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Estrada Index of stars

Bingjun Li
Department of Mathematics, Hunan Institute of Humanities, Science and Technology Loudi, Hunan, P.R. China, 417000.

ABSTRACT: *Let G be a simple graph with n vertices, and $\lambda_1, \cdots, \lambda_n$ be the eigenvalues of its adjacent matrix. The Estrada index of G is a graph invariant, defined as $EE(G)=\Sigma_{i=1}^{n} e^{\lambda_i}$, is proposed as a Molecular structure descriptor. In this paper, we obtain the Estrada index of star S_n, and show that $EE(C_n)< EE(S_n)$ for $n>6$, where C_n is the cycle on n vertices.*

KEYWORDS: *Estrada index; star; cycle*

I. INTRODUCTION

Let G be a simple graph with vertex set $V = \{v_1; ...; v_n\}$ and the edge set E. Let $A(G)$ be the adjacent matrix of G, which is a symmetric (0; 1) matrix. The spectrum of G is the eigenvalues of its adjacency matrix, which are denoted by $\lambda_1, \cdots, \lambda_n$. A graph-spectrum-based molecular structure descriptor, put forward by Estrada [2], is defined as

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

EE is usually referred as the Estrada index. Although invented in 2000, the Esteada index has been successfully related to chemical properties of organic molecules, especially proteins [2-3]. Estrada and Rodriguez-Velazquez [4-5] showed that *EE* provides a measure of the centrality of complex (communication, social, metabolic, etc.) networks. It was also proposed as a measure of molecular branching [6]. Within groups of isomers, *EE* was found to increase with the increasing extent of branching of carbon-atom skeleton. In addition, EE characterizes the structure of alkanes via electronic partition function. Therefore it is natural to investigate the relations between the Estrada index and the graph-theoretic properties of *G*.

Let $d(u)$ denote the degree of vertex u. A vertex of degree 1 is called a pendant vertex or a leaf. A connected graph without any cycle is a tree. The path P_n is a tree of order n with exactly two pendant vertices. Let $d(u)$ denote the degree of vertex u. A vertex of degree 1 is called a pendant vertex. A connected graph without any cycle is a tree. The path P_n is a tree of order n with exactly two pendant vertices. The star of order n, denoted by S_n, is a tree with $n - 1$ pendant vertices.

A walk in a graph G is a finite non-null sequence $w = v_0e_1v_1e_2v_{2...}v_{k-1}e_kv_k$, whose terms are alternately vertices and edges, such that, for every $1 \le i \le k$, the ends of e_i are v_{i-1} and v_i. We say that w is a walk from v_0 to v_k, or a $(v_0, v_k)-$walk. The vertices v_0 and v_k are called the initial and final vertices of w, respectively, and $v_1, ..., v_{k-1}$ its internal vertices. The integer k is the length of w. The walk is closed if $v_0 = v_k$.

Some mathematical properties of the Estrada index were established. One of most important properties is the following:

$$EE= \Sigma_{k\geqslant 0}(M_k (G))/k!$$

$M_k(G)$ is called the k-th spectral moment of the graph G. $M_k(G)$ is equal to the number of closed walks of length k in G. Thus, if for two graphs G_1 and G_2, we have $M_k(G_1)\geqslant M_k(G_2)$ for all $k \geqslant 0$, then $EE(G_1)\geqslant EE(G_2)$. Moreover, if there is at least one positive integer t such that $M_t(G_1) > M_t(G_2)$, then $EE(G_1) > EE(G_2)$.

In [1], Gutman examine the Estrada index of cycles and paths, and found analytical expression for them. In this paper. We examine a frequently encountered graph S_n, and compare $EE(S_n)$ with $EE(C_n)$, where C_n is the cycle on n vertices.

II. MAIN RESULTS

The adjacent matrix $A(S_n)$ of the star S_n is:

$$A(S_n)=\begin{pmatrix} 0 & 1 & 1 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 0 & \cdots & 0 \\ \vdots & & & & \vdots \\ 1 & 0 & 0 & \cdots & 0 \end{pmatrix}$$

The solutions of the characteristic equation are $\sqrt{n-1}, 0, \cdots, -\sqrt{n-1}$

Therefore,

$$EE(S_n) = \Sigma_{i=1}^{n} e^{\lambda_i} = e^{\sqrt{n-1}} + e^{-\sqrt{n-1}} + (n-2) = 2\cosh(\sqrt{n-1}) + (n-2) \cdots\cdots (1)$$

In [1], the author showed that

$$EE(C_n) = \sum_{k=1}^{n} e^{2\cos(2k\pi/n)} \approx 2.2795853 \quad n \cdots\cdots (2)$$

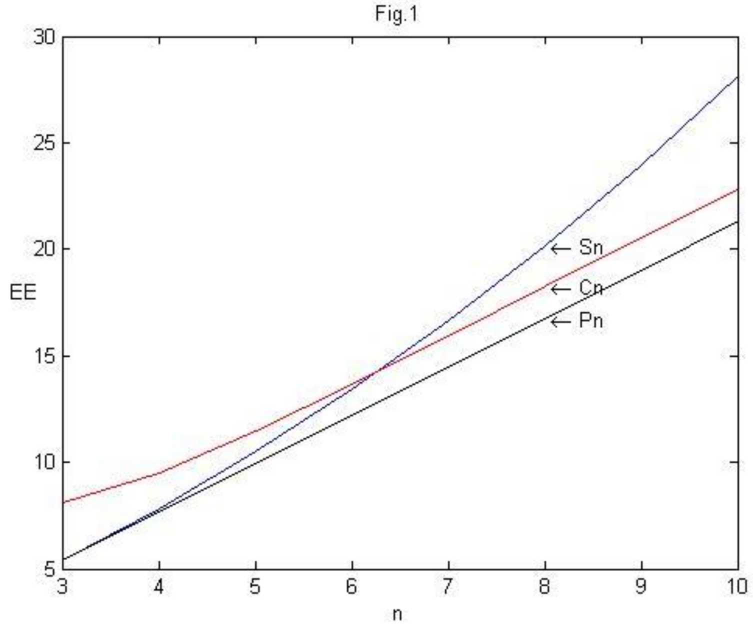
$$EE(P_n) = \sum_{k=1}^{n} e^{2\cos(k\pi/(n+1))} \approx (n+1)2.2795853 \quad - \cosh(2) \cdots\cdots (3)$$

We calculate *EE(P_n)*, *EE(C_n)* and *EE(S_n)* for n=3,4,..., 9 by MATLAB.

n	3	4	5	6	7	8	9
S_n	5.356367113	7.82915488	10.52439138	13.46334694	16.66877282	20.16498213	23.97793443
C_n	8.124814981	9.524391382	11.49618632	13.69671392	15.96024206	18.23712561	20.51632252
P_n	5.356367113	7.635733838	9.91531615	12.19490143	14.47448673	16.75407203	19.03365733

We plot *EE(P_n)*, *EE(C_n)* and *EE(S_n)* in one figure.

Fig.1



In this picture, we see that *EE(C_n)>EE(P_n)* because we can obtain C_n by adding a new edge between two end vertices in P_n. Therefore, there are more closed walk in Cn than in P_n.

In the following, we will compere *EE(S_n)* with *EE(C_n)*, where C_n is the cycle on n vertices.

Theorem 2.1 $EE(C_n) < EE(S_n)$ for any $n \geq 7$.

proof. The precision of the approximation(equation (2)) expression is of a remarkable accuracy. It is reasonable to use this approximation in the following.

$$f(n) = EE(C_n) - EE(S_n)$$

$$= 2.2795853 \quad n - 2\cosh(\sqrt{n-1}) - n + 2$$

$$= 1.2795853 \quad n - 2\cosh(\sqrt{n-1}) + 2$$

$$f(x) = 1.2795853 \quad x - 2\cosh\sqrt{n-1} + 2 = 1.2795853 \quad x - e^{\sqrt{n-1}} - e^{-\sqrt{n-1}} + 2$$

Let $\sqrt{x-1} = t$,then

$$f(x) = g(t) = 1.2795853 \quad t^2 + 1.2795853 \quad - e^t - e^{-t} + 2$$

$g'(t) = 2 * 1.2795853 \quad t - 1.2795853 \quad - e^{t} + e^{-t}$

We assume that n>6. Hence t>2 we have

$g'(2) < 0$, and $g''(t) < 0$.

So $f(x) < 0$ for any $x \geq 7$.

Therefore, $EE(C_n) < EE(S_n)$ for any $n \geq 7$, as desired.

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