Extremal Schultz Index Of Acyclic Molecular Graphs With Diameter 4

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Abstract

Let $G = (V, E)$ be a simple connected graph, d_v is the degree of vertex v, $d_G u, v)$ is the distance between u and v. The Schultz index of G is defined as $\mathcal{W}_+(G) = \sum_{u,v \subset V(G)} (d_u + d_v) d_G(u, v)$. In this paper, we investigate the Schultz index of a class tree with diameter not more than 4.

1 Introduction

Let $G = (V, E)$ be a simple connected graph with the vertex set V and the edge set E. For any $v \in V$, $N(v)$ denotes the neighbors of v, and $d_v = |N(v)|$ is the degree of v, $\Delta(G)$ be the maximum degree of G. The distance between u and v is the smallest length of any $u - v$ path in G and is denoted by $d_G(u, v)$ or simply $d(u, v)$ if the graph G under consideration is clear. Hence if $d(u, v) = k$, then there exists a $u - v$ path $P : u = v_0, v_1, \cdots, v_k = v$ of length k in G, but no $u - v$ path of smaller length exists in G. The diameter of a graph, denoted by *diam(G)*, is the maximum distance between any two vertices. Graph theory was successfully provided the chemist with a variety of very useful tools, namely, topological index. Numbers reflecting certain structural features of organic molecules that are obtained from the molecular graph are usually called graph invariants or more commonly topological indices. The Schultz molecular topological index of a (chemical) graph G introduced by Schultz [3] in 1989 was a graph-theoretical descriptor for characterizing alkanes by an integer. He named this descriptor the molecular topological index and denoted it by $\mathcal{W}_+(G)$ or simply by MTI. Later, $\mathcal{W}_+(G)$ became much better known under the name the Schultz index, defined as

$$\mathcal{W}_+(G) = \sum_{u,v \subset V(G)} (d_u + d_v) d_G(u, v)$$

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Schultz in his initial paper described it as MTI, von Knop and his group [4] gave the mathematical formulation of MTI in the same year 1989.

It has been demonstrated that $\mathcal{W}_+(G)$ and W are closely mutually related for certain classes of molecular graphs [6-11]. In [6,9] the authors derived the explicit relation between $\mathcal{W}_+(G)$ and W for trees :

$$\mathcal{W}_+(G) = 4W(G) - n(n-1)$$

A.A.Dobrynin et al., [7] get the explicit relation between the Wiener index and the Schultz index of catacondensed benzenoid graphs:

$$\mathcal{W}_+(G) = 5W(G) - (12h^2 - 14h + 5).$$

A.A.Dobrynin et al., [8] showed that the Schultz index has the same discriminating power with the Wiener index, i.e., $\mathcal{W}_+(G_1) = \mathcal{W}_+(G_2)$ if and only if $W(G_1) = W(G_2)$ for an arbitrary catacondensed benzenoid graph pair. Other related references see [10-16].

In this paper, we shall investigate the Schultz index of a class tree with diameter not more than 4, and determine the extremal Schultz index the trees.

2 Preliminaries

Denote by $D(G) = [d_1, d_2, \cdots, d_n]$ the degree sequence of the graph G, where d_i stands the degree of the i-th vertex of G, and $d_1 \geq d_2 \geq \cdots \geq d_n$. Furthermore, $D(G) = [d_1^{a_1}, d_2^{a_2}, \cdots, d_t^{a_t}]$ means that G has a_i vertices of degree d_i, where $i = 1, 2, \cdots, t$.

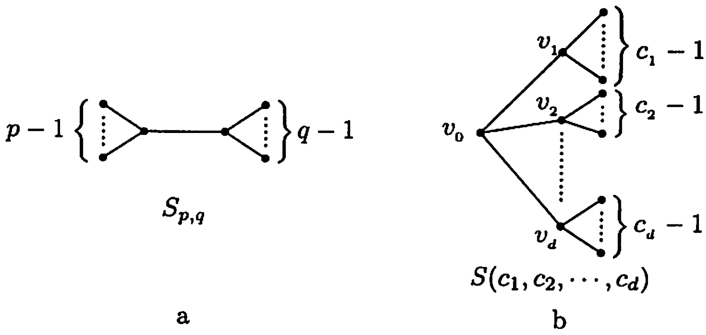
A tree is called a *a double star* $S_{p,q}$(see Figure 1(a)), if it is obtained from $K_{1,p}$ and $K_{1,q-1}$ by identifying a pendent vertex of $K_{1,p}$ with the center of $K_{1,q-1}$, where $1 < p \leq q$. Then for a double star $S_{p,q}$ with n vertices, we have $p + q = n$, and $p \leq \lfloor \frac{n}{2} \rfloor$. We call a double star $S_{p,q}$ *balanced*, if $p = \lfloor \frac{n}{2} \rfloor$ and $q = \lceil \frac{n}{2} \rceil$.

Definition. Let $(c_1, c_2, \cdots, c_d)$ be a partition of n, the *starlike tree* is constructed in the following way:

(1) Let $S_1, S_2, \cdots, S_d$ be the stars with edge number $c_1-1, c_2-1, \cdots, c_d-1$ respectively, and $v_1, v_2, \cdots, v_d$ be their center vertices;

(2) Add a vertex v_0, which join the center vertices $v_1, v_2, \cdots, v_d$ of $S_1, S_2, \cdots, S_d$ respectively.

Then, we can get a tree T with diameter not more than 4. The degree of $v_1, v_2, \cdots, v_d$ are $c_1, c_2, \cdots, c_d$, resp. $|V(T)| = n + 1$, $|E(T)| = d + (c_1 - 1) + (c_2 - 1) + \cdots + (c_d - 1) = c_1 + c_2 + \cdots + c_d = n$. We denote it as $S(c_1, c_2, \cdots, c_d)$ is shown in Figure 1(b).



a b

Figure 1.

From above description, we have

Theorem 2.1. Let $S(c_1, c_2, \cdots, c_d)$ be the graph depicted above. Then

$$\mathcal{W}_+(S(c_1, c_2, \cdots, c_d)) = 7n^2 - 4nd + 3n - 4\sum_{i=1}^{d} c_i^2$$

Proof. For all pairs (x, y) of vertices in $S(c_1, c_2, \cdots, c_d)$, we have $d(x, y) \leq 4$. Thus we only have to count the number of pairs (x, y) with $d(x, y) = k$, for $1 \leq k \leq 4$. We divided the vertices into three groups- the center v_0, the neighbors v_1, $v_2, \cdots, v_d$ of the center, and the leaves $w_1, w_2, \cdots, w_{n-d}$.

By the definition of Schultz index, we have

(1) Obviously, there are n pairs with $d(x, y) = 1$, all the total pairs for the contribution to the Schultz index are:

$$\sum_{i=1}^{d}(c_i + 1)(c_i - 1) + \sum_{i=1}^{d}(c_i + d) = \sum_{i=1}^{d} c_i^2 + \sum_{i=1}^{d} c_i + d^2 - d$$

(2) All pairs of the form $(x, y) = (v_0, w_i)$, $(x, y) = (v_i, v_j)$, or $(x, y) = (w_i, w_j)$ (where w_i, w_j are neighbors of the same v_k, for $1 \leq k \leq d$) satisfy $d(x, y) = 2$. The total pairs for the contribution to the Schultz index are:

$$2 \times [2 \cdot \sum_{i=1}^{d} \binom{c_i - 1}{2} + (d + 1)(n - d) + (d - 1)\sum_{i=1}^{d} c_i]$$

(3) For all pairs of the form $(x, y) = (v_i, w_j)$ with $v_i \not\sim w_j$ we have $d(x, y) = 3$. The total pairs for the contribution to the Schultz index are:

$$3 \times [\sum_{i=1}^{d}(c_i + 1)\sum_{i=1}^{d}(c_i - 1) - \sum_{i=1}^{d}(c_i^2 - 1)]$$

(4) Finally, $d(w_i, w_j) = 4$ if and only if w_i and w_j are not the neighbors of the same v_k $(1 \leq k \leq d)$. The total pairs for the contribution to the Schultz index are:

$$4 \times 2 \times [\binom{n-d}{2} - \sum_{i=1}^{d} \binom{c_i - 1}{2}]$$

Summing up, let $G = S(c_1, c_2, \cdots, c_d)$ then the Schultz index of G is

$$\begin{aligned}
&\mathcal{W}_+(G) \\
= &\sum_{u,v \subset V(G)} (d_u + d_v) d_G(u, v) \\
= &\sum_{i=1}^{d} c_i^2 + \sum_{i=1}^{d} c_i + d^2 - d + 2 \times [2 \cdot \sum_{i=1}^{d} \tbinom{c_i - 1}{2} + (d+1)(n-d) \\
&+(d-1) \sum_{i=1}^{d} c_i] + 3 \times [\sum_{i=1}^{d} (c_i + 1) \sum_{i=1}^{d} (c_i - 1) - \sum_{i=1}^{d} (c_i^2 - 1)] \\
&+4 \times 2 \times [\tbinom{n-d}{2} - \sum_{i=1}^{d} \tbinom{c_i - 1}{2}] \\
= &7n^2 - 4nd + 3n - 4 \sum_{i=1}^{d} c_i^2
\end{aligned}$$

3 Extremal Schultz index of starlike trees

This section will be denoted to the characterization of the star-like tree of maximal Schultz index. First, we note the following:

Lemma 3.1. If a partition contains two parts c_i, c_j such that $c_i \geq c_j + 2$, the corresponding Schultz index of $S(c_1, c_2, \cdots, c_d)$ increases if they are replaced by $c_i - 1$, $c_j + 1$

Proof. Obviously, if n and d remain unchanged, the only term in the Schultz index of $S(c_1, c_2, \cdots, c_d)$ that changes is the sum $\sum_{i=1}^{d} c_i^2$, and the difference is

$$-4[(c_i - 1)^2 + (c_j + 1)^2 - c_i^2 - c_j^2] = 8(c_i - 1 - c_j) > 0$$

Therefore, if a partition satisfies the condition of the lemma, its Schultz index cannot be maximal. So we only have to consider partitions consisting of two different parts k and $k + 1$.

Next, we shall discuss the extremal Schultz index of $S(c_1, c_2, \cdots, c_d)$.

Let $\mathcal{A}(n, d) = \{S(c_1, c_2, \cdots, c_d) | c_1 + c_2 + \cdots + c_d = n\}$ be the sets of $S(c_1, c_2, \cdots, c_d)$, then

Theorem 3.2. Let $G \in \mathcal{A}(n, d)$, if the partition length d is fixed, then $S(n - d + 1, 1, 1, \cdots, 1)$; $S(n - d, 2, 1, 1, \cdots, 1)$, if $2 \leq d \leq n - 2$;

$S(n-d-1,3,1,1,\cdots,1)$, if $2 \le d \le n-4$ or $S(2,2,2,1,\cdots,1)$, if $d = n-3$; $S(k+1,k+1,\cdots,k+1,k,k,\cdots,k)$, $k = \lfloor \frac{n}{d} \rfloor$ has the smallest, the second smallest, the third smallest and the largest Schultz index, respectively.

Proof. Let $G \in \mathcal{A}(n,d)$, we choose G such that $\mathcal{W}_+(G)$ is as large as possible. If the partition is different from $(k+1,k+1,\cdots,k+1,k,k,\cdots,k)$, we can find a partition c_i, c_j such that $c_i \ge c_j + 2$, if we replace them by $c_i - 1$, $c_j + 1$, the Schultz index increases by lemma 3.1, such that $\mathcal{W}_+(G') > \mathcal{W}_+(G)$, which contradict to the choice of G. Analogously, we choose G such that $\mathcal{W}_+(G)$ is as small as possible. If a partition of fixed length d is different from $(n-d+1,1,1,\cdots,1)$, the partition must contains c_i, c_j such that $c_i \ge c_j + 2$, if we replace them by $c_i + 1$, $c_j - 1$ and get a graph G', after operation, the Schultz index decreases by lemma 3.1, such that $\mathcal{W}_+(G') < \mathcal{W}_+(G)$, which contradict to the choice of G as well. This proves the statements for maximum and minimum.

For $d = n-1$ and $d = 1$, the partition is uniquely determined by its length. Thus there is no second smallest Schultz index in this case. Therefore, we consider the case $2 \le d \le n-2$. Now, suppose that there is a graphs G, and the partition of G is different from $(n-d+1,1,1,\cdots,1)$ and $(n-d,2,1,1,\cdots,1)$, $\mathcal{W}_+(G)$ is as small as possible, then the partition in G must contain either two parts $c_i \ge c_j \ge 3$ or three parts $c_i \ge c_j \ge c_k \ge 2$. In both case, we replace c_i, c_j by $c_i + 1$, $c_j - 1$, then we obtain the partition different from $(n-d+1,1,1,\cdots,1)$, and the Schultz index decreases in this case, repeating this operation, we shall get the partition $(n-d,2,1,1,\cdots,1)$, which obtain the second smallest Schultz index.

If $d \ge n-2$ or $d = 1$, there are no further partitions. If $d = n-3$, there is only one partition remaining, namely $(2,2,2,1,\cdots,1)$. Thus it is also the partition giving the third smallest Schultz index. Eventually, if $1 \le d \le n-4$, Similar to the discussion of above two cases, we obtain a partition $(n-d-1,3,1,1,\cdots,1)$, which different from $(n-d+1,1,1,\cdots,1)$ $(n-d,2,1,1,\cdots,1)$. It follows that $S(n-d-1,3,1,1,\cdots,1)$, if $2 \le d \le n-4$ or $S(2,2,2,1,\cdots,1)$, if $d = n-3$ obtains the third smallest Schultz index.

The proof of the theorem is completed.

Lemma 3.3. The Schultz index of a double star $S_{p,q}$ is monotonously increasing in p.

Proof. Similar to above proof, by simple calculation, we have

$$\begin{aligned} & \mathcal{W}_+(S_{p,q}) \\ = \ & n^2 + n - 2 - 2pq + 2[2pq - 2 + (p-1)(p-2) + (q-1)(q-2)] \\ & +6(p-1)(q-1) \\ = \ & 3n^2 - 11n + 4pq + 8 \end{aligned}$$

from the definition of $S_{p,q}$, we have $p + q = n, 1 < p \leq q$, thus,

$$\mathcal{W}_{+}(S_{p,q}) = -4p^2 + 4np + 3n^2 - 11n + 8$$

and $\frac{d(\mathcal{W}_{+}(S_{p,q}))}{dp} = 4n - 8p \geq 0$, it suffices to see that, $\mathcal{W}_{+}(S_{p,q})$ is monotonously increasing in p. Thus, the lemma holds.

Note 3.4. The balanced double star $S_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ has the maximum values of Schultz index among all double star $S_{p,q}$ with n vertices.

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