

A Lower Bound on the Degree Distance in a Tree

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Abstract

For a graph $G = (V, E)$, the degree distance of G is defined as

$$DD(G) = \sum_{\{u,v\} \subseteq V(G)} (d_G(u) + d_G(v))d_G(u, v)$$

where $d_G(u)$ (or $d(u)$) is the degree of the vertex u in G , and $d_G(u, v)$ is the distance between u and v . This paper gets a lower bound on the degree distance in a tree in terms of the order and diameter of the tree.

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1 Introduction

We use Bondy and Murty [1] for terminologies and notions not defined here. Let $G = (V, E)$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$ and $|V| = n$, $|E(G)| = m$ are the vertex and edge number of G , *resp.* For any $u, v \in V$, $d_G(u)$ (or simply by $d(u)$) and $d_G(u, v)$ denote the degree of u and the distance (i.e., the number of edges on the shortest path) between u and v , respectively. The distance $d(x, y)$ from a vertex x to another vertex y is the minimum number of edges in an $x - y$ path. The distance $d_G(x, S)$ from a vertex x to the set S is $\min_{y \in S} d(x, y)$. Let P_n , C_n and S_n be the path, cycle and the star on n vertices.

The oldest and most thoroughly examined use of a topological index in chemistry was by Wiener [2] in the study of paraffin boiling points, and the topological index was called Wiener index or Wiener number. The Wiener index of the graph G , is equals to the sum of distances between all pairs of vertices of the respective molecular graph, i.e., $W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v)$. In connection with certain investigations in mathematical chemistry, Dobrynin

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and Kochetova [3] introduced firstly in connection with certain chemical applications, and at the same time by Gutman [4] who named it the *Schultz index*, defined as $DD(G) = \sum_{\{u,v\} \subseteq V(G)} (d_G(u) + d_G(v))d_G(u,v)$. This name was eventually accepted by most authors. Here, we refer to [5] for a clarification of the notion.

The degree distance attracted much attention after it was discovered. It has been demonstrated that $DD(G)$ and $W(G)$ are closely mutually related for certain classes of molecular graphs [4, 6-10]. Klein *et al* [6] derived an explicit relation between $DD(G)$ and $W(G)$ for trees. In [7], the authors derived relations between $W(G)$ and $DD(G)$, for the (unbranched) hexagonal chain composed of n fused hexagons. In [8], A. I. Tomescu characterized the connected unicyclic and bicyclic graphs in terms of the degree sequence, as well as the graphs in these classes minimal with respect to the degree distance are given. In [9], O. Bucicovschi and S. M. Cioabă studied the degree distance of graphs with given order and size, and determined the minimum degree distance of a connected graph of order n and size m .

2 Preliminary Notes

Definition 2.1 For any triple integers (p, d, q) where $d \geq 2, n \geq d + 1, p + d + q = n + 1, 1 \leq p \leq q \leq \lceil \frac{n+1-d}{2} \rceil$. Let $T(p, d, q)$ denote the graph constructed from $P_{d-1} : x_1, x_2, \dots, x_{d-1}$ by attaching p pendent edges at x_1 and q pendent edges at x_{d-1} . Then $T(p, d, q)$ is a tree of order n and diameter d , and it contains precisely two stems x_1 and x_{d-1} with p and q leaves, resp.

When $d = 2$, the graph $T(p, 2, q) \cong S_n$; $d = 3$, the graph $T(p, 2, q) \cong S(p, q)$ which we named it as *star-like tree*.

3 Main Results

These are the main results of the paper.

Theorem 3.1 For any pair of integers (n, d) , where $d \geq 2, n \geq d + 1$.

$$\begin{aligned} & DD(T(p, d, q)) \\ &= \frac{2}{3}d^3 + (2d^2 - 4d - 1)(p + q) + 2(2d - 1)pq + 3(p^2 + q^2) - 3d^2 + \frac{13}{3}d - 2 \end{aligned}$$

Proof. For the convenience of the computation, we classified the vertices of $T(p, d, q)$ into three types. The first type: the vertices attached at vertex x_1 ; the second type: the vertices attached at vertex x_{d-1} ; the third type: the vertices in P_{d-1} .

(i) for the vertices lies in the first type, all the vertices for the contribution to the degree distance is $2 \times 2 \times \binom{p}{2} = 2p^2 - 2p$;

(ii) for the vertices lies in the second type, all the vertices for the contribution to the degree distance is $\frac{2}{3}d^3 + (\frac{1}{2}d^2 - \frac{3}{2}d + 1)(p + q) - 3d^2 + \frac{13}{3}d - 2$;

(iii) for the vertices lies in the third type, all the vertices for the contribution to the degree distance is $2 \times 2 \times \binom{q}{2} = 2q^2 - 2q$;

(iv) for the vertices lies between the first type and the second type, all the vertices for the contribution to the degree distance is $p \times q \times 2 \times d = 2dpq$;

(v) for the vertices lies between the first type and the third type, all the vertices for the contribution to the degree distance is $\frac{3}{2}d^2p + dpq - \frac{5}{2}dp + p^2 - pq$;

(vi) for the vertices lies between the second type and the third type, all the vertices for the contribution to the degree distance is

$$\begin{aligned} & q \times (q + 2) + q \times 3 \times [2 + \cdots + (d - 2)] + q \times (p + 2)(d - 1) \\ &= \frac{3}{2}d^2q + dpq - \frac{5}{2}dq + q^2 - pq \end{aligned}$$

Summing up, we get the result.

Theorem 3.2 For the fixed n, d , $DD(T(p, d, q))$ is monotone increasing in p .

Proof. By theorem 3.1, we have

$$DD(T(p, d, q)) - DD(T(p-1, d, q+1)) = 4(d-2)(q+1-p) \geq 0 \text{ (since } d \geq 2, q \geq p+1)$$

From above theorem, we can get following Lemma easily.

Lemma 3.3 For the fixed n, d , $T(1, d, n-d)$ has the smallest degree distance among $T(p, d, q)$.

By simple calculation, we have

$$DD(T(1, d, n-d)) = -\frac{4}{3}d^3 + 2(n+1)d^2 - 6dn + 3n^2 - 3n + \frac{10}{3}d$$

Theorem 3.4 For the fixed n, d , $DD(T(1, d, n-d))$ is monotone increasing in d with $d \geq 2$.

Proof. From above, we have

$$\begin{aligned} & DD(T(1, d, n-d)) - DD(T(1, d-1, n+1-d)) \\ &= -\frac{4}{3}d^3 + 2(n+1)d^2 - 6dn + 3n^2 - 3n + \frac{10}{3}d \\ &\quad - [-\frac{4}{3}(d-1)^3 + 2(n+1)(d-1)^2 - 6(d-1)n + 3n^2 - 3n + \frac{10}{3}(d-1)] \\ &= 4(d-2)(n-d) \geq 0 \end{aligned}$$

Combing all cases above, we shall get a lower bound on the degree distance in $T(p, d, q)$.

Theorem 3.5 $T(1, 2, n-2)$ has the smallest degree distance among $T(p, d, q)$ with $d \geq 2$.

Nextly, we shall investigate the degree distance in $S(p, q)$.

Theorem 3.6 *Let $S(p, q)$ be the graph described above, then $DD(S(p, q)) = 3n^2 - 7n + 4 + 4pq$.*

Proof. By simple calculation, we arrive at the result.

Theorem 3.7 *$DD(S(p, q))$ is monotone increasing in p .*

Proof. By theorem 3.6, we have $\frac{\partial(DD(S(p,q)))}{\partial p} = 4q > 0$.

Theorem 3.8 *The order of $DD(S(p, q))$ is:*

$$DD(S(1, n-3)) < DD(S(2, n-4)) < \cdots < DD(S(\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil))$$

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