Discrete Applied Mathematics 157 (2009) 2773–2777

Contents lists available at ScienceDirect

Discrete Applied Mathematics

journal homepage: www.elsevier.com/locate/dam

On the degree distance of a graph

P. Dankelmann [a,*], I. Gutman [b], S. Mukwembi [a], H.C. Swart [a]

[a] University of KwaZulu-Natal, Durban, South Africa

[b] University of Kragujevac, Kragujevac, Serbia

ARTICLE INFO

Article history:
Received 19 January 2009
Received in revised form 1 April 2009
Accepted 8 April 2009
Available online 17 May 2009

Keywords:
Distance
Degree distance
Diameter

ABSTRACT

If G is a connected graph with vertex set V, then the degree distance of G, $D'(G)$, is defined as $\sum_{\{u,v\}\subseteq V}(\deg u + \deg v)\, d(u, v)$, where $\deg w$ is the degree of vertex w, and $d(u, v)$ denotes the distance between u and v. We prove the asymptotically sharp upper bound $D'(G) \le \frac{1}{4} nd(n-d)^2 + O(n^{7/2})$ for graphs of order n and diameter d. As a corollary we obtain the bound $D'(G) \le \frac{1}{27} n^4 + O(n^{7/2})$ for graphs of order n. This essentially proves a conjecture by Tomescu [I. Tomescu, Some extremal properties of the degree distance of a graph, Discrete Appl. Math. (98) (1999) 159– 163].

1. Introduction

In this paper we are concerned with an invariant of connected graphs called the *degree distance*. Let G be a connected graph of order n and $V(G)$ its vertex set. We denote the degree of a vertex $w \in V(G)$ by $\deg w$ and the distance between vertices $v \in V(G)$ and $u \in V(G)$ by $d(v, u)$. Then the degree distance of G is defined as

$$D'(G) = \sum_{\{u,v\}\subseteq V(G)} (\deg u + \deg v) d(u, v).$$

The degree distance seems to have been considered first by Dobrynin and Kochetova [6] and practically at the same time by Gutman [7], who used a different name for it (see below). In the mathematical literature $D'(G)$ was investigated by Tomescu [20], Tomescu [21] and Bucicovschi and Cioabă [2]. However, somewhat earlier, the same quantity was encountered in connection with certain chemical applications.

In 1989 H.P. Schultz put forward a so-called "*molecular topological index*", *MTI*, defined as follows [15]: Let G be a (molecular) graph of order n whose vertices are labelled by $v_1, v_2, \ldots, v_n$. Then

$$MTI = MTI(G) = \sum_{i=1}^{n} [\mathbf{v}(\mathbf{A} + \mathbf{D})]_i$$

where $\mathbf{A}$ and $\mathbf{D} = \|d(v_i, v_j)\|$ are, respectively, the adjacency and distance matrices of G, and where $\mathbf{v} = (\deg v_1, \deg v_2, \ldots, \deg v_n)$. For chemical research on *MTI* see [12–16,18,19,17].

It is easy to show that [7]

$$MTI(G) = M(G) + S(G) \qquad (1)$$

where

$$M(G) = \sum_{i=1}^{n} (\deg v_i)^2$$

* Corresponding author.
E-mail address: dankelma@ukzn.ac.za (P. Dankelmann).

0166-218X/$ – see front matter
doi:10.1016/j.dam.2009.04.006

and

$$S(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}(\deg v_i + \deg v_j)\, d(v_i, v_j).$$

The first term on the right-hand side of (1) has received much attention in the chemical literature, where it is known as the "*Zagreb index*" (see [8] and the references cited therein). For mathematical research on $M(G)$ see [4]. $M(G)$ is related in a simple manner to the variance of the vertex degrees of G (see [1]).

The second term on the right-hand side of (1) is the degree distance of G. In the chemical literature the name "*Schultz index*" was proposed for it in [7], and was eventually accepted by most other authors (see, for instance, [5,22]), including the members of the Schultz family (see [17]).

The relation between the degree distance and the Wiener index was investigated in [5,7,9–11,14]. Recall that the Wiener index of a graph G is defined as

$$W(G) = \sum_{\{u,v\}\subseteq V} d(u, v).$$

One such relation is provided by the following identity (see [7,11]): If T is a tree of order n, then

$$D'(T) = 4\,W(T) - n(n-1).$$

2. An upper bound on the degree distance

In [20], Tomescu proved that the degree distance of a connected graph of order n cannot exceed $\frac{2}{27}n^4 + O(n^3)$. He conjectured that this bound can be improved to $\frac{1}{27}n^4 + O(n^3)$, and he constructed a family of graphs that attain this bound. In [2], Bucicovschi and Cioabă comment that "this conjecture seems difficult at present time". Our main result implies this conjecture, except for a weakening of the $O(n^3)$ error term to $O(n^{7/2})$.

We will make use of the following lemma (see [3]).

Lemma 1. *Let v be a vertex of eccentricity d, and let k be a real, $k > 2$. Let A_k be the number of distance layers of v that contain only vertices of degree less than k. Then*

$$A_k \geq (d+1)\frac{k+1}{k-2} - \frac{3n}{k-2}.$$

Theorem 1. *Let G be a connected graph of order n and diameter d. Then*

$$D'(G) \leq \frac{1}{4}nd(n-d)^2 + O(n^{7/2}).$$

Proof. Let $P = u_0, u_1, \ldots, u_d$ be a diametral path. We will find it convenient to identify P with the set of its vertices. Let $\mathcal{C}$ be a maximum set of disjoint pairs of vertices in $V - P$ at distance at least 3. If $\{a, b\} \in \mathcal{C}$, then we say that a and b are partners. Finally let $M \subset V$ be the set of vertices that are neither in a pair of vertices in $\mathcal{C}$ nor on P. Let $m = |M|$ and $|\mathcal{C}| = c$.

For a vertex v of G define $D(v) = \sum_{w\in V} d(v, w)$ and $D'(v) = \deg v D(v)$. We will make use of the following equation, observed by Tomescu [20].

$$D'(G) = \sum_{v\in V} D'(v). \tag{2}$$

Claim 1: $\sum_{u\in P} D'(u) = O(n^{7/2})$.

Partition the set P into two sets P_1 and P_2, where $P_1 = \{v \in P \mid \deg v \leq \sqrt{n}\}$, and $P_2 = P - P_1$. Substituting $\sqrt{n}$ for k and u_0 for v in Lemma 1 yields that $|P_1| \geq (d+1)\frac{k+1}{k-2} - \frac{3n}{k-2} = d - O(\sqrt{n})$, and thus $|P_2| = O(\sqrt{n})$. Hence

$$\sum_{u\in P} D'(u) = \sum_{u\in P_1} \deg u\, D(u) + \sum_{u\in P_2} \deg u\, D(u) \leq |P_1| n^2\sqrt{n} + |P_2| nn^2 = O(n^{7/2}). \tag{3}$$

Case 1: $m \leq 1$.

We first show that, for all $\{a, b\} \in \mathcal{C}$,

$$D'(a) + D'(b) \leq \frac{1}{2}nd(n-d) + O(n^2). \tag{4}$$

Since a has $\deg a$ vertices at distance 1, and no vertex has distance greater than d from a, $D(a) \leq \deg a + 2 + 3 + \cdots + (d-1) + (n - \deg a - d + 1)d = d(n - \frac{1}{2}d - \deg a) + O(n)$, and thus $D'(a) \leq d \deg a(n - \frac{1}{2}d - \deg a) + O(n^2)$. (We note that throughout the proof we will replace small additive constants by $O(1)$ in order to keep the calculations simple. These $O(1)$ terms will lead to higher order error terms $O(n)$, $O(n^2)$, etc.) Similarly we have $D'(b) \leq d \deg b(n - \frac{1}{2}d - \deg b) + O(n^2)$, and thus

$$\begin{aligned} D'(a)+D'(b) &\le d\left(\deg a\left(n-\frac{1}{2}d-\deg a\right)+\deg b\left(n-\frac{1}{2}d-\deg b\right)\right)+O(n^2),\\ &= d\Big(f(\deg a)+f(\deg b)\Big)+O(n^2), \end{aligned}$$

where f is the real function defined by $f(x)=x(n-\frac{1}{2}d-x)$. Let $K=\deg a+\deg b$. Elementary calculations show that $f(x_1)+f(x_2)$ is maximised, subject to $x_1+x_2=K$, if $x_1=x_2=\frac{1}{2}K$. Hence

$$D'(a)+D'(b)\le Kd\left(n-\frac{1}{2}d-\frac{1}{2}K\right)+O(n^2). \tag{5}$$

Now $\deg a+\deg b\le n-d+5$ since a and b have no common neighbours, and each of a and b is adjacent to at most 3 vertices on P. Hence $K\le n-d+O(1)$. Since the right-hand side of (5) is increasing for $K\le n-\frac{1}{2}d$, we obtain (4) by substituting $K=n-d+O(1)$.

We now bound $D'(G)$. By $m\le 1$ and $D'(v)\le n^3$ for all $v\in M$, we have $\sum_{v\in M}D'(v)\le n^3$. Hence

$$\begin{aligned} D'(G) &= \sum_{\{a,b\}\in\mathcal{C}}(D'(a)+D'(b))+\sum_{v\in M}D'(v)+\sum_{x\in P}D'(x)\\ &\le \frac{1}{2}cnd(n-d)+O(n^{7/2}). \end{aligned}$$

Now $n=2c+d+1+m$, so $c=\frac{1}{2}(n-d)+O(1)$. Substituting this now yields the theorem for Case 1.

Case 2: $m\ge 2$.

Fix a vertex $v\in M$. From each pair $\{a,b\}\in\mathcal{C}$ choose the vertex closer to v, or if $d(v,a)=d(v,b)$ choose one of the vertices arbitrarily, and let A be the set of vertices thus chosen, and let B be the set of partners of the vertices in A. So $|A|=|B|=c$. Let A_1 (B_1) be the set of vertices x in A (B) whose partner is at distance at most 9 from x, and let $c_1=|A_1|=|B_1|$.

Claim 2: $d_G(x,y)\le 8$ for all $x,y\in A\cup M$.

By the maximality of $\mathcal{C}$, the distance between any two vertices of M is at most 2. We show that $d(v,a)\le 4$ for each $a\in A$. Suppose to the contrary that there exists an $a\in A$ with $d(v,a)\ge 5$. Let $b\in V$ be the partner of a. Then also $d(v,b)\ge 5$. Choose a vertex $v'\in M-\{v\}$. By $d(v,v')\le 2$, we get $d(a,v')\ge 3$ and $d(b,v')\ge 3$. Hence removing the pair $\{a,b\}$ from $\mathcal{C}$ and replacing it by the pairs $\{a,v\}$ and $\{b,v'\}$, we obtain a larger number of pairs at distance at least 3, contradicting the maximality of $\mathcal{C}$. Hence we have $d(v,a)\le 4$ for all $a\in A$. Now let $x,y\in A\cup M$. From the above it follows that $d(x,v)\le 4$ and $d(v,y)\le 4$, and thus $d(x,y)\le 8$.

Claim 3: Let $\{a,b\}\in\mathcal{C}$. If $d(a,b)\ge 10$ then

$$D'(a)+D'(b)\le d\left(\left(n-\frac{1}{2}d-m-c\right)(m+c)+\left(n-\frac{1}{2}d-c\right)c-(m+c)c_1\right)+O(n^2).$$

We may assume that $a\in A$. Consider a first. Since all vertices in $A\cup M$ are within distance 8 of a, and further c_1 vertices of B_1 are within distance 17 of a, we have

$$\begin{aligned} D(a) &\le 8|A\cup M|+17|B_1|+18+19+\cdots+(d-1)+(n-d-m-c-c_1)d+O(n)\\ &= d\left(n-\frac{1}{2}d-m-c-c_1\right)+O(n). \end{aligned}$$

Vertex a has at most c neighbours in $A\cup B$ since a cannot be adjacent to a vertex in $A\cup B$ and its partner. Also a has at most 3 neighbours on P, and at most m neighbours in M. Hence $\deg a\le m+c+O(1)$, and so

$$D'(a)\le (m+c)d\left(n-\frac{1}{2}d-m-c-c_1\right)+O(n^2).$$

Now consider b.

$$\begin{aligned} D'(b) &\le \deg b(\deg b+2+3+\cdots+d+(n-d-\deg b)d)+O(n^2)\\ &= \deg b\left(n-\frac{1}{2}d-\deg b\right)d+O(n^2). \end{aligned}$$

Define the real function f by $f(x)=xd(n-\frac{1}{2}d-x)$. Then $f'(x)=d(n-\frac{1}{2}d-2x)$, and so $f(x)$ is increasing for $x\le\frac{1}{2}n-\frac{1}{4}d$. Now b has at most c neighbours in $A\cup B$, at most 3 neighbours in P, and no neighbours in M since $d(a,b)\ge 10$. Hence $\deg b\le c+3$. Since $\frac{1}{2}n-\frac{1}{4}d=c+\frac{1}{2}m+\frac{1}{4}d+\frac{1}{2}\ge c+2$, we have

$$D'(b)\le\max(f(c+2),f(c+3))+O(n^2)=c\left(n-\frac{1}{2}d-c\right)d+O(n^2).$$

Adding the two bounds yields Claim 3.

CLAIM 4: Let $\{a, b\} \in \mathcal{C}$. If $d(a, b) \le 9$ then

$$D'(a) + D'(b) \le d(n-d)\left(n - \frac{1}{2}d - c - m - c_1\right) + O(n^2).$$

We may assume that $a \in A$. By Claim 2, each of the $c + m$ vertices in $A \cup M$ is within distance 8 of a, and each vertex in B_1 is within distance 9 of some vertex of A. Hence the distance between any two vertices of $A \cup M \cup B_1$ does not exceed 26. Hence, for each $x \in \{a, b\}$,

$$\begin{aligned} D(x) &\le (c + m + c_1)26 + 27 + 28 + \cdots + (d-1) + (n - d - c - m - c_1)d + O(n) \\ &= d\left(n - \frac{1}{2}d - c - m - c_1\right) + O(n). \end{aligned}$$

Now a and b have no common neighbour, and at most 3 neighbours each on P, so $\deg a + \deg b \le n - d + O(1)$. Hence

$$\begin{aligned} D'(a) + D'(b) &\le (\deg a + \deg b)\left(d\left(n - \frac{1}{2}d - c - m - c_1\right) + O(n)\right) \\ &\le d(n-d)\left(n - \frac{1}{2}d - c - m - c_1\right) + O(n^2), \end{aligned}$$

as desired.

CLAIM 5: $D'(u) \le (n - d - c)d(n - \frac{1}{2}d - c - c_1 - m) + O(n^2)$ for all $u \in M$.

Each of the $c + m$ vertices in $A \cup M$ is within distance 8 of each vertex $u \in M$, the c_1 vertices in B_1 are within distance 17 of u. Since all vertices in $A \cup M \cup B_1$ are within distance 17 of u, the sum of the distances from u to the remaining vertices is at most $18 + 19 + \cdots + (d-1) + (n - c - c_1 - m - d + 18)d$. So

$$\begin{aligned} D(u) &\le (c + m)8 + 17c_1 + 18 + 19 + \cdots + (d-1) + (n - d - c - c_1 - m)d + O(n) \\ &= d\left(n - \frac{1}{2}d - c - c_1 - m\right) + O(n). \end{aligned}$$

Now u is adjacent to at most 3 vertices of P, and to at most c vertices of $A \cup B$. Hence $\deg u \le n - d - c + O(1)$, and thus

$$D'(u) \le (n - d - c)d\left(n - \frac{1}{2}d - c - c_1 - m\right) + O(n^2).$$

From Claims 3 and 4 we obtain

$$\begin{aligned} D'(G) &= \sum_{\{a,b\}\in\mathcal{C}} (D'(a) + D'(b)) + \sum_{v\in M} D'(v) + \sum_{x\in P} D'(x) \\ &\le (c - c_1)d\left(\left(n - \frac{1}{2}d - m - c\right)(m + c) + \left(n - \frac{1}{2}d - c\right)c - (m + c)c_1\right) \\ &\quad + c_1 d(n-d)\left(n - \frac{1}{2}d - c - c_1 - m\right) + m(n - d - c)d\left(n - \frac{1}{2}d - c - c_1 - m\right) + O(n^{7/2}). \end{aligned}$$

Since $c - c_1 \ge 0$ and $n - \frac{1}{2}d - m - c \ge 0$, the right-hand side of the last inequality is at most

$$\begin{aligned} &\left\{(c - c_1)d\left(\left(n - \frac{1}{2}d - m - c\right)(m + 1 + c) + \left(n - \frac{1}{2}d - c\right)c - (m + c)c_1\right)\right. \\ &\quad \left.+\ c_1 d(n-d)\left(n - \frac{1}{2}d - c - c_1 - m\right)\right\} + m(n - d - c)d\left(n - \frac{1}{2}d - c - c_1 - m\right) + O(n^{7/2}). \end{aligned}$$

Let $f(n, d, c, c_1)$ be the above expression, without the $O(n^{7/2})$ term. Thus
$D'(G) \le f(n, d, c, c_1) + O(n^{7/2})$. By first replacing m in the expression of f in curly brackets by $n - 2c - d - 1$ and then differentiating we get

$$\frac{\mathrm{d}f}{\mathrm{d}c_1} = d\left(-(2c + 2)c_1 - 2c\left(n - d - \frac{3}{2}c - 1\right) - m(n - d - c)\right) < 0.$$

Hence f is decreasing with respect to c_1, and so

$$\begin{aligned} D'(G) &\le f(n, d, c, 0) + O(n^{7/2}) \\ &= cd\left(\left(n - \frac{1}{2}d - m - c\right)(m + 1 + c) + \left(n - \frac{1}{2}d - c\right)c\right) + m(n - d - c)d\left(n - \frac{1}{2}d - c - m\right) + O(n^{7/2}) \end{aligned}$$

$$= d\left\{\left(c+\frac{1}{2}d\right)(n-d-c)^2 + c^2\left(n-\frac{1}{2}d-c\right)\right\} + O(n^{7/2}).$$

Denote the term in curly brackets by $g(c)$. Differentiating and simplifying yield

$$g'(c) = (n-2d)(n-d-2c),$$

so g is maximised for $c = \frac{1}{2}(n-d)$. Substituting back yields, after simplification, the theorem. □

To see that this bound is best possible, except for the $O(n^{7/2})$ error term, consider the graph $G_{n,d}$ obtained from two disjoint complete graphs H_1 and H_2 of orders $\lceil \frac{n-d+1}{2} \rceil$ and $\lfloor \frac{n-d+1}{2} \rfloor$, respectively, and a path P on $d-1$ vertices, by joining one of the two end vertices of P to all vertices in H_1, and the other end vertex of P to all vertices in H_2. It is easy to verify that

$$D'(G_{n,d}) = \frac{1}{4}nd(n-d)^2 + O(n^3).$$

A simple maximisation of the bound in Theorem 1 yields the following.

Corollary 1. *Let G be a connected graph of order n. Then*

$$D'(G) \le \frac{1}{27}n^4 + O(n^{7/2}).$$

As pointed out by Tomescu [20], the graph $G_{n,n/3}$ shows that, apart from the $O(n^{7/2})$ term, this bound is best possible.

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