

# On extremal cacti with minimal degree distance

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**Abstract.** Let  $Diag(G)$  and  $D(G)$  be the degree-diagonal matrix and distance matrix of  $G$ , respectively. Define the multiplier  $Diag(G)D(G)$  as degree distance matrix of  $G$ . The degree distance of  $G$  is defined as  $D'(G) = \sum_{x \in V(G)} d_G(x)D_G(x)$ , where  $d_G(x)$  is the degree of vertex  $x$ ,  $D_G(x) = \sum_{u \in V(G)} d_G(u, x)$  and  $d_G(u, x)$  the distance between  $u$  and  $x$ . Obviously,  $D'(G)$  is also the sum of elements of degree distance matrix  $Diag(G)D(G)$  of  $G$ . A connected graph  $G$  is a cactus if any two of its cycles have at most one common vertex. Let  $\mathcal{G}(n, r)$  be the set of cacti of order  $n$  and with  $r$  cycles. In this paper, we give the sharp lower bound of the degree distance of cacti among  $\mathcal{G}(n, r)$ , and characterize the corresponding extremal cactus.

**Keywords:** degree distance; cactus; degree distance matrix

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## 1. Introduction

Let  $G = (V(G), E(G))$  be a connected simple graph with vertex set  $V(G) = \{v_1, v_2, \dots, v_n\}$  and edge set  $E(G)$ . Set  $N(v_i) = \{u | uv_i \in E(G)\}$ ,  $N[v_i] = N(v_i) \cup \{v_i\}$ . Let  $d_G(v_i) (= |N(v_i)|)$  be the degree of vertex  $v_i$  of  $G$ . The number  $\delta(G) = \min\{d_G(v) | v \in V(G)\}$  is the minimum degree of  $G$ , the number  $\Delta(G) = \max\{d_G(v) | v \in V(G)\}$  its maximum degree. If  $d_G(v) = k$ , we name  $v$  as  $k$ -degree vertex. Denote by  $Diag(G)$  the diagonal matrix of vertex degrees of  $G$ . For vertices  $v_i, v_j \in V(G)$ , the distance  $d_G(v_i, v_j)$  is defined as the length of the shortest path between  $v_i$  and  $v_j$  in  $G$ . Let  $D(G) = (d_{ij})_{v_i, v_j \in V(G)}$  be the distance matrix of  $G$ , where  $d_{ij} = d_G(v_i, v_j)$ . Define the multiplier  $Diag(G)D(G)$  as degree distance matrix of  $G$ .

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The degree distance  $D'(G)$  of  $G$ , which was introduced by Dobrynin and Kochetova [3] and Gutman [5], is defined as

$$D'(G) = \sum_{x \in V(G)} d_G(x) D_G(x) \quad (1.1)$$

where  $d_G(x)$  is the degree of vertex  $x$ ,  $D_G(x) = \sum_{u \in V(G)} d_G(u, x)$  and  $d_G(u, x)$  the distance between  $u$  and  $x$ . Obviously,  $D'(G)$  is also the sum of elements of degree distance matrix  $Diag(G)D(G)$  of  $G$ . Besides as a topological index itself, the degree distance is also the non-trivial part of the molecular topological index (MTI) (or Schultz index) [10], which may be expressed as  $D'(G) + \sum_{u \in V(G)} d_G(u)^2$ , for characterization of alkanes [5, 8, 9]. Some properties for the degree distance may be found, e.g., in [8, 9, 14] in the text of MTI.

The degree distance of graphs is well studied in the literature. In [12], Tomescu presented the graph with minimum degree distance among all connected graphs and disproved a conjecture posed in [3], and in [13] some properties of graphs having minimum degree distance in the class of connected graphs of order  $n$  and size  $m \geq n - 1$  were deduced. In [2] the authors reported the minimum degree distance of graphs with given order and size. Dankelmann et al. [4] presented an asymptotically sharp upper bound of the degree distance of graphs with given order and diameter. Hou and Chang [6] obtained the maximum degree distance among unicyclic graphs on  $n$  vertices. In [11], Tomescu obtained the minimum degree distance of unicyclic and bicyclic graphs, and the authors in [7] characterized  $n$ -vertex unicyclic graphs with girth  $k$ , having minimum and maximum degree distance, and the maximum degree distance among bicyclic graphs, respectively.

In this paper, we will further study the degree distance of cacti. We call  $G$  a cactus if it is connected and all of blocks of  $G$  are either edges or cycles, i.e., any two of its cycles have at most one common vertex. Denote  $\mathcal{G}(n, r)$  the set of cacti of order  $n$  and with  $r$  cycles. Specifically,  $\mathcal{G}(n, 0)$  is the set of trees of order  $n$  and  $\mathcal{G}(n, 1)$  is the set of unicyclic graphs of order  $n$ . In this paper, we will give the sharp lower bound of the degree distance of cacti among  $\mathcal{G}(n, r)$ , and characterize the corresponding extremal cactus.

In order to state our results, we introduce some notation and terminology. For other undefined notation we refer to Bollobás [1]. If  $W \subset V(G)$ , we denote by  $G - W$  the subgraph of  $G$  obtained by deleting the vertices of  $W$  and the edges incident with them, and by  $G[W]$  the induced subgraph of  $G$ . Similarly, if  $E \subset E(G)$ , we denote by  $G - E$  the subgraph of  $G$

obtained by deleting the edges of  $E$ . If  $W = \{v\}$  and  $E = \{xy\}$ , we write  $G - v$  and  $G - xy$  instead of  $G - \{v\}$  and  $G - \{xy\}$ , respectively.

Now we give some lemmas that will be used in the proof of our main results.

**Lemma 1.1.** [13] *If  $T \in \mathcal{G}(n, 0)$ , then  $D'(T) \geq 3n^2 - 7n + 4$ , the equality holds if and only if  $T \cong S_n$ .*

Denote by  $C_k(1^{n-k})$  the graph obtained by attaching  $n - k$  pendent edges to one vertex of  $C_k$ .

**Lemma 1.2.** [13] *If  $G \in \mathcal{G}(n, 1)$ , then  $D'(G) \geq 3n^2 - 3n - 6$ , the equality holds if and only if  $G \cong C_3(1^{n-3})$ .*

For a connected graph  $G$  with  $u \in V(G)$ , we define

$$D_G^*(u) = \sum_{x \in V(G)} d_G(x)d_G(x, u).$$

**Lemma 1.3.** [7] *Let  $G$  be a connected graph and  $v$  be a pendent vertex of  $G$  with  $uv \in E(G)$ . Then*

$$D'(G) = D'(G - v) + D_{G-v}(u) + D_G(v) + D^*(v).$$

Let  $G_1, G_2$  be two connected graphs,  $G_1 \cup G_2 = (V(G_1) \cup V(G_2), E(G_1) \cup E(G_2))$ .

**Lemma 1.4.** [7] *Let  $G$  be a connected graph with a cut-vertex  $v$  such that  $G_1$  and  $G_2$  are two connected subgraphs of  $G$  having  $v$  as the only common vertex and  $G = G_1 \cup G_2$ . Let  $n_i = |V(G_i)|$  and  $m_i = |E(G_i)|$  for  $i = 1, 2$ . Then  $D'(G) = D'(G_1) + D'(G_2) + 2m_1D_{G_2}(v) + 2m_2D_{G_1}(v) + (n_1 - 1)D_{G_2}^*(v) + (n_2 - 1)D_{G_1}^*(v)$ .*

Let  $G^0(n, r)$  be the graph as shown in Figure 1.

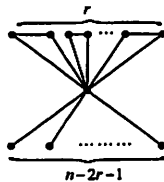


Figure 1: The graph  $G^0(n, r)$

**Lemma 1.5.** *Let  $G$  be a graph in  $\mathcal{G}(n, r)$  with  $a$  1-degree vertices and  $A = \{v \in V(G) : d_G(v) = 1\}$ , then  $n \geq 2r + a + 1$ .*

*Proof.* It is easy to see that there are at least  $2r + 1$  vertices on the  $r$  cycles in  $G$  and  $|A| = a$ , then  $n \geq a + 2r + 1$ . □

## 2. The minimum degree distance of cacti

In the section, we will study a sharp lower bound on the degree distance of cacti. First, we give some lemmas that will be used.

**Lemma 2.1.** *Let  $G^0(n, r)$  be the graph shown in Figure 1, then*

$$D'(G^0(n, r)) = 3n^2 + 4nr - 7n - 10r + 4.$$

*Proof.* For simplicity, let  $A = G^0(n, r)$ . By (1.1), we have

$$\begin{aligned} D'(G^0(n, r)) &= \sum_{v \in V(A)} d_A(v) D_A(v) \\ &= \sum_{v \in V(A), d_A(v)=1} D_A(v) + 2 \sum_{v \in V(A), d_A(v)=2} D_A(v) + (n-1) \sum_{v \in V(A), d_A(v)=n-1} D_A(v) \\ &= 3n^2 + 4nr - 7n - 10r + 4. \end{aligned}$$

□

**Lemma 2.2.** *Let  $G \in \mathcal{G}(n, r)$  and  $v$  be a pendent vertex of  $G$  with  $uv \in E(G)$ , then  $D^*(v) \geq 3n + 4r - 5$ . The equality holds if and only if  $G \cong G^0(n, r)$ .*

*Proof.* By the definition of  $D^*(v)$ , we have

$$\begin{aligned} D^*(v) &= \sum_{x \in V(G)} d_G(x) d_G(x, v) \\ &= \sum_{x \in V(G) - \{u, v\}} d_G(x) [d_G(x, u) + 1] + d_G(u) \\ &= \sum_{x \in V(G) - \{u, v\}} d_G(x) d_G(x, u) + 2[(n-1) + r] - 1 \\ &\geq \sum_{x \in V(G) - \{u, v\}} d_G(x) + 2[(n-1) + r] - 1. \end{aligned}$$

We can assume that there are  $a$  1-degree vertices in  $G$ . Then

$$\begin{aligned}\sum_{x \in V(G) - \{u, v\}} d_G(x) &= a - 1 + \sum_{x \in V(G) - \{u, v\}, d_G(x) \geq 2} d_G(x) \\ &\geq a - 1 + 2[n - 1 - a] = 2n - a - 3.\end{aligned}$$

Further, we have  $D^*(v) \geq 4n + 2r - a - 6$ . By Lemma 1.5, we have  $-a \geq 2r + 1 - n$ , then  $D^*(v) \geq 3n + 4r - 5$ . The equality holds if and only if  $d_G(x) = 2$  for any  $x \in \{y \in V(G) - \{u, v\}, d_G(y) \geq 2\}$  and  $d_G(x, u) = 1$  for any  $x \in V(G) - u$ , that is,  $G \cong G^0(n, r)$ .  $\square$

**Lemma 2.3.** Let  $C_k = u_1 u_2 \dots u_k u_1$  ( $k \geq 4$ ) and  $Q = C_k - u_1 u_2 + u_2 u_k$ , then

- (i)  $\sum_{u \in V(C_k)} d_{C_k}(u, u_1) - \sum_{u \in V(Q)} d_Q(u, u_1) = \begin{cases} 1 - l, & \text{if } k = 2l, \\ -l, & \text{if } k = 2l + 1. \end{cases}$
- (ii)  $\sum_{u \in V(C_k)} d_{C_k}(u, u_k) - \sum_{u \in V(Q)} d_Q(u, u_k) = \lfloor \frac{k}{2} \rfloor - 1;$
- (iii)  $\sum_{u \in V(C_k)} d_{C_k}(u, u_1) - \sum_{u \in V(Q)} d_Q(u, u_k) = \lfloor \frac{k}{2} \rfloor - 1;$
- (iv) If  $k = 4$  or  $k \geq 6$ ,  $\sum_{x \in V(C_k) - \{u_1, u_k\}} \sum_{u \in V(C_k)} d_{C_k}(u, x) - \sum_{x \in V(C_k) - \{u_1, u_k\}} \sum_{u \in V(Q)} d_Q(u, x) \geq 0$ .

*Proof.* By direct calculation, it is easy to obtain the following results:

If  $k = 2l$  ( $l \geq 2$ ), where  $l$  is an integer, then

$$\begin{aligned}\sum_{u \in V(C_k)} d_{C_k}(u, u_1) &= \sum_{u \in V(C_k)} d_{C_k}(u, u_k) \\ &= 2[1 + 2 + \dots + (l - 1)] + l\end{aligned}\tag{2.2}$$

$$\sum_{u \in V(Q)} d_Q(u, u_k) = 2[1 + 2 + \dots + (l - 1)] + 1\tag{2.3}$$

$$\sum_{u \in V(Q)} d_Q(u, u_1) = 2[1 + 2 + \dots + (l - 1)] + 2l - 1\tag{2.4}$$

If  $k = 2l + 1$  ( $l \geq 2$ ), where  $l$  is an integer, then

$$\begin{aligned}\sum_{u \in V(C_k)} d_{C_k}(u, u_1) &= \sum_{u \in V(C_k)} d_{C_k}(u, u_k) \\ &= 2(1 + 2 + \dots + l)\end{aligned}\tag{2.5}$$

$$\sum_{u \in V(Q)} d_Q(u, u_k) = 2[1 + 2 + \dots + (l - 1)] + l + 1\tag{2.6}$$

$$\sum_{u \in V(Q)} d_Q(u, u_1) = 2[1 + 2 + \dots + (l - 1)] + l + 2l\tag{2.7}$$

$$\begin{aligned} \sum_{\partial \in V(\partial)^n} d_{\partial}^{\partial} (n, n_{l+1}) &= \sum_{\partial \in V(\partial)^n} d_{\partial}^{\partial} (n, n_{l+1}) \\ \sum_{\partial \in V(\partial)^n} d_{\partial}^{\partial} (n, n_l) &= \sum_{\partial \in V(\partial)^n} d_{\partial}^{\partial} (n, n_{l+2}) \\ &\vdots \\ \sum_{\partial \in V(\partial)^n} d_{\partial}^{\partial} (n, n_2) &= \sum_{\partial \in V(\partial)^n} d_{\partial}^{\partial} (n, n_{2l+1}) \end{aligned}$$

If  $k = 2l + 1$  ( $l \geq 3$ ), for  $x = n_2, \dots, n_{2l}$ , we have

$$\sum_{x \in V(C_k)} d_{C_k}^{\partial} (n, x) - \sum_{x \in V(C_k) - \{n_1, n_k\}} d_{C_k}^{\partial} (n, x) = \sum_{x \in V(C_k) - \{n_1, n_k\}} d_{C_k}^{\partial} (n, x) = (l-1)(l-2) \geq 0.$$

Then

$$\sum_{\partial \in V(C_k)} d_{C_k}^{\partial} (n, n_2) = \dots = \sum_{\partial \in V(C_k)} d_{C_k}^{\partial} (n, n_k) = 2[l+2+\dots+(l-1)] + l.$$

and by symmetry, we have

$$\begin{aligned} \sum_{\partial \in V(\partial)} d_{\partial}^{\partial} (n, n_l) &= \sum_{\partial \in V(\partial)} d_{\partial}^{\partial} (n, n_{l+1}) \\ &\vdots \\ \sum_{\partial \in V(\partial)} d_{\partial}^{\partial} (n, n_2) &= \sum_{\partial \in V(\partial)} d_{\partial}^{\partial} (n, n_{2l-1}) \end{aligned}$$

we have

(iv) Let  $x \in V(C_k) - \{n_1, n_k\}$ . If  $k = 2l$  ( $l \geq 2$ ), for  $x = n_2, \dots, n_{2l-1}$ ,

$$\sum_{\partial \in V(C_k)} d_{C_k}^{\partial} (n, n_1) - \sum_{\partial \in V(\partial)} d_{\partial}^{\partial} (n, n_k) = \lfloor \frac{2}{k} \rfloor - 1.$$

(iii) Similarly, by (2.2), (2.3), (2.5) and (2.6), it is easy to obtain that

$$\sum_{\partial \in V(C_k)} d_{C_k}^{\partial} (n, n_k) - \sum_{\partial \in V(\partial)} d_{\partial}^{\partial} (n, n_k) = l - 1 = \lfloor \frac{2}{k} \rfloor - 1.$$

(ii) By (2.2), (2.3), (2.5) and (2.6), it is easy to obtain that

$$\sum_{\partial \in V(C_k)} d_{C_k}^{\partial} (n, n_1) - \sum_{\partial \in V(\partial)} d_{\partial}^{\partial} (n, n_1) = \begin{cases} 1 - l, & \text{if } k = 2l, \\ -l, & \text{if } k = 2l + 1. \end{cases}$$

(i) By (2.2) and (2.4), (2.5) and (2.7), we have

and by symmetry, we have

$$\sum_{u \in V(C_k)} d_{C_k}(u, u_2) = \cdots = \sum_{u \in V(C_k)} d_{C_k}(u, u_k) = 2(1 + 2 + \cdots + l).$$

Then

$$\begin{aligned} & \sum_{x \in V(C_k) - \{u_1, u_k\}} \sum_{u \in V(C_k)} d_{C_k}(u, x) - \sum_{x \in V(C_k) - \{u_1, u_k\}} \sum_{u \in V(Q)} d_Q(u, x) \\ &= l^2 - 3l + 1 > 0. \end{aligned}$$

This completes the proof.  $\square$

Let  $H$  be a connected graph and  $C_k = u_1 u_2 \dots u_k u_1$  ( $k = 4$  or  $k \geq 6$ ). Suppose that  $w$  is a vertex of  $H$ , let  $G_1$  be the graph obtained from  $H$  and  $C_k$  by identifying  $w$  with  $u_k$  and  $G_2 = G_1 - u_1 u_2 + u_2 u_k$ .

**Lemma 2.4.** *Let  $G_1, G_2$  be graphs as description above, then  $D'(G_1) > D'(G_2)$ .*

*Proof.* Let  $V_1 = \{u_1, u_2, \dots, u_k\}$ ,  $V_2 = V(G_1) - V_1$ . It is obvious that we have the following results:

- (i)  $d_{G_1}(u_1) = 2$ ,  $d_{G_2}(u_1) = 1$ ,  $d_{G_2}(u_k) = d_{G_1}(u_k) + 1$  and  $d_{G_2}(x) = d_{G_1}(x) = 2$  for  $x \in V(G_1) - \{u_1, u_k\}$ ;
- (ii)  $d_{G_1}(u, u_k) = d_{G_2}(u, u_k)$  for  $u \in V_2$ .

By (1.1), we have

$$\begin{aligned} D'(G_1) &= d_{G_1}(u_1)D_{G_1}(u_1) + d_{G_1}(u_k)D_{G_1}(u_k) + \sum_{x \in V_2} d_{G_1}(x)D_{G_1}(x) + \\ & \quad \sum_{x \in V_1 - \{u_1, u_k\}} d_{G_1}(x)D_{G_1}(x), \\ D'(G_2) &= d_{G_2}(u_1)D_{G_2}(u_1) + d_{G_2}(u_k)D_{G_2}(u_k) + \sum_{x \in V_2} d_{G_2}(x)D_{G_2}(x) + \\ & \quad \sum_{x \in V_1 - \{u_1, u_k\}} d_{G_2}(x)D_{G_2}(x). \end{aligned}$$

Note that

$$\begin{aligned} A_1 &= d_{G_1}(u_1)D_{G_1}(u_1) - d_{G_2}(u_1)D_{G_2}(u_1) = 2D_{G_1}(u_1) - D_{G_2}(u_1) \\ &= \left\{ \sum_{u \in V_2} [d_{G_1}(u, u_k) + 1] + \sum_{u \in V_1} d_{G_1}(u, u_1) \right\} + \left\{ \sum_{u \in V_1} d_{G_1}(u, u_1) - \right. \\ & \quad \left. \sum_{u \in V_1} d_{G_2}(u, u_1) \right\}; \end{aligned}$$

$$\begin{aligned}
A_2 &= d_{G_1}(u_k)D_{G_1}(u_k) - d_{G_2}(u_k)D_{G_2}(u_k) \\
&= d_{G_1}(u_k)D_{G_1}(u_k) - [d_{G_1}(u_k) + 1]D_{G_2}(u_k) \\
&= d_{G_1}(u_k)\left[\sum_{u \in V_1} d_{G_1}(u, u_k) - \sum_{u \in V_1} d_{G_2}(u, u_k)\right] - \left[\sum_{u \in V_2} d_{G_2}(u, u_k) + \sum_{u \in V_1} d_{G_2}(u, u_k)\right].
\end{aligned}$$

Then if  $k = 2l$ , by Lemma 2.3 (i)-(iii), we have

$$\begin{aligned}
A_1 + A_2 &= \left\{ \sum_{u \in V_2} [d_{G_1}(u, u_k) + 1] + \sum_{u \in V_1} d_{G_1}(u, u_1) \right\} + \left\{ \sum_{u \in V_1} d_{G_1}(u, u_1) \right. \\
&\quad \left. - \sum_{u \in V_1} d_{G_2}(u, u_1) \right\} + \left\{ d_{G_1}(u_k) \left[ \sum_{u \in V_1} d_{G_1}(u, u_k) - \sum_{u \in V_1} d_{G_2}(u, u_k) \right] - \left[ \sum_{u \in V_2} d_{G_2}(u, u_k) + \sum_{u \in V_1} d_{G_2}(u, u_k) \right] \right\} \\
&= n - 2l + (l - 1)d_{G_1}(u_k) > 0.
\end{aligned}$$

Furthermore, by Lemma 2.3 (ii), we have

$$\begin{aligned}
A_3 &= \sum_{x \in V_2} d_{G_1}(x)[D_{G_1}(x) - D_{G_2}(x)] \\
&= \sum_{x \in V_2} d_{G_1}(x) \left\{ \sum_{u \in V_2} d_{G_1}(u, x) + \sum_{u \in V_1} [d_{G_1}(u, u_k) + d_{G_1}(u_k, x)] \right. \\
&\quad \left. - \left[ \sum_{u \in V_2} d_{G_2}(u, x) + \sum_{u \in V_1} (d_{G_2}(u, u_k) + d_{G_2}(u_k, x)) \right] \right\} \\
&= \sum_{x \in V_2} d_{G_1}(x) \left[ \sum_{u \in V_1} d_{G_1}(u, u_k) - \sum_{u \in V_1} d_{G_2}(u, u_k) \right] \\
&= (l - 1) \sum_{x \in V_2} d_{G_1}(x) > 0.
\end{aligned}$$

For any vertex  $x \in V_1 - \{u_1, u_k\}$ , we have

$$\begin{aligned}
&d_{G_1}(x)D_{G_1}(x) - d_{G_2}(x)D_{G_2}(x) \\
&= 2D_{G_1}(x) - 2D_{G_2}(x) \\
&= 2 \sum_{u \in V_2} [d_{G_1}(u_k, x) - d_{G_2}(u_k, x)] + 2 \left[ \sum_{u \in V_1} d_{G_1}(u, x) - \sum_{u \in V_1} d_{G_2}(u, x) \right] \\
&= 2(n - k)[d_{G_1}(u_k, x) - d_{G_2}(u_k, x)] + 2 \left[ \sum_{u \in V_1} d_{G_1}(u, x) - \sum_{u \in V_1} d_{G_2}(u, x) \right]
\end{aligned}$$

and it is easy to see that  $d_{G_1}(u_k, x) - d_{G_2}(u_k, x) \geq 0$ . Further by Lemma



2.3 (iv), we have

$$\begin{aligned}
A_4 &= \sum_{x \in V_1 - \{u_1, u_k\}} d_{G_1}(x) D_{G_1}(x) - \sum_{x \in V_1 - \{u_1, u_k\}} d_{G_2}(x) D_{G_2}(x) \\
&= \sum_{x \in V_1 - \{u_1, u_k\}} \{2(n-k)[d_{G_1}(u_k, x) - d_{G_2}(u_k, x)] + 2[\sum_{u \in V_1} d_{G_1}(u, x) - \\
&\quad \sum_{u \in V_1} d_{G_2}(u, x)]\} \geq 0.
\end{aligned}$$

If  $k = 2l + 1$ , similarly, we have

$$\begin{aligned}
A_1 + A_2 &= n - k + (l - 1) + (l - 1)d_{G_1}(u_k) > 0; \\
A_3 &= (l - 1) \sum_{x \in V_2} d_{G_1}(x) > 0; \\
A_4 &= \sum_{x \in V_1 - \{u_1, u_k\}} \{2(n-k)[d_{G_1}(u_k, x) - d_{G_2}(u_k, x)] + \\
&\quad 2[\sum_{u \in V_1} d_{G_1}(u, x) - \sum_{u \in V_1} d_{G_2}(u, x)]\} \geq 0.
\end{aligned}$$

Hence

$$D'(G_1) - D'(G_2) = A_1 + A_2 + A_3 + A_4 > 0.$$

□

**Theorem 2.5.** *Let  $G \in \mathcal{G}(n, r)$ , then  $D'(G) \geq 3n^2 + 4nr - 7n - 10r + 4$ . The equality holds if and only if  $G \cong G^0(n, r)$ .*

*Proof.* By induction on  $n + r$ . If  $r = 0$  or  $1$ , then the theorem holds clearly by lemmas 1.1-1.2. Now, we assume that  $r \geq 2$  and  $n \geq 5$ . If  $n = 5$ , then the theorem holds clearly by the facts that there is only one graph in  $\mathcal{G}(5, 2)$ . Let  $G \in \mathcal{G}(n, r)$ ,  $n \geq 6$  and  $r \geq 2$  in what follows.

**Case 1.**  $\delta(G) = 1$ .

Let  $v \in V(G)$  with  $d_G(v) = 1$  and  $wv \in E(G)$ . Note that  $G - v \in \mathcal{G}(n - 1, r)$ . Then

$$D_{G-v}(u) = \sum_{x \in V(G)-v} d_G(x, u) \geq n - 2 \quad (2.8)$$

$$\begin{aligned}
D_G(v) &= \sum_{x \in V(G)} d_G(x, v) = \sum_{x \in V(G)-v} [d_G(x, u) + 1] \\
&= n - 1 + \sum_{x \in V(G)-v} d_G(x, u) \geq 2n - 3 \quad (2.9)
\end{aligned}$$

By lemmas 1.3, 2.2, the inductive assumption, (2.8) and (2.9), we have

$$\begin{aligned} D'(G) &= D'(G-v) + D_{G-v}(u) + D_G(v) + D^*(v) \\ &\geq [3(n-1)^2 + 4(n-1)r - 7(n-1) - 10r + 4] + (n-2) + \\ &\quad (2n-3) + (3n+4r-5) = 3n^2 + 4nr - 7n - 10r + 4. \end{aligned}$$

The equality holds if and only if  $G \cong G^0(n, r)$ .

**Case 2.**  $\delta(G) \geq 2$ .

By the definition of cactus,  $\delta(G) \geq 2$  and  $r \geq 2$ , we can choose a cycle  $C_k = u_1u_2 \dots u_ku_1$  of  $G$  such that  $d_G(u_1) = \dots = d_G(u_{k-1}) = 2$  and  $d_G(u_k) \geq 3$ .

**Subcase 2.1.** If  $k = 3$ , let  $G_1 = G - \{u_1, u_2\}$  and  $G_2 = C_3$ , then  $G_1 \in \mathcal{G}(n-2, r-1)$ . By Lemma 1.4, we have

$$\begin{aligned} D'(G) &= D'(G_1) + D'(G_2) + 2m_1D_{G_2}(u_3) + 2m_2D_{G_1}(u_3) + \\ &\quad (n_1-1)D_{G_2}^*(u_3) + (n_2-1)D_{G_1}^*(u_3). \end{aligned}$$

Note that

$$\begin{aligned} D'(G_2) &= 12, & D_{G_2}(u_3) &= 2, & D_{G_2}^*(u_3) &= 4, \\ m_1 &= [(n-1) + r] - 3 = n + r - 4, & m_2 &= 3, & n_1 &= n - 2, & n_2 &= 3. \end{aligned}$$

Furthermore

$$D_{G_1}(u_3) = \sum_{x \in V(G_1)} d_{G_1}(x, u_3) \geq n_1 - 1 = n - 3 \quad (2.10)$$

$$D_{G_1}^*(u_3) \geq \sum_{x \in V(G_1) - u_3} d_{G_1}(x) \geq 2(n-3) \quad (2.11)$$

By the inductive assumption, we have

$$\begin{aligned} &D'(G_1) \\ &\geq 3(n-2)^2 + 4(n-2)(r-1) - 7(n-2) - 10(r-1) + 4 \quad (2.12) \end{aligned}$$

Then

$$D'(G) \geq 3n^2 + 4nr - 5n - 14r + 2 \quad (2.13)$$

The equality holds in (2.10) if and only if  $d_{G_1}(u_3) = n_1 - 1$ ; In (2.11), the first equality holds if and only if  $d_{G_1}(x, u_3) = 1$  for any  $x \in V(G_1) - u_3$ , and since  $\delta(G_1) \geq 2$ , then the second equality holds if and only if  $d_{G_1}(x) = 2$

for any  $x \in V(G_1) - u_3$ . The equality holds in (2.12) if and only if  $G_1 \cong G^0(n-2, r-1)$ . Then we have  $d_G(u_3) = n-1$  and  $2r = n-1$ . Note that

$$3n^2 + 4nr - 5n - 14r + 2 - (3n^2 + 4nr - 7n - 10r + 4) = 2(n-1-2r) = 0.$$

Hence  $D'(G) \geq 3n^2 + 4nr - 7n - 10r + 4$ , the equality holds in (2.13) if and only if  $G \cong G^0(n, r)$ .

**Subcase 2.2.** If  $k = 5$ , let  $G_1 = G - \{u_1, u_2, u_3, u_4\}$  and  $G_2 = C_5$ , then  $G_1 \in \mathcal{G}(n-4, r-1)$ . By Lemma 1.4, we have

$$\begin{aligned} D'(G) &= D'(G_1) + D'(G_2) + 2m_1 D_{G_2}(u_5) + 2m_2 D_{G_1}(u_5) + \\ &\quad (n_1 - 1)D_{G_2}^*(u_5) + (n_2 - 1)D_{G_1}^*(u_5). \end{aligned}$$

Note that

$$\begin{aligned} D'(G_2) &= 60, \quad D_{G_2}(u_5) = 6, \quad D_{G_2}^*(u_5) = 12, \\ m_1 &= [(n-1) + r] - 5 = n + r - 6, \quad m_2 = 5, \quad n_1 = n - 4, \quad n_2 = 5. \end{aligned}$$

Furthermore

$$\begin{aligned} D_{G_1}(u_5) &= \sum_{x \in V(G_1)} d_{G_1}(x, u_5) \geq n_1 - 1 = n - 5 \\ D_{G_1}^*(u_5) &= \sum_{x \in V(G_1)} d_{G_1}(x) d_{G_1}(x, u_5) \geq \sum_{x \in V(G_1) - u_5} d_{G_1}(x) \geq 2(n-5) \end{aligned}$$

By the inductive assumption, we have

$$D'(G_1) \geq 3(n-4)^2 + 4(n-4)(r-1) - 7(n-4) - 10(r-1) + 4$$

Then

$$D'(G) \geq 3n^2 + 4nr + 7n - 14r - 56.$$

By Lemma 1.5 we have  $n \geq 2r + 1$ , then

$$\begin{aligned} &3n^2 + 4nr + 7n - 14r - 56 - (3n^2 + 4nr - 7n - 10r + 4) \\ &= 14n - 4r - 60 \geq 24r - 46 > 0. \end{aligned}$$

Hence  $D'(G) > 3n^2 + 4nr - 7n - 10r + 4$ .

**Subcase 2.3.** If  $k = 4$  or  $k \geq 6$ , let  $G' = G - u_1 u_2 + u_2 u_k$ , obviously,  $G' \in \mathcal{G}(n, r)$ . By Lemma 2.4, we have  $D'(G) > D'(G')$ . Note that  $\delta(G') = 1$ , by case 1, we have

$$D'(G') \geq 3n^2 + 4nr - 7n - 10r + 4.$$

This completes the proof.  $\square$

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## References

- [1] B. Bollobás, *Modern Graph Theory* (Springer-Verlag, 1998).
- [2] O. Bucicovschi, S.M. Cioabă, The minimum degree distance of graphs of given order and size, *Discrete Appl. Math.* 156 (2008) 3518-521.
- [3] A. A. Dobrynin, A. A. Kochetova, Degree distance of a graph: A degree analogue of the Wiener index, *J. Chem. Inf. Comput. Sci.* 34 (1994) 1082-1086.
- [4] P. Dankelmann, I. Gutman, S. Mukwembi, H.C. Swart, On the degree distance of a graph, *Discrete Appl. Math.* 157 (2009) 2773-2777.
- [5] I. Gutman, Selected properties of the Schulz molecular topological index, *J. Chem. Inf. Comput. Sci.* 34 (1994) 1087-1089.
- [6] Y. Hou, A. Chang, The unicyclic graphs with maximum degree distance, *J. Math. Study* 39 (2006) 18-24.
- [7] A. Ilić, D. Stevanović, L. Fengd, G. Yu, P. Dankelmann, Degree distance of unicyclic and bicyclic graphs, *Discrete Appl. Math.* 159 (2011) 779-788.
- [8] D. J. Klein, Z. Mihalić, D. Plavšić, N. Trinajstić, Molecular topological index: A relation with Wiener index, *J. Chem. Inf. Comput. Sci.* 32 (1992) 304-305.
- [9] S. Klavžar, I. Gutman, A comparison of the Schultz molecular topological index with the Wiener index, *J. Chem. Inf. Comput. Sci.* 36 (1996) 1001-1003.
- [10] H. P. Schultz, Topological organic chemistry. 1. Graph theory and topological indices of alkanes, *J. Chem. Inf. Comput. Sci.* 29 (1989) 227-228.
- [11] A. I. Tomescu, Unicyclic and bicyclic graphs having minimum degree distance, *Discrete Appl. Math.* 156 (2008) 125-130.
- [12] I. Tomescu, Some extremal properties of the degree distance of a graph, *Discrete Appl. Math.* 98 (1999) 159-163.
- [13] I. Tomescu, Properties of connected graphs having minimum degree distance, *Discrete Math.* 309 (2009) 2745-2748.
- [14] B. Zhou, Bounds for Schultz molecular topological index, *MATCH Commun. Math. Comput. Chem.* 56 (2006) 189-194.