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# Cycles, the Degree Distance, and the Wiener Index\*

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## ABSTRACT

The degree distance of a graph  $G$  is  $D'(G) = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n (d_i + d_j) L_{i,j}$ , where  $d_i$  and  $d_j$  are the degrees of vertices  $v_i, v_j \in V(G)$ , and  $L_{i,j}$  is the distance between them. The Wiener index is defined as  $W(G) = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n L_{i,j}$ . An elegant result (Gutman; Klein, Mihalić, Plavšić and Trinajstić) is known regarding their correlation, that  $D'(T) = 4W(T) - n(n-1)$  for a tree  $T$  with  $n$  vertices. In this note, we extend this study for more general graphs that have frequent appearances in the study of these indices. In particular, we develop a formula regarding their correlation, with an error term that is presented with explicit formula as well as sharp bounds for unicyclic graphs and cacti with given parameters.

**Keywords:** Degree Distance; Wiener Index; Cacti

## 1. Introduction

The Wiener index of a graph  $G$  is the sum of the distances between all pairs of vertices, denoted by

$W(G) = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n L_{i,j}$  where  $L_{i,j}$  is the distance between two vertices  $v_i, v_j \in V(G) := \{v_1, v_2, \dots, v_n\}$ . Such topological indices are defined as molecular descriptors that describe the structure/shape of molecules, helping to predict the activity and properties of molecules in complex experiments. Among these indices,  $W(G)$  was introduced by and named after Wiener [1] as one of the most well-known such concepts.

Dobrynin and Kochetova [2] introduced the degree distance as a “degree analogue of the Wiener index”, denoted by

$$\begin{aligned} D'(G) &= \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n ((d_i + d_j) L_{i,j}) \\ &= \sum_{i=1}^n \sum_{j=1}^n (d_i L_{i,j}) \end{aligned}$$

where  $d_i$  is the degree of the vertex  $v_i$ .

The properties of  $W(G)$  and  $D'(G)$  of various types of graphs are vigorously studied, see for instance [3-9] and the references there for such results on trees,

unicyclic and bicyclic graphs, and cacti. In many cases their extremal values are achieved by the same structures. Then it is natural to consider the correlation between  $W(G)$  and  $D'(G)$ . An elegant result for trees was achieved in as early as 1992, that

**Theorem 1.1.** ([10,11])  $D'(T) = 4W(T) - n(n-1)$  for a tree  $T$  with  $n$  vertices.

We generalize Theorem 1.1 to unicyclic graphs and cacti in general. In Section 2, we provide an observation where an “error term” is defined to simplify notations. With this observation, we provide the relation between  $D'(T)$  and  $W(T)$  for unicyclic graphs and cacti in Section 3.

## 2. The “Error Term” and a Simple Observation

Theorem 1.1 also follows from the fact that  $e(T) = 0$  (for a tree  $T$ ) in the following:

**Lemma 2.1.** Let an “error term” be

$e(G) := D'(G) - 4W(G) + 2n|E(G)| - n(n-1)$ . Then

$$e(G) = \sum_{i=1}^n \left( \sum_{\substack{j=1 \\ j \neq i}}^n (d_i - 1)(L_{i,j} + 1) + d_i \right) - 2W(G). \quad (1)$$

*Proof.* From the definition we have

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$$\begin{aligned}
 D'(G) &= \sum_{i=1}^n \sum_{j=1}^n ((d_i - 1)(L_{i,j} + 1) + L_{i,j} - d_i + 1) \\
 &= \sum_{i=1}^n \sum_{\substack{j=1 \\ j \neq i}}^n ((d_i - 1)(L_{i,j} + 1)) + 2W(G) \\
 &\quad - 2n|E(G)| + n^2 \\
 &= \sum_{i=1}^n \left( \sum_{\substack{j=1 \\ j \neq i}}^n ((d_i - 1)(L_{i,j} + 1)) + d_i \right) \\
 &\quad + 2W(G) - 2n|E(G)| + n(n-1).
 \end{aligned}$$

□

To understand (1), note that for any two non-adjacent vertices  $x$  and  $y$  in  $V(G)$ , the sum

$$\begin{aligned}
 &\sum_{i=1}^n \left( \sum_{\substack{j=1 \\ j \neq i}}^n (d_i - 1)(L_{i,j} + 1) + d_i \right) \\
 &= \sum_{i=1}^n \left( \sum_{\substack{j=1 \\ j \neq i}}^n (d_i - 1)(L_{i,j} + 1) \right) + \sum_{i=1}^n d_i
 \end{aligned} \tag{2}$$

counts the distance between  $x$  and  $y$  once when  $v_i$  is a neighbor of  $x$  on the shortest path between  $x$  and  $y$  and  $v_j = y$ , and once when  $v_i$  is a neighbor of  $y$  on the shortest path between  $x$  and  $y$  and  $v_j = x$ . When  $d_i$  is summed over all  $i$  we get twice the number of edges, which double counts all pairs of vertices distance 1 apart.

Throughout this note, we will focus on the distances that are counted more than twice in (2), the sum of which gives us  $e(G)$ . Theorem 1.1 follows from Lemma 2.1 through the fact that all distances are counted exactly twice in a tree. Also, note that the sum of distances of pairs of adjacent vertices are counted exactly twice by  $\sum_{i=1}^n d_i$ . Hence, we only need to consider the distances between non-adjacent vertices.

### 3. Unicyclic Graphs and Cacti

In this section, we extend this result to unicyclic graphs and cacti. Although the unicyclic graphs can be considered as a special case of cacti, it is convenient to illustrate the proof by studying a unicyclic graph first. The “error term”  $e(G)$  enables us to present the general formula in a “neat” manner, then we focus on its explicit form and bounds.

A *cactus* is a connected graph  $G$  where any two cycles share at most one vertex. Trees, cycles, and unicyclic graphs are all special cases of cacti. Let  $s$  be the number of cycles in  $G$ , then  $s=1$  in cycles and unicyclic graphs.

#### 3.1. Unicyclic Graphs

**Theorem 3.1.**  $D'(G) = 4W(G) - n(n+1) + e(G)$  for a

unicyclic graph  $G$  on  $n$  vertices.

$$\begin{aligned}
 2(n - \lambda) + n(\lambda + 1) &\leq e(G) \\
 &\leq (n - \lambda + 1)^2 + n\lambda + \lambda - 1
 \end{aligned} \tag{3}$$

where  $\lambda$  is the length of the unique cycle.

*Proof.* The formula for  $D'(G)$  follows immediately since  $|E(G)| = |V(G)| = n$ .

**1) We first establish a formula for  $e(G)$ .** Let  $x_1, x_2, \dots, x_\lambda$  be the vertices on the cycle labeled in a clockwise fashion and let  $X_1, X_2, \dots, X_\lambda$  be the corresponding components after removing all edges on the cycle. Note that  $X_k$  is a tree for  $k = 1, 2, \dots, \lambda$ .

First notice that the distances between any two vertices in  $X_k$  are counted exactly twice since  $X_k$  is a tree, for  $k = 1, 2, \dots, \lambda$ . Suppose that  $v_i \in X_k$  and  $v_j \in X_l$ , and  $1 \leq k < l \leq \lambda$ . For  $v_i \neq x_k$ , the shortest paths between  $v_j$  and all but one neighbors of  $v_i$  must contain the shortest path from  $v_i$  to  $v_j$ . Then the distance between  $v_j$  and all neighbors of  $v_i$  not on the path between  $v_j$  and  $v_i$  is counted exactly twice.

If  $v_i = x_k$ , let  $\lambda$  be even (the case for odd  $\lambda$  is similar). If  $l - k \leq \frac{\lambda}{2} - 2$  or  $l - k \leq \frac{\lambda}{2} + 2$ , then the shortest paths between  $v_j$  and all but one neighbors of  $x_k$  must contain the shortest path from  $x_k$  to  $v_j$ . Then the distance between  $v_j$  and any vertex adjacent to  $x_k$  not on the shortest path between  $v_j$  and  $x_k$  is counted exactly twice.

When  $l - k = \frac{\lambda}{2} - 1$ , the distance between  $v_j$  and any neighbor of  $x_k$  in  $V(X_k)$  are counted twice as above. However, the distance between  $x_{k-1}$  and  $v_j$  is counted as

$$\begin{aligned}
 1 + L(x_k, v_j) &= 1 + L(x_k, x_l) + L(x_l, v_j) \\
 &= \frac{\lambda}{2} + L(x_l, v_j)
 \end{aligned}$$

where  $L(v, u)$  is the distance between  $v$  and  $u$ . Note that this distance is also counted for the case

$l - k = \frac{\lambda}{2} + 1$ , hence over counted once for every

$v_j \in V(X_l)$ . Then the total contribution to  $e(G)$  as  $l$  ranges from 1 to  $\lambda$  is

$$\begin{aligned}
 &\sum_{l=1}^{\lambda} \sum_{v \in V(X_l)} \left( \frac{\lambda}{2} + L(x_l, v) \right) \\
 &= n \left( \frac{\lambda}{2} \right) + \sum_{l=1}^{\lambda} \sum_{v \in V(X_l)} L(x_l, v).
 \end{aligned}$$

When  $l - k = \frac{\lambda}{2}$ , the distance between  $x_{k-1}$  or  $x_{k+1}$

and  $v_j \in V(X_l)$  is miscounted once as  $\frac{\lambda}{2} + 1 + L(x_l, v)$ .

Then the contribution to  $e(G)$  is given by

$$\begin{aligned} & \sum_{l=1}^{\lambda} \sum_{v \in V(X_l)} \left( \frac{\lambda}{2} + 1 + L(x_l, v) \right) \\ &= n \left( \frac{\lambda}{2} + 1 \right) + \sum_{l=1}^{\lambda} \sum_{v \in V(X_l)} L(x_l, v). \end{aligned}$$

Then

$$\begin{aligned} e(G) &= 2 \sum_{l=1}^{\lambda} \sum_{v \in V(X_l)} L(x_l, v) + n(\lambda + 1) \\ &= 2 \sum_{l=1}^{\lambda} D_l + n(\lambda + 1). \end{aligned}$$

Here  $D_l = \sum_{v \in V(X_l)} L(x_l, v)$  is often referred to as the distance function of  $x_l$  in  $X_l$ .

2) Next we analyze the value  $e(G)$ . It is known that, with given number of vertices,  $D_l$  is minimized by the center of a star and maximized by one end of a path. Hence

$$|V(X_l)| - 1 \leq D_l \leq \frac{1}{2} |V(X_l)| (|V(X_l)| - 1).$$

The sharp bounds of  $e(G)$  are given by

$$\begin{aligned} 2 \sum_{l=1}^{\lambda} (|V(X_l)| - 1) + n(\lambda + 1) &\leq e(G) \\ &\leq \sum_{l=1}^{\lambda} (|V(X_l)| (|V(X_l)| - 1)) + n(\lambda + 1). \end{aligned}$$

The sharp lower bound can be achieved by any cycle with pendant edges attached, the sharp upper bound can be achieved by appending a path to a cycle, proving (3).  $\square$

In the case of a cycle,  $D_l = 0$  and  $\lambda = n$ , we have a simple corollary as follows.

**Corollary 3.2.**

$D'(C_n) = 4W(C_n) = 4W(C_n) - n(n+1) + e(C_n)$  for a cycle  $C_n$  on  $n$  vertices, where  $e(C_n) = n(n+1)$ .

Note that Corollary 3.2 can be directly verified from the definitions,

$$\begin{aligned} D'(G) &= \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n (d_i + d_j) L_{i,j} = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n (2+2) L_{i,j} \\ &= 2 \sum_{i=1}^n \sum_{j=1}^n L_{i,j} = 4W(G). \end{aligned}$$

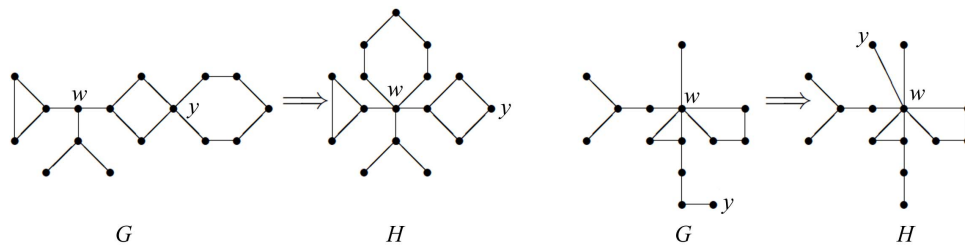


Figure 1. Two operations that decreases  $e(G)$ .

**3.2.  $e(G)$  for General Cacti**

Let  $G$  be a cactus with  $s$  cycles and  $r$  edges not on any cycle. Label the cycles  $c_\alpha$  for  $\alpha = 1, 2, \dots, s$ , let  $\lambda_\alpha$  be the length of  $c_\alpha$  and  $x_l^\alpha$  be a vertex on  $c_\alpha$  with component  $X_l^\alpha$  (the component containing  $x_l^\alpha$  after the removal of the edges on  $c_\alpha$ ) for  $l = 1, 2, \dots, \lambda_\alpha$ . Define the distance function of  $x_l^\alpha$  by

$$D_l^\alpha = \sum_{v \in X_l^\alpha} L(x_l^\alpha, v).$$

Since  $|E(G)| = n + s - 1$ , we immediately have

$$D'(G) = 4W(G) - n(n + 2s - 1) + e(G).$$

As was the case for the unicyclic graph, for every cycle in  $G$  we have a contribution of

$$2 \sum_{l=1}^{\lambda_\alpha} \sum_{v \in V(X_l^\alpha)} L(x_l^\alpha, v_j) + n(\lambda_\alpha + 1)$$

to  $e(G)$ . Then an explicit formula is given by

$$\begin{aligned} e(G) &= \sum_{\alpha=1}^s \left( 2 \sum_{l=1}^{\lambda_\alpha} D_l^\alpha + n(\lambda_\alpha + 1) \right) \\ &= 2 \sum_{\alpha=1}^s \sum_{l=1}^{\lambda_\alpha} D_l^\alpha + n(n - r + 2s - 1). \end{aligned} \tag{4}$$

With (4), we claim that, with given  $n, s, r$  and cycle lengths, the star-shaped cactus (a cactus that has only one cut vertex as its center) minimizes  $e(G)$ .

**Claim 3.1.** For any cactus  $G$  with order  $n$ ,  $s$  cycles,  $r$  edges and any vertex  $w \in V(G)$ , there exists a star-shaped cactus  $S$  with the same parameters and cycle lengths with center  $u$ , such that

$$\sum_{v \in V(S)} L(v, u) \leq \sum_{v \in V(G)} L(v, w).$$

One can easily see the idea from Figure 1, where either operation from  $G$  to  $H$  will reduce  $\sum_{v \in V(G)} L(v, w)$  unless we have a star-shaped cactus.

Then  $e(G)$  is minimized when  $G$  is a star-shaped cactus. Consequently  $D_l^\alpha = 0$  for all but one  $l$ , for any given  $\alpha$ .

$$\begin{aligned} e(G) &= 2 \sum_{\alpha=1}^s \sum_{l=1}^{\lambda_\alpha} D_l^\alpha + n(n - r + 2s - 1) \\ &\geq 2 \sum_{\alpha=1}^s \left( \left\lfloor \frac{\lambda_\alpha}{2} \right\rfloor \left\lfloor \frac{\lambda_\alpha + 1}{2} \right\rfloor \right) + 2rs + n(n - r + 2s - 1). \end{aligned}$$

**Remark 3.3.** *If one does not specify the cycle lengths, then bounds similar to the unicyclic case can be achieved. Also, it is interesting to see that  $e(G)$  is minimized by a star-shaped cactus, which minimizes a number of graphical indices including  $W(G)$  ([7]) among cacti.*

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