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Estrada index of dendrimers

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Let G be a graph and λ_1, λ_2, … λ_n be the eigenvalues of G. The Estrada index EE(G) of the graph G is defined as the sum of e^{λ_i}, 1 ≤ i ≤ n. In this paper some upper and lower bounds for the Estrada index of a general dendrimer is presented.

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1. Introduction

Dendrimers are highly branched macromolecules. They are being investigated for possible uses in nanotechnology, gene therapy, and other fields. The nanostar dendrimer is part of a new group of macromolecules that appear to be photon funnels just like artificial antennas. The topological study of these macromolecules is the aim of this article [1-3].

In this paper, the word graph refers to a finite, undirected graph without loops and multiple edges. Let G be a graph and $\{v_1, ..., v_n\}$ be the set of all vertices of G. The adjacency matrix of G is a 0−1 matrix $A(G) = [a_{ij}]$, where a_{ij} is the number of edges connecting v_i and v_j. The spectrum of a graph G is the set of eigenvalues of A(G), together with their multiplicities. A graph of order n has exactly n real eigenvalues $\lambda_1 \le \lambda_2 \dots \le \lambda_n$. The basic properties of graph eigenvalues can be found in the famous book of Cvetkovic, Doob and Sachs [4].

The Estrada index EE(G) of the graph G is defined as the sum of e^{λ_i}, $1 \le i \le n$. This quantity, introduced by Ernesto Estrada [5,6] has noteworthy chemical applications [7−16].

Throughout this paper our notation is standard and taken mainly from the standard book of graph theory. A walk is a sequence of graph vertices and graph edges such that the graph vertices and graph edges are adjacent. A closed walk is a walk in which the first and the last vertices are the same. A closed walk has backtracking if, in the closed walk, an edge appears twice in immediate succession.

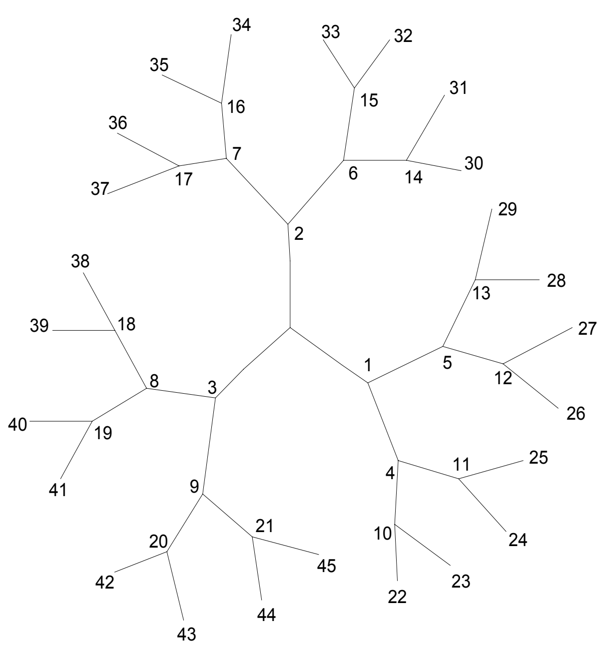

Fig. 1. The fourth generation of dendrimer molecule D[4].

2. Main results and discussion

Suppose D[n] is the molecular graph of the dendrimer molecule depicted in Fig. 1. In this section, at first some formulae for $\sum_{i=1}^{n} \lambda_i^k$, $1 \le k \le 10$, are given. Then we apply these values to estimate the Estrada index of dendrimer molecule D[n]. For the sake of completeness, we mention here a well-known theorem of algebraic graph theory[4] as follows:

Theorem A. Let G be a graph with m edges and t triangles, $A(G) = [a_{ij}]$ and $A^k(G) = [b_{ij}]$. Then the number of walks from u to v in G with length k is b_{uv}. Moreover, $Tr(A) = 0$, $Tr(A^2) = 2m$ and $Tr(A^3) = 6t$.

We assume that $\lambda_1, \lambda_2, \ldots, \lambda_N$ are eigenvalues of dendrimer molecule D[n]. A well-known theorem in linear algebra states that $Tr(A^k) = \sum_{i=1}^{N} \lambda_i^k$ = the number of closed walks in D[n]. Since there are no odd closed walks in D[n], one can prove the following theorem:

Lemma 1. $\sum_{i=1}^{N} \lambda_i^{2k-1} = 0.$

In the following simple lemma, $\sum_{i=1}^{N} \lambda_i^2$ and $\sum_{i=1}^{N} \lambda_i^4$ are computed.

Lemma 2. $\sum_{i=1}^{N} \lambda_i^2 = 6 \times 2^n - 6$ and $\sum_{i=1}^{N} \lambda_i^4 = 48 \times 2^n - 30.$

Proof. Since $\sum_{i=1}^{N} \lambda_i^2 = 2m$, the first part is trivial. For the proof of second part, we notice that every closed walk of length 4 in the dendrimer molecule D[n] constructed from one edge or a path of length 2. Therefore we must count the following type of sequences:

a) $v_1v_2v_1v_2v_1$;
b) $v_1v_2v_3v_2v_1$;
c) $v_2v_1v_2v_3v_2$.

There are $6\times2^{n+1} - 6$ sequences of type (a), $12\times N - 36\times2^n$ sequences of type (b) and $3N-9\times2^n$ sequences of type (c), proving the second part of lemma.

Lemma 3. $\sum_{i=1}^{N} \lambda_i^6 = 474 \times 2^n - 372$.

Proof. We apply a similar argument as Lemma 2 to count the number of closed walk of length 6 in D[n]. Such walks constructed from an edge, a path of length 2, a path of length 3, a star S_4 or a hexagon. If v_i's are distinct vertices of D[n] then we must count the sequences given in Table 1. In this table, we also give the number of walks in each case and we have $\sum_{i=1}^{N} \lambda_i^6 = 474 \times 2^n - 372$, as desired.

Lemma 4. $\sum_{i=1}^{n} \lambda_i^8 = 1176 \times 2^n - 1062$.

Proof. We count the number of closed walk of length 8 in D[n]. In Table 2, we calculate this number for different types of walks. From this table, one can see that $\sum_{i=1}^{n} \lambda_i^8 = 1176 \times 2^n - 1062$, proving the lemma.

Lemma 5. $\sum_{i=1}^{n} \lambda_i^{10} = 6448 \times 2^n - 6654$.

Proof. By counting the number of closed walks of length 10 in D[n] and Table 3, one can see that $\sum_{i=1}^{n} \lambda_i^{10} = 6448 \times 2^n - 6654$, proving the lemma.

Theorem. There are real numbers $C_1, C_2, \ldots, C_n$, $-3 < C_i \le 3$, such that the Estrada index of a dendrimer D[n] is computed as follows:

$$EE(D[n]) = EE(D[n]) = \frac{161291}{28380}2^n - \frac{2899919}{604800} + \sum_{i=1}^{n} \frac{\lambda_i^{12} e^{C_i}}{12!}.$$

Proof. The proof is follows from Lemmas 1–5 and Taylor's Theorem.

Corollary. With the notation of main theorem, $\left(\frac{1308}{12!e^3} + \frac{161291}{28380}\right)2^n - \frac{2899919}{604800} < EE(C_n) < \left(\frac{e^3 3^{12}}{12!} + \frac{161291}{28380}\right)2^n - \frac{2899919}{604800}$,

Table 1. The walks of length 6.

Type	Sequence	No
A	$v_1v_2v_1v_2v_1v_2v_1$	$12.2^n–6$
B	$v_1v_2v_1v_2v_3v_2v_1$	$42\|V\|-126.2^n$
C	$v_2v_1v_2v_1v_2v_3v_2$	$42\|V\|–126.2^n$
D	$v_1v_2v_3v_4v_3v_2v_1$	$60\|V\|–240.2^n$
E	$v_2v_1v_2v_3v_4v_3v_2$	$24\|V\| – 96.2^n$
F	$v_1v_2v_3v_2v_4v_2v_1$	$6\|V\| – 18.2^n$
G	$v_2v_1v_2v_4v_2v_3v_2$	$6\|V\| – 18.2^n$

Table 2. The walks of length 8.

Type	Sequence	No
A	$v_1v_2v_1v_2v_1v_2v_1v_2v_1$	$12.2^n – 6$
B	$v_1v_2v_1v_2v_3v_2v_3v_2v_1$	$42\|V\| – 126.2^n$
C	$v_2v_1v_2v_3v_2v_3v_2v_1v_2$	$42\|V\| – 126.2^n$
D	$v_1v_2v_1v_2v_3v_2v_4v_2v_1$	$60\|V\| – 240.2^n$
E	$v_2v_1v_2v_1v_2v_3v_2v_4v_2$	$120\|V\| – 480.2^n$
F	$v_1v_2v_1v_2v_3v_2v_4v_2v_1$	$36\|V\| – 108.2^n$
G	$v_2v_1v_2v_1v_2v_3v_2v_4v_2$	$36\|V\| – 108.2^n$
H	$v_1v_2v_3v_4v_5v_4v_3v_2v_1$	$24\|V\| – 108.2^n$
I	$v_2v_1v_2v_3v_4v_5v_4v_3v_2$	$48\|V\| – 216.2^n$
J	$v_3v_2v_1v_2v_3v_4v_5v_2v_3$	$24\|V\| – 108.2^n$
K	$v_1v_2v_3v_4v_3v_5v_3v_2v_1$	$12\|V\| – 48.2^n$
L	$v_2v_1v_2v_3v_4v_3v_5v_3v_2$	$24\|V\| – 96.2^n$
M	$v_3v_2v_1v_2v_3v_4v_3v_5v_3$	$36\|V\| – 144.2^{n–1}$
N	$v_4v_3v_5v_3v_2v_1v_2v_3v_4$	$24\|V\| – 96.2^n$

Table 3. The walks of length 10.

Type	Sequence	No
A	$v_1v_2v_1v_2v_1v_2v_1v_2v_1v_2v_1$	$12.2^n - 6$
B	$v_1v_2v_1v_2v_3v_2v_3v_2v_1v_2v_1$	$90\|V\| - 270.2^n$
C	$v_2v_1v_2v_3v_2v_3v_2v_1v_2v_1v_2$	$90\|V\| - 270.2^n$
D	$v_1v_2v_1v_2v_3v_2v_3v_4v_2v_2v_1$	$216\|V\| - 864.2^n$
E	$v_2v_1v_2v_1v_2v_3v_2v_3v_4v_3v_2$	$540\|V\| - 2160.2^n$
F	$v_1v_2v_3v_2v_3v_2v_4v_2v_3v_2v_1$	$150\|V\| - 450.2^n$
G	$v_2v_1v_2v_1v_2v_3v_2v_3v_2v_4v_2$	$150\|V\| - 450.2^n$
H	$v_1v_2v_3v_4v_5v_4v_5v_4v_3v_2v_1$	$168\|V\| - 756.2^n$
I	$v_2v_1v_2v_1v_2v_3v_4v_5v_4v_3v_2$	$288\|V\| - 1296.2^n$
J	$v_3v_2v_1v_2v_3v_4v_5v_4v_3v_4v_3$	$192\|V\| - 864.2^n$
K	$v_1v_2v_3v_4v_3v_4v_3v_5v_3v_2v_1$	$96\|V\| - 384.2^n$
L	$v_2v_1v_2v_1v_2v_3v_4v_3v_5v_3v_2$	$360\|V\| - 480.2^n$
M	$v_3v_2v_1v_2v_3v_4v_3v_5v_3v_4v_3$	$216\|V\| - 864.2^{n-1}$
N	$v_4v_3v_4v_3v_5v_3v_2v_1v_2v_3v_4$	$240\|V\| - 960.2^n$
O	$v_1v_2v_3v_4v_5v_6v_5v_4v_3v_2v_1$	$48\|V\| - 240.2^n$
P	$v_2v_1v_2v_3v_4v_5v_6v_5v_4v_3v_2$	$96\|V\| - 4802^n$
Q	$V_3v_2v_1v_2v_3v_4v_5v_6v_5v_4v_3$	$96\|V\| - 480.2^n$
R	$v_1v_2v_3v_4v_5v_4v_6v_4v_3v_2v_1$	$24\|V\| - 108.2^n$
S	$v_2v_1v_2v_3v_4v_5v_4v_6v_4v_3v_2$	$48\|V\| - 216.2^n$
T	$v_3v_2v_1v_2v_3v_4v_5v_4v_6v_4v_3$	$48\|V\| - 216.2^n$
U	$v_4v_3v_2v_1v_2v_3v_4v_5v_4v_6v_4$	$72\|V\| - 324.2^n$
V	$v_5v_4v_6v_4v_3v_2v_1v_2v_3v_4v_5$	$48\|V\| - 216.2^n$
W	$v_1v_2v_3v_6v_3v_4v_5v_4v_3v_2v_1$	$48\|V\| - 192.2^n$
X	$v_2v_1v_2v_3v_4v_5v_4v_3v_6v_3v_2$	$72\|V\| - 216.2^n$
Y	$v_3v_2v_1v_2v_3v_4v_5v_4v_3v_6v_3$	$72\|V\| - 324.2^n$
Z	$v_6v_3v_4v_5v_4v_3v_2v_1v_2v_3v_6$	$24\|V\| - 108.2^n$
AA	$v_1v_2v_3v_4v_3v_6v_3v_2v_5v_2v_1$	$24\|V\| - 104.2^n$
AB	$v_2v_1v_2v_3v_4v_3v_6v_3v_2v_5v_2$	$72\|V\| - 216.2^n$

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