$ in (5), we have

$$EE(G) \leq n - 2 - \lambda_1 - \sqrt{2m - \lambda_1^2} + e^{\lambda_1} + e^{\sqrt{2m-\lambda_1^2}}$$

$$EE(G) \leq n - 2 - \lambda_1 - \sqrt{2m - \lambda_1^2} + t - \frac{\lambda_1^3}{6} - \frac{\left(\sqrt{2m - \lambda_1^2} \right)^3}{6} + e^{\lambda_1} + e^{\sqrt{2m-\lambda_1^2}} .$$

Acknowledgement. This work was supported by the National Natural Science Foundation of China (no. 10671076).

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