The Balaban and sum-Balaban indices of the nanostar dendrimer NS[n]

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The Balaban and sum-Balaban indices of a connected graph G=(V,E) with m edges are $J(G)=\frac{m}{\mu+1}\sum_{uv\in E}\frac{1}{\sqrt{D(u)D(v)}}$ and $SJ(G)=\frac{m}{\mu+1}\sum_{uv\in E}\frac{1}{\sqrt{D(u)+D(v)}}$, where μ is the cyclomatic number of G and D(v) is the summation of all distances between a vertex v and all other vertices of G, respectively. In this paper, explicit formulas for the Balaban and sum-Balaban indices index of the nanostar dendrimer NS[n] is derived according to a recursive relation of distances. Numerical values show that the Balaban index of NS[n] is not more than two and is decreasing, and its sum-Balaban index is increasing on n.

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1. Introduction

A topological index is a numerical quantity derived in a unambiguous manner from the structure graph of a molecule. It does not depend on the labeling or the pictorial representation of a graph, i.e., a graph structural invariant. Despite the considerable loss of information by compressing in a single number of a whole structure, such descriptors found broad applications in QSPR/QSAR and aimed to elucidate the relation between the structure of a molecule and its properties or biological activities.

The Balaban index was proposed by A. T. Balaban [1,2], which also called the average distance-sum connectivity or J index. It appears to be a very useful molecular descriptor with attractive properties. For a simple and connected graph G with vertex-set V(G) and edge-set E(G), $d_G(u,v)$ denotes the distance between vertices u and v in G, and $D_G(u)=\sum_{v\in V(G)} d_G(u,v)$ is the distance sum of vertex u in G, i.e., the row sum of distance matrix of G corresponding to u. The Balaban index of G is defined as $J(G)=\frac{m}{\mu+1}\sum_{uv\in E}\frac{1}{\sqrt{D_G(u)D_G(v)}}$, where m is the number of edges and μ is the cyclomatic number of G, respectively. It was shown in [3] that the ordering induced by the Balaban index parallels the ordering induced by the Wiener index for the constitutional isomers of alkanes with 6 through 9 carbon atoms, but reduces the degeneracy of the latter index and provides a much higher discriminating ability.

Very recently, a new topological index is the sum-Balaban index, which was first introduced in [4]. It is defined as $SJ(G)=\frac{m}{\mu+1}\sum_{uv\in E}\frac{1}{\sqrt{D_G(u)+D_G(v)}}$. This index has been successfully correlated with physo-chemical properties of organic molecules. Indeed, the sum-Balaban index is correlated well with some physico-chemical properties and other topological indices (Balaban index, second Zagreb index, Wiener index, Schultz molecular topological index, Gutman molecular topological index, Kirchhoff number etc.) of octanes and lower benzenoids. For details of mathematical properties, as well as basic computational techniques, the readers are suggested to refer to [4,5].

Dendrimers [6] are highly branched macromolecules. They can be precisely designed and manufactured for a wide variety of applications, such as nanotechnology, drug delivery, gene delivery, diagnostics and other fields. The first dendrimers [7] were made by divergent synthesis in 1978. Dendrimers thereafter experienced an explosion of scientific interest because of their unique molecular architecture. Some works for computing other topological indices of some dendrimers can be found in papers [8-14]. The aim of this paper is computing the Balaban and sum-Balaban indices of an infinite class of dendrimers, depicted in Fig. 1. Numerical values show that its sum-Balaban index is increasing on the step of growth, and its Balaban index is decreasing and not more than two. Unlike the constitutional isomers of alkanes in [3], the ordering induced by the Balaban index is not parallel to the ordering induced by the Wiener index for this type of dendrimer.

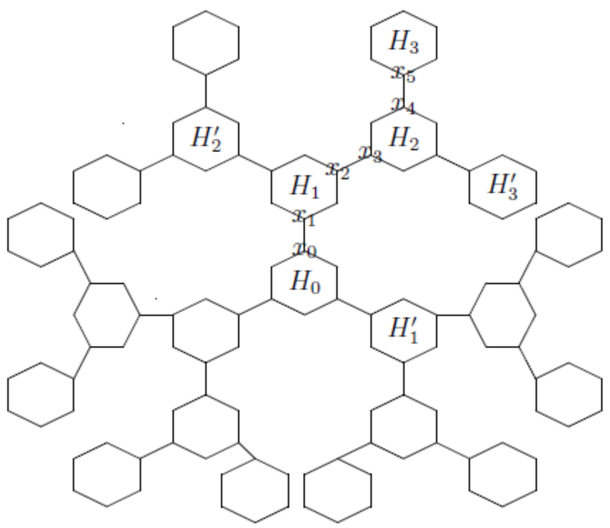

Fig. 1. The nanostar dendrimer NS[n=3].

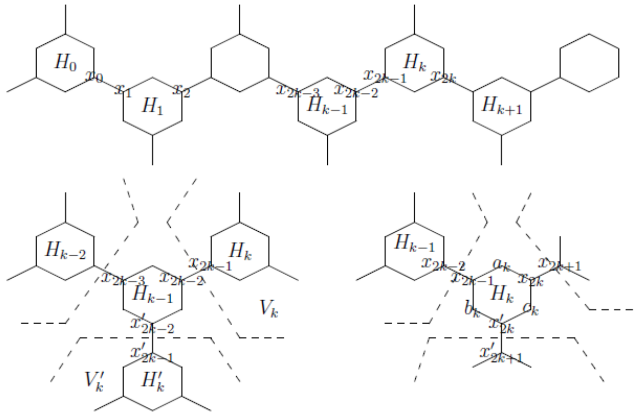

Fig. 2.

2. Results and discussion

In this section, we will first give a recursive relation of distances, and then obtain explicit closed-form formulas for the Balaban and sum-Balaban indices of the nanostar dendrimer NS[n], depicted in Figs. 1, where n denotes the step of growth in this type of dendrimer. It is easy to see that the number of vertices and the number of edges in NS[n] are $|V|=18\times 2^n-12$, $m=|E|=21\times 2^n-15$ and $\mu=|E|-|V|+1=3\times 2^n-2$.

Let H_0 be the central hexagon of NS[n] and $V(H_0)=\{x_0, x'_0, x''_0, a_0, b_0, c_0\}$. H_k is a hexagon in the k-th generation, $x_{2k-2}x_{2k-1}$ is the edge connecting H_{k-1} and H_k, $V(H_k)=\{x_{2k-1}, x_{2k}, x'_{2k}, a_k, b_k, c_k\}$, $1\le k\le n$, depicted in Fig. 2. G_k is the component containing x_{2k-1} of NS[n]-$x_{2k-2}x_{2k-1}$, $V_k=V(G_k)$ and $|V_k|=6\times 2^{n-k+1}-6$. For any $x\in V$, $D(x)=\sum_{y\in V} d(x,y)$, then

$$D(x_{2k-1})-D(x_{2k-2})=\sum_{y\in V_k}(d(x_{2k-1},y)-d(x_{2k-2},y))+\sum_{y\notin V_k}(d(x_{2k-1},y)-d(x_{2k-2},y))$$
$$=-|V_k|+(|V|-|V_k|)=|V|-2|V_k|$$

i.e., $D(x_{2k-1}) = D(x_{2k-2}) + |V| - 2|V_k|$. (1)

In specially,

$$D(x_1) = D(x_0) + |V| - 2|V_1| = D(x_0) + 3\times 2^{n+1}.$$

$$D(x_{2k-2}) - D(x_{2k-2}) = \sum_{y\in V_k}(d(x_{2k-2},y) - d(x_{2k-3},y)) + \sum_{y\in V'_k}(d(x_{2k-2},y) - d(x_{2k-3},y))$$
$$+ \sum_{y\notin V_{k-1}}(d(x_{2k-2},y) - d(x_{2k-3},y)) + \sum_{y\in V(H_{k-1})}(d(x_{2k-2},y) - d(x_{2k-3},y))$$
$$= -2|V_k| + 0 + 2(|V| - |V_{k-1}|) + 0 = 2(|V| - |V_k| - |V_{k-1}|)$$

i.e., $D(x_{2k-2}) = D(x_{2k-3}) + 2(|V| - |V_k| - |V_{k-1}|)$. (2)

From (1) and (2), we have

$$D(x_{2k-1}) = D(x_{2k-3}) + 3|V| - 4|V_k| - 2|V_{k-1}|$$
$$= D(x_{2k-3}) + 27\times 2^{n+1} - 3\times 2^{n-k+5}$$
$$= D(x_{2k-5}) + (27\times 2^{n+1} - 3\times 2^{n-k+6}) + (27\times 2^{n+1} - 3\times 2^{n-k+5})$$
$$= \cdots$$
$$= D(x_1) + 27(k-1)\times 2^{n+1} - 3\times 2^{n-k+5}\times(1+2+2^2+\cdots+2^{k-2})$$
$$= D(x_1) + (27k-51)\times 2^{n+1} - 3\times 2^{n-k+5}$$
$$= D(x_0) + 27(k-48)\times 2^{n+1} - 3\times 2^{n-k+5}$$

i.e., $D(x_{2k-1}) = D(x_0) + 27(k-48)\times 2^{n+1} - 3\times 2^{n-k+5}$ (3)

and

$D(x_{2k-2}) = D(x_{2k-1}) - |V| + 2|V_k| = D(x_0) + (27k-57)\times 2^{n+1} + 15\times 2^{n-k+3}$,

$$D(x_{2k}) = D(x_0) + (27k-30)\times 2^{n+1} - 3\times 2^{n-k+2} \quad (4)$$

$$D(a_k) - D(x_{2k-1}) = D(b_k) - D(x_{2k-1})$$
$$= \sum_{y\notin V_k}(d(a_k,y) - d(x_{2k-1},y)) + \sum_{y\in V_{k+1}}(d(a_k,y) - d(x_{2k-1},y))$$
$$+ \sum_{y\in V'_{k+1}}(d(a_k,y) - d(x_{2k-1},y)) + \sum_{y\in V(H_k)}(d(a_k,y) - d(x_{2k-1},y))$$
$$= (|V| - |V_k|) - |V_{k+1}| + |V'_{k+1}| + 0 = |V| - |V_k|$$

i.e., $D(a_k) = D(b_k) = D(x_{2k-1}) + |V| - |V_k|$. And by (3),

$$D(a_k) = D(b_k) = D(x_0) + (27k-39)\times 2^{n+1} + 21\times 2^{n-k+2} - 6 \quad (5)$$

Similarly,

$$D(c_k) - D(x_{2k-1})$$
$$= \sum_{y\notin V_k}(d(c_k,y) - d(x_{2k-1},y)) + \sum_{y\in V_{k+1}}(d(c_k,y) - d(x_{2k-1},y))$$
$$+ \sum_{y\in V'_{k+1}}(d(c_k,y) - d(x_{2k-1},y)) + \sum_{y\in V(H_k)}(d(c_k,y) - d(x_{2k-1},y))$$
$$= 3(|V| - |V_k|) - |V_{k+1}| - |V'_{k+1}| + 0 = 3|V| - 3|V_k| - 2|V_{k+1}|$$

i.e., $D(c_k) = D(x_{2k-1}) + 3|V| - 3|V_k| - 2|V_{k+1}|$.

And by (3),

$$D(c_k) = D(x_0) + (27k-21)\times 2^{n+1} + 3\times 2^{n-k+4} - 6 \quad (6)$$

Now, we compute $D(x_0)$.

$$d(x_0, x_{2k-1}) = d(x_0, x_1) + d(x_1, x_2) + d(x_2, x_3) + d(x_3, x_4) + \cdots + d(x_{2k-2}, x_{2k-1})$$
$$= 1+2+1+2+\cdots+1 = 3k-2$$

$$d(x_0, b_k) = d(x_0, a_k) = d(x_0, x_{2k-1}) + d(x_{2k-1}, a_k) = 3k-1$$

$$d(x_0, x'_{2k}) = d(x_0, x_{2k}) = d(x_0, x_{2k-1}) + d(x_{2k-1}, x_{2k}) = 3k$$

$$d(x_0, c_k) = d(x_0, x_{2k-1}) + d(x_{2k-1}, c_k) = 3k-1.$$

For $k\ge 1$, $d(x_0, H_k) = \sum_{y\in H_k} d(x_0, y) = 18k-3$,

and

$$\sum_{y\in V_1} d(x_0,y) = \sum_{k=1}^{n} 2^{k-1} d(x_0, H_k) = \sum_{k=1}^{n}(18k-3)\times 2^{k-1} = (18n-21)\times 2^n + 21.$$

By the symmetry of NS[n], we have

$$\sum_{y\in V'_1} d(x'_0,y) = \sum_{y\in V''_1} d(x''_0,y) = \sum_{y\in V_1} d(x_0,y) = (18n-21)\times 2^n + 21$$

.

And,

$$D(x_0) = \sum_{y\in V_1} d(x_0,y) + \sum_{y\in V'_1}(d(x'_0,y) + d(x_0,x'_0)) + \sum_{y\in V''_1}(d(x''_0,y) + d(x_0,x''_0)) + \sum_{y\in V(H_0)} d(x_0,y)$$
$$= 3\sum_{y\in V_1} d(x_0,y) + 2|V'_1| + 2|V''_1| + \sum_{y\in V(H_0)} d(x_0,y)$$
$$= 3((18n-21)\times 2^n + 21) + 4\times 6(2^n - 1) + 9$$
$$= (54n-39)\times 2^n + 48$$

i.e., $D(x_0) = 27n\times 2^{n+1} - 39\times 2^n + 48$ (7)

From (3)-(6), we have

$$D(x_{2k-2}) = 3(16 - 51\times 2^n + 5\times 2^{n-k+3} + 9k\times 2^{n+1} + 9n\times 2^{n+1})$$

$$D(x_{2k-1}) = 3(16 - 45\times 2^n + 2^{n-k+5} + 9k\times 2^{n+1} + 9n\times 2^{n+1})$$

$$D(x_{2k}) = D(x'_{2k}) = 3(16 - 33\times 2^n + 5\times 2^{n-k+2} + 9k\times 2^{n+1} + 9n\times 2^{n+1})$$

$$D(a_k) = D(b_k) = 3(14 - 39\times 2^n + 7\times 2^{n-k+2} + 9k\times 2^{n+1} + 9n\times 2^{n+1})$$

$$D(c_k) = 3(14 - 27\times 2^n + 7\times 2^{n-k+2} + 9k\times 2^{n+1} + 9n\times 2^{n+1})$$

Let

$$\mathrm{J}(\mathrm{H}_0)=\frac{1}{\sqrt{D(x_0)D(a_0)}}+\frac{1}{\sqrt{D(x'_0)D(a_0)}}+\frac{1}{\sqrt{D(x'_0)D(b_0)}}+\frac{1}{\sqrt{D(x''_0)D(b_0)}}+\frac{1}{\sqrt{D(x''_0)D(c_0)}}+\frac{1}{\sqrt{D(x_0)D(c_0)}},$$

$$\mathrm{J}(\mathrm{H}_k)=\frac{1}{\sqrt{D(x_{2k-2})D(x_{2k-1})}}+\frac{1}{\sqrt{D(x_{2k-1})D(a_k)}}+\frac{1}{\sqrt{D(a_k)D(x_{2k})}}+\frac{1}{\sqrt{D(x_{2k})D(c_k)}}+\frac{1}{\sqrt{D(c_k)D(x'_{2k})}}+\frac{1}{\sqrt{D(x'_{2k})D(b_k)}}+\frac{1}{\sqrt{D(x_{2k-1})D(b_k)}}.$$

By the definition of Balaban index,

$$J(NS[n])=\frac{m}{\mu+1}[J(H_0)+\sum_{k=1}^{n}(3\times 2^{k-1}\times J(H_k))]$$
$$=\frac{21\times 2^n-15}{3\times 2^n-1}[\frac{2}{\sqrt{(16-13\times 2^n+9n\times 2^{n+1})(14-11\times 2^n+9n\times 2^{n+1})}}$$
$$+\sum_{k=1}^{n}(\frac{2^k}{\sqrt{(16-33\times 2^n+5\times 2^{n-k+2}+9k\times 2^{n+1}+9n\times 2^{n+1})(14-39\times 2^n+7\times 2^{n-k+2}+9k\times 2^{n+1}+9n\times 2^{n+1})}}$$
$$+\frac{2^k}{\sqrt{(16-33\times 2^n+5\times 2^{n-k+2}+9k\times 2^{n+1}+9n\times 2^{n+1})(14-27\times 2^n+2^{n-k+4}+9k\times 2^{n+1}+9n\times 2^{n+1})}}$$
$$+\frac{2^k}{\sqrt{(14-39\times 2^n+7\times 2^{n-k+2}+9k\times 2^{n+1}+9n\times 2^{n+1})(16-45\times 2^n+n\times 2^{n-k+5}+9k\times 2^{n+1}+9n\times 2^{n+1})}}$$
$$+\frac{2^k}{\sqrt{(16-51\times 2^n+5\times 2^{n-k+3}+9k\times 2^{n+1}+9n\times 2^{n+1})(16-45\times 2^n+2^{n-k+5}+9k\times 2^{n+1}+9n\times 2^{n+1})}})]$$

Similarly, let

$$\mathrm{SJ}(\mathrm{H}_0)=\frac{1}{\sqrt{D(x_0)+D(a_0)}}+\frac{1}{\sqrt{D(x'_0)+D(a_0)}}+\frac{1}{\sqrt{D(x'_0)+D(b_0)}}+\frac{1}{\sqrt{D(x''_0)+D(b_0)}}+\frac{1}{\sqrt{D(x''_0)+D(c_0)}}+\frac{1}{\sqrt{D(x_0)+D(c_0)}},$$

$$\mathrm{SJ}(\mathrm{H}_k)=\frac{1}{\sqrt{D(x_{2k-2})+D(x_{2k-1})}}+\frac{1}{\sqrt{D(x_{2k-1})+D(a_k)}}+\frac{1}{\sqrt{D(a_k)+D(x_{2k})}}+\frac{1}{\sqrt{D(x_{2k})+D(c_k)}}+\frac{1}{\sqrt{D(c_k)+D(x'_{2k})}}+\frac{1}{\sqrt{D(x'_{2k})+D(b_k)}}+\frac{1}{\sqrt{D(x_{2k-1})+D(b_k)}}.$$

then

$$SJ(NS[n])=\frac{m}{\mu+1}[SJ(H_0)+\sum_{k=1}^{n}(3\times 2^{k-1}\times SJ(H_k))]$$
$$=\frac{21\times 2^n-15}{3\times 2^n-1}[\frac{1}{\sqrt{5/2-2^{n+1}+3n\times 2^n}}+\sum_{k=1}^{n}(\frac{2^{k-1}}{\sqrt{5/2-5\times 2^n+3\times 2^{n-k}+3k\times 2^n+3n\times 2^n}}$$
$$+\frac{2^{k-1}}{\sqrt{5/2-7\times 2^n+5\times 2^{n-k}+3k\times 2^n+3n\times 2^n}}+\frac{2^{k-1}}{\sqrt{5/2-3\times 2^{n+1}+2^{n-k+2}+3k\times 2^n+3n\times 2^n}}$$
$$+\frac{2^{k-2}}{\sqrt{8/3-2^{n+3}+3\times 2^{n-k+1}+3k\times 2^n+3n\times 2^n}})]$$

Theorem. The Balaban and sum-Balaban indices of NS[n] are

$$J(NS[n])=\frac{21\times 2^n-15}{3\times 2^n-1}[\frac{2}{\sqrt{(16-13\times 2^n+9n\times 2^{n+1})(14-11\times 2^n+9n\times 2^{n+1})}}$$
$$+\sum_{k=1}^{n}(\frac{2^k}{\sqrt{(16-33\times 2^n+5\times 2^{n-k+2}+9k\times 2^{n+1}+9n\times 2^{n+1})(14-39\times 2^n+7\times 2^{n-k+2}+9k\times 2^{n+1}+9n\times 2^{n+1})}}$$
$$+\frac{2^k}{\sqrt{(16-33\times 2^n+5\times 2^{n-k+2}+9k\times 2^{n+1}+9n\times 2^{n+1})(14-27\times 2^n+2^{n-k+4}+9k\times 2^{n+1}+9n\times 2^{n+1})}}$$
$$+\frac{2^k}{\sqrt{(14-39\times 2^n+7\times 2^{n-k+2}+9k\times 2^{n+1}+9n\times 2^{n+1})(16-45\times 2^n+n\times 2^{n-k+5}+9k\times 2^{n+1}+9n\times 2^{n+1})}}$$
$$+\frac{2^k}{\sqrt{(16-51\times 2^n+5\times 2^{n-k+3}+9k\times 2^{n+1}+9n\times 2^{n+1})(16-45\times 2^n+2^{n-k+5}+9k\times 2^{n+1}+9n\times 2^{n+1})}})]$$

$$SJ(NS[n])=\frac{21\times 2^n-15}{3\times 2^n-1}[\frac{1}{\sqrt{5/2-2^{n+1}+3n\times 2^n}}+\sum_{k=1}^{n}(\frac{2^{k-1}}{\sqrt{5/2-5\times 2^n+3\times 2^{n-k}+3k\times 2^n+3n\times 2^n}}$$
$$+\frac{2^{k-1}}{\sqrt{5/2-7\times 2^n+5\times 2^{n-k}+3k\times 2^n+3n\times 2^n}}+\frac{2^{k-1}}{\sqrt{5/2-3\times 2^{n+1}+2^{n-k+2}+3k\times 2^n+3n\times 2^n}}$$
$$+\frac{2^{k-2}}{\sqrt{8/3-2^{n+3}+3\times 2^{n-k+1}+3k\times 2^n+3n\times 2^n}})]$$

On the other hand, we can also obtain the Wiener index of NS[n] in the following. From (3)-(6),

$$D(H_k)=\sum_{y\in V(H_k)}D(y)=D(x_{2k-1})+D(x_{2k})+D(x'_{2k})+D(a_k)+D(b_k)+D(c_k)$$
$$=[D(x_0)+(27k-48)\times 2^{n+1}+3\times 2^{n-k+5}]+2[D(x_0)+(27k-30)\times 2^{n+1}+15\times 2^{n-k+2}]$$
$$+2[D(x_0)+(27k-39)\times 2^n+21\times 2^{n-k+2}-6]+[D(x_0)+(27k-21)\times 2^{n+1}+3\times 2^{n-k+4}-6]$$
$$=6D(x_0)+(162k-207)\times 2^{n+1}+27\times 2^{n-k+4}-18,$$

i.e.,

$$D(H_k)=6D(x_0)+(162k-207)\times 2^{n+1}+27\times 2^{n-k+4}-18. \quad (8)$$

From (7) and (8), we have

$$W(NS[n])=\frac{1}{2}[D(H_0)+\sum_{k=1}^{n}(3\times 2^{k-1}\times D(H_k))]=270(9n\times 4^{n+1}-27\times 2^{2n+1}+65\times 2^n-10).$$

This result is also obtained in [12].

In the Table 1, the three indices of NS[n] are computed, for some n.

Table 1. Three indices of NS[n] for some k.

n	W	J	SJ
0	27	2	4.24264
1	1296	1.44054	10.1879
2	14526	0.949114	14.2539
3	107082	0.661111	18.2517
4	649890	0.486717	22.9993
5	3539538	0.375614	29.1073
6	18027954	0.301359	37.2194
7	87813234	0.249547	48.1336
8	414505458	0.211985	62.9045
9	1911928050	0.183819	82.9605
10	8665131762	0.162069	110.256

It is evident that there exist strong correlation between W and J, SJ:

$$W = 3.2977 \times J^{-0.1375}, \qquad R = -0.994334$$

$$W = 2.8863 \times SJ^{0.1566}, \qquad R = 0.996795$$

where R is the coefficient of correlation. And these numerical values show that its sum-Balaban index is increasing on the step of growth, and its Balaban index is decreasing and not more than two. Unlike the constitutional isomers of alkanes in [3], the ordering induced by the Balaban index is not parallel to the ordering induced by the Wiener index for this type of dendrimer. The latter assertion cannot be considered as proven in a rigorous mathematical manner. Such a proof awaits to be achieved in the future.

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