Kragujevac J. Sci. 29 (2007) 67-72. UDC 541.66:547.318

A LOWER BOUND FOR THE ESTRADA INDEX OF BIPARTITE MOLECULAR GRAPHS

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(Received December 19, 2006)

ABSTRACT. The Estrada index is a novel molecular structure-descriptor, defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$, where $\lambda_1, \lambda_2, ..., \lambda_n$ are the eigenvalues of the molecular graph *G*. It was recently shown that *EE* of a benzenoid graph with *n* vertices and *m* edges is bounded from below as $EE > n \cosh \sqrt{2m/n}$. We now demonstrate that for all bipartite graphs, $EE > n_0 + (n - n_0) \cosh \sqrt{2m/(n - n_0)}$, where n_0 is the number of the zero eigenvalues.

INTRODUCTION

This paper sheds some new lights on the mathematical properties of the Estrada index. The Estrada index was originally defined [1] as a molecular structure-descriptor [2], but this quantity can be considered as a graph invariant that can be defined for any graph.

Let *G* be a graph, possessing *n* vertices and *m* edges and let $\lambda_1, \lambda_2, ..., \lambda_n$ be its eigenvalues [3,4]. These eigenvalues will be labeled so that $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_n$. The Estrada index is then defined as

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

In a very short period the Estrada index has found several applications. Some of them were chemical, where this index was used as molecular-structure descriptor [1, 5-7]. There are some other, fully unrelated, applications of *EE,* put forward by Estrada and

Rodríguez–Velázquez [8,9]. They showed that *EE* provides a measure of the average centrality, i. e., the quality of connectedness, of complex (reaction, communication, social, metabolic, etc) networks.

Investigations of the mathematical properties of the Estrada index started short time ago, and have been accomplished only to a limited degree [8-11].

We first recall two mathematical functions that we use in our considerations. The *hyperbolic cosine* and *hyperbolic sine* are defined as

$$\cosh(x) = \frac{e^x + e^{-x}}{2} \qquad \text{and} \qquad \sinh(x) = \frac{e^x - e^{-x}}{2},$$

respectively. Note that the first derivative of $\cosh(x)$ is equal to $\sinh(x)$, and the first derivative of $\sinh(x)$ is equal to $\cosh(x)$.

In what follows we use some results from graph spectral theory [3]. It is known that the eigenvalues of G are not mutually independent and there exist several relations between them. We use two of these. The paring theorem [3,4,12] holds for the eigenvalues of a bipartite graph:

$$\lambda_i + \lambda_{n+1-i} = 0 \quad \text{for} \quad i = 1,2,...,n. \tag{2}$$

Another well known relation is that the sum of squares of the eigenvalues of a graph with m edges is equal to $2m$. For bipartite graphs, in view of Eq. (2), this relation can be written as

$$\sum_{+} (\lambda_i)^2 = m \tag{3}$$

with the summation going over all positive eigenvalues.

If G has n_0 zero eigenvalues, then because of Eq. (2) the graph G has $(n - n_0)/2$ positive and $(n - n_0)/2$ negative eigenvalues. Bearing this fact in mind, Eq. (1) can be written as [9]

$$EE(G) = n_0 + 2\sum_{+} \cosh(\lambda_i)$$

with the summation going over all positive eigenvalues.

A LOWER BOUND FOR THE ESTRADA INDEX

In the paper [11] the dependence of *EE* on the structure of benzenoid hydrocarbons was examined and a lower bound for *EE* established. This lower bound was deduced by means of a method that earlier was applied in the case of total π-electron energy [13], and that resulted in the famous McClelland upper bound for the total π-electron energy [14,15]. Applying the same method one could deduce a lower bound for *EE* of benzenoid systems. In [11] it was shown that for Kekulèan benzenoid hydrocarbons (whose molecular graphs are bipartite and for which n_0 = 0), the inequality $EE > n\cosh\sqrt{2m/n}$ holds. Now we are applying an analogous reasoning to find a lower bound valid for all bipartite graphs.

In order to deduce the extremal value *EE** of *EE* we employ the standard Lagrange-multiplier technique: First we constuct the auxiliary function *F*:

$$F := n_0 + 2\sum_{+}\cosh(\lambda_i) - \alpha\left(\sum_{+}(\lambda_i)^2 - m\right) \qquad (4)$$

where α is the Lagrange multiplier. Then the condition

$$\frac{\partial F}{\partial \lambda_k} = 0$$

is imposed for all $k = 1,2,...,(n-n_0)/2$, which leeds to the equations

$$2\sinh(\lambda_k) - 2\alpha\lambda_k = 0$$

that must hold for all $k = 1,2,...,(n-n_0)/2$.

The function sinh(*x*) monotonically increases in the entire interval (-∞,+∞) and is equal to zero for *x*=0. Its first derivative at *x*=0 is equal to unity. Bearing these facts in mind, one can easily see that for α>1 the equation $2\sinh(x) - 2\alpha x = 0$ has a single positive-valued solution. Denote it by x_0. This results in $\alpha = \sinh(x_0)/x_0$.

Because of Eq. (3) and because of the choice $\lambda_k = x_0$ for $k = 1,2,...,(n-n_0)/2$, we readily arrive at

$$x_0 = \sqrt{\frac{2m}{n-n_0}}$$

and therefore

$$EE^* = n_0 + (n - n_0)\cosh\left(\sqrt{\frac{2m}{n - n_0}}\right). \qquad (5)$$

Theorem 1. The Estrada index of a bipartite graph with n vertices, m edges ($m \geq 1$) and n_0 zero eigenvalues is always greater than $n_0 + (n - n_0)\cosh\left(\sqrt{\frac{2m}{n - n_0}}\right)$.

Proof. We already know that the expression on the right-hand side of Eq. (5) is an extremal value of the Estrada index. In order to prove Theorem 1 we have to verify that it is a minimum. For this we examine the Hessian matrix $\boldsymbol{H}(F)$ of the function F, Eq. (4). Note that in our case $\boldsymbol{H}(F)$ is a square matrix of order $(n\text{-}n_0)/2$. Because of

$$\frac{\partial F}{\partial \lambda_k} = 2\sinh(\lambda_k) - 2\alpha\lambda_k$$

it is

$$\frac{\partial^2 F}{\partial \lambda^2{}_k} = 2\cosh(\lambda_k) - 2\alpha$$

and

$$\frac{\partial^2 F}{\partial \lambda_k \partial \lambda_{k'}} = 0$$

for $k \neq k'$. Therefore $\boldsymbol{H}(F)$ is a diagonal matrix whose all diagonal elements are equat to

$$2\cosh(x_0) - 2\alpha \quad \text{i. e.,} \quad 2\cosh(x_0) - 2\frac{\sinh(x_0)}{x_0}$$

By using the definitions of the hyperbolic cosine and sine, we obtain

$$2\cosh(x_0) - 2\frac{\sinh(x_0)}{x_0} = \frac{(x_0 - 1)e^{x_0} + (x_0 + 1)e^{-x_0}}{x_0}. \qquad (6)$$

If $x_0 \geq 1$, then the right-hand side of Eq. (6) is evidently positive-valued. This in turn means that all eigenvalues of $\boldsymbol{H}(F)$ are positive-valued, implying that the function F attains a minimum.

In order to complete the proof it remains to demonstrate that for all bipartite graphs $x_0 \geq 1$. Because $2m/n$ is the average vertex degree of the respective graph, it is obvious that $x_0 \geq 1$ holds for all graphs (both bipartite and non-bipartite) in which all vertices have degree at least one, i. e., in which there are no isolated vertices. Then, of course, also $x_0 = \sqrt{\frac{2m}{n - n_0}}$ is greater than or equal to unity.

Let G be a graph possessing exactly p isolated vertices. Then G can be written as $G' \cup p\,K_1$ and G' is a graph with n-p vertices, possessing the same number m of edges as the graph G. The number of zero eigenvalues of G is equal to the number of zero eigenvalues of G' plus p . Therefore

$$x_0(\mathrm{G}) = 2m(G)/[n(G)-n_0(G)] = 2m(G')/[n(G')+p - n_0(G')-p]$$
$$= 2m(G')/[n(G') - n_0(G')] = x_0(G')$$

and $x_0(G') \geq 1$ because G' is a graph without isolated vertices. Therefore also $x_0(G) \geq 1$.

This completes the proof of Theorem 1. ■

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