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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 $D'(G)=\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left(d_i+d_j\right)L_{i,j}$, 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 $v_i, v_j \in V(G) := \{v_1, v_2, \cdots, v_n\}$. 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

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

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*

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

Proof. From the definition we have

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

□

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

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

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.*

$$2(n-\lambda)+n(\lambda+1)\le e(G)\le(n-\lambda+1)^2+n\lambda+\lambda-1 \tag{3}$$

where λ 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 $x_1,x_2,\cdots,x_\lambda$ be the vertices on the cycle labeled in a clockwise fashion and let $X_1,X_2,\cdots,X_\lambda$ be the corresponding components after removing all edges on the cycle. Note that X_k is a tree for $k=1,2,\cdots,\lambda$.

First notice that the distances between any two vertices in X_k are counted exactly twice since X_k is a tree, for $k=1,2,\cdots,\lambda$. Suppose that $v_i\in X_k$ and $v_j\in X_l$, and $1\le k<l\le\lambda$. 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 λ be even (the case for odd λ is similar). If $l-k\le\frac{\lambda}{2}-2$ or $l-k\le\frac{\lambda}{2}+2$, 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

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

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 λ is

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

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

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

Then

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

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

$$|V(X_l)|-1\le D_l\le\frac{1}{2}|V(X_l)|\left(|V(X_l)|-1\right).$$

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

$$2\sum_{l=1}^{\lambda}\left(|V(X_l)|-1\right)+n(\lambda+1)\le e(G) \le\sum_{l=1}^{\lambda}\left(|V(X_l)|\left(|V(X_l)|-1\right)\right)+n(\lambda+1).$$

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). □

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,

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

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_α for $\alpha=1,2,\cdots,s$, let λ_α be the length of c_α and x_l^α be a vertex on c_α with component X_l^α (the component containing x_l^α after the removal of the edges on c_α) for $l=1,2,\cdots,\lambda_\alpha$. Define the distance function of x_l^α 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

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

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

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 α.

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

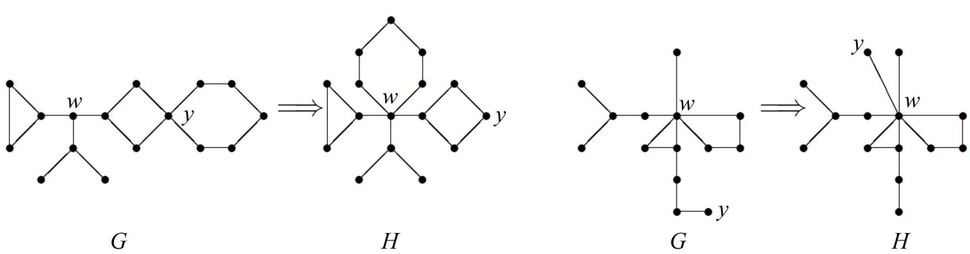

Figure 1. Two operations that decreases *e*(*G*).

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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