

DEGREE DISTANCE AND MINIMUM DEGREE

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Abstract

Let G be a finite connected graph of order n , minimum degree δ and diameter d . The degree distance $D'(G)$ of G is defined as $\sum_{\{u,v\} \subseteq V(G)} (\deg u + \deg v) d(u, v)$, where $\deg w$ is the degree of vertex w and $d(u, v)$ denotes the distance between u and v . In this paper, we find an asymptotically sharp upper bound on the degree distance in terms of order, minimum degree and diameter. In particular, we prove that

$$D'(G) \leq \frac{1}{4} dn \left(n - \frac{d}{3}(\delta + 1) \right)^2 + O(n^3).$$

As a corollary, we obtain the bound $D'(G) \leq n^4/(9(\delta + 1)) + O(n^3)$ for a graph G of order n and minimum degree δ . This result, apart from improving on a result of Dankelmann *et al.* [‘On the degree distance of a graph’, *Discrete Appl. Math.* **157** (2009), 2773–2777] for graphs of given order and minimum degree, completely settles a conjecture of Tomescu [‘Some extremal properties of the degree distance of a graph’, *Discrete Appl. Math.* **98** (1999), 159–163].

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1. Introduction

Let G be a connected graph with vertex set V and edge set E . The *degree distance* $D'(G)$ of 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 in G .

The degree distance, a Schultz-type molecular topological index and a variant of the well-known and much studied Wiener index, seems to have been considered first by Dobrynin and Kochetova [5] in 1994 and practically at the same time by

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Gutman [6], who introduced it as a kind of a vertex-valency-weighted sum of the distances between all pairs of vertices in a graph. Gutman revealed that in the case of acyclic structures, the index is closely related to the Wiener index and reflects precisely the same structural features of a molecular graph as the Wiener index does.

Before 1994, the degree distance was encountered in connection with certain chemical applications [11, 12]. After 1994, the degree distance was investigated by several authors, for instance, Bucicovschi and Cioabă [1], Dankelmann *et al.* [3], Ilić *et al.* [8], Tomescu [13], and Tomescu [14]. In this paper we are concerned with upper bounds on the degree distance. Sharp upper and lower bounds on the degree distance for trees of given order have been completely determined (see, for example the recent survey in [4]). For general graphs, Dobrynin and Kochetova [5] conjectured that the largest degree distance of all connected graphs of order n equals $n^4/32 + O(n^3)$. This was refuted by Tomescu [13], who showed that graphs consisting of two cliques of order approximately $n/3$ joined by a path on approximately $n/3$ vertices, have degree distance $n^4/27 + O(n^3)$. He then made the following attractive conjecture.

CONJECTURE 1.1 [13]. *Let G be a connected graph of order n . Then*

$$D'(G) \leq \frac{n^4}{27} + O(n^3).$$

Nine years after the announcement of this conjecture, Bucicovschi and Cioabă [1] commented that Tomescu's conjecture 'seems difficult at present time'. In the following year, Dankelmann *et al.* [3] considered this problem, and though they came close to proving the conjecture, their proof was unable to deal with the $O(n^3)$ error term. They proved the following bound.

THEOREM 1.2 [3]. *If G is a connected graph of order n , then*

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

Recently the method developed in [3] was improved by M. J. Morgan, S. Mukwembi and H. C. Swart ('On a conjecture by Tomescu', submitted for publication), leading to a complete solution of Tomescu's conjecture.

Since the degree distance can be considered as a weighted version of the Wiener index, comparisons between the two indices are inevitable. For trees of given order, these two parameters actually determine each other: Klein *et al.* [9] and Gutman [6] showed that, for every tree T of order n , $D'(T) = 4W(T) - n(n-1)$, where $W(G) = \sum_{\{u,v\} \subseteq V} d(u,v)$ is the Wiener index of G . Since its introduction in the late 1940s by the chemist Harold Wiener in an attempt to analyse the chemical properties of paraffins (alkanes) [15], the mathematical properties of the Wiener index have been studied by several authors. One of the oldest results on upper bounds of this quantity is that amongst all connected graphs of given order, the path has the maximum Wiener index. For graphs of given minimum degree, this result was improved independently

by several authors, among them Kouider and Winkler [10] and Dankelmann and Entringer [2], who proved the following bound.

THEOREM 1.3 [2, 10]. *Let G be a graph of order n and minimum degree δ . Then*

$$W(G) \leq \frac{n^3}{2(\delta + 1)} + O(n^2),$$

and this bound is best possible.

In light of Theorem 1.3 and the fact that the degree distance can be considered as a weighted version of the Wiener index, it is natural to look for a best upper bound on the degree distance of a connected graph of given order and minimum degree. To date, no work answering this question has been reported. The purpose of this paper is to contribute towards filling this gap. Our method is an improvement of the method initiated in [3]. We obtain an asymptotically sharp upper bound on the degree distance of a graph of given order and minimum degree. Our result, apart from being a strengthening of Theorem 1.2 and a theorem by Morgan *et al.* (see above), confirms and improves on Tomescu's conjecture (Conjecture 1.1) if minimum degree is prescribed.

The notation that we use is as follows. For a vertex v of G , we denote by $D(v)$ the total distance or the status of v . That is, $D(v) = \sum_{x \in V(G)} d(v, x)$. The quantity $\deg v D(v)$ is denoted by $D'(v)$. We denote the open neighbourhood of v by $N(v)$, that is, $N(v) = \{x \in V(G) \mid d(x, v) = 1\}$. The closed neighbourhood of v in G , that is, $N(v) \cup \{v\}$, is denoted by $N[v]$. Here and in the following, we assume that the minimum degree δ is fixed.

The useful equation

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

was first observed by Tomescu [13].

2. Results

We begin by presenting a very simple but handy observation.

FACT 2.1. *Let G be a connected graph of order n , diameter d and minimum degree δ . If $v \in V(G)$, then $d \leq (3/(\delta + 1))(n - \deg v) + 6$.*

PROOF. Assume that $v \in V(G)$ and let $P = v_0, v_1, \dots, v_d$ be a diametric path of G . Let

$$S := \left\{ v_{3i+1} \mid i = 0, 1, \dots, \left\lfloor \frac{d-1}{3} \right\rfloor \right\}.$$

For each $x \in S$, choose any δ neighbours $x_1, x_2, \dots, x_\delta$ of x and denote the set $\{x, x_1, x_2, \dots, x_\delta\}$ by $M[x]$. Let $M = \bigcup_{x \in S} M[x]$. Then

$$|M| = (\delta + 1) \left(\left\lfloor \frac{d-1}{3} \right\rfloor + 1 \right).$$

Note that by construction of S , $N[v] \cap M$ has at most $2\delta + 1$ vertices. Hence

$$\begin{aligned} n &\geq |M| + |N[v]| - |M \cap N[v]| \\ &\geq (\delta + 1) \left(\left\lfloor \frac{d-1}{3} \right\rfloor + 1 \right) + \deg v + 1 - (2\delta + 1) \\ &\geq (\delta + 1) \frac{d}{3} + \deg v - 2\delta, \end{aligned}$$

and rearranging the terms completes the proof. □

We will often use the following simple and straightforward result or a variation on it.

PROPOSITION 2.2. *Let G be a connected graph of order n , diameter d and fixed minimum degree δ . If $v \in V(G)$, then*

$$D(v) \leq d \left(n - \frac{d}{6}(\delta + 1) - \deg v \right) + O(n).$$

PROOF. Denote the eccentricity of v by e . For all $i = 1, 2, \dots, e$, let $N_i := \{x \in V(G) \mid d(v, x) = i\}$ and $|N_i| = k_i$. Note that if $x \in N_i$, $i = 2, 3, \dots, e - 1$, then $N[x] \subseteq N_{i-1} \cup N_i \cup N_{i+1}$ so that

$$k_{i-1} + k_i + k_{i+1} \geq \delta + 1.$$

Clearly,

$$D(v) = 1k_1 + 2k_2 + \dots + ek_e. \tag{2.1}$$

We look at three cases separately.

Case 1: $e \equiv 0 \pmod{3}$. Subject to

$$k_1 = \deg v, \quad k_i \geq 1 \quad \text{for } i = 2, 3, \dots, e,$$

and

$$k_2 + k_3 + k_4 \geq \delta + 1, \quad k_5 + k_6 + k_7 \geq \delta + 1, \dots, \quad k_{e-4} + k_{e-3} + k_{e-2} \geq \delta + 1,$$

(2.1) is maximised for

$$\begin{aligned} k_1 &= \deg v, \quad k_2 = 1 = k_3, \quad k_4 = \delta - 1, \quad k_5 = 1 = k_6, \\ k_7 &= \delta - 1, \dots, \quad k_{e-4} = 1 = k_{e-3}, \quad k_{e-2} = \delta - 1, \quad k_{e-1} = 1 \end{aligned}$$

and

$$k_e = n - \deg v - \frac{1}{3}(e - 3)(\delta + 1) - 1 - 1.$$

This gives

$$\begin{aligned} D(v) &\leq \deg v + 2 + 3 + 4(\delta - 1) + 5 + 6 + 7(\delta - 1) \\ &\quad + \dots + (e - 4) + (e - 3) + (e - 2)(\delta - 1) + (e - 1) \\ &\quad + e \left(n - \deg v - \frac{1}{3}(e - 3)(\delta + 1) - 2 \right) \\ &= e \left(n - \frac{e}{6}(\delta + 1) - \deg v \right) + O(n). \end{aligned}$$

If $e = d - c$, where $c \in \{0, 1, \dots, 5\}$, then

$$\begin{aligned} D(v) &\leq (d - c)\left(n - \frac{d - c}{6}(\delta + 1) - \deg v\right) + O(n) \\ &= d\left(n - \frac{d}{6}(\delta + 1) - \deg v\right) + O(n), \end{aligned}$$

as desired. So assume that $e \leq d - 6$. The function

$$f(e) = e\left(n - \frac{e}{6}(\delta + 1) - \deg v\right)$$

is increasing in e for all $e \leq (3/(\delta + 1))(n - \deg v)$. Note from Fact 2.1 that $d - 6 \leq (3/(\delta + 1))(n - \deg v)$. Hence

$$D(v) \leq f(d - 6) = d\left(n - \frac{d}{6}(\delta + 1) - \deg v\right) + O(n),$$

and the proposition is proved for this case. This completes Case 1.

The other cases, $e \equiv 1 \pmod{3}$ and $e \equiv 2 \pmod{3}$, are treated similarly. □

THEOREM 2.3. *Let G be a connected graph of order n , diameter d and fixed minimum degree δ . Then*

$$D'(G) \leq \frac{1}{4} dn\left(n - \frac{d}{3}(\delta + 1)\right)^2 + O(n^3).$$

Moreover, this inequality is asymptotically tight.

PROOF. Let $P : v_0, v_1, \dots, v_d$ be a diametric path of G and let $S \subset V(P)$ be the set

$$S := \left\{v_{3i+1} : i = 0, 1, 2, \dots, \left\lfloor \frac{d-1}{3} \right\rfloor\right\}.$$

For each $v \in S$, choose any δ neighbours $u_1, u_2, \dots, u_\delta$ of v and denote the set $\{v, u_1, u_2, \dots, u_\delta\}$ by $M[v]$. Let $M = \bigcup_{v \in S} M[v]$. Then

$$|M| = (\delta + 1)\left(\left\lfloor \frac{d-1}{3} \right\rfloor + 1\right).$$

CLAIM 1.

$$\sum_{u \in M} D'(u) \leq O(n^3).$$

PROOF OF CLAIM 1. Let $S_1 \subset S$ be the set $S_1 = \{v_j \in S : j \equiv 1 \pmod{6}\}$. Let $S_2 = S - S_1$. Then for each $u, v \in S_1$, $u \neq v$, we have $M[u] \cap M[v] = \emptyset$ and the neighbourhoods of $M[u]$ and $M[v]$ are also disjoint. Write the elements of S_1 as $S_1 = \{w_1, w_2, \dots, w_{|S_1|}\}$. For each $w_j \in S_1$, let $M[w_j] = \{w_j, u_1^j, u_2^j, \dots, u_\delta^j\}$, where $u_1^j, u_2^j, \dots, u_\delta^j$ are neighbours of w_j . Then

$$n \geq (\deg w_1 + 1) + (\deg w_2 + 1) + \dots + (\deg w_{|S_1|} + 1)$$

and, for $t = 1, 2, \dots, \delta$,

$$n \geq (\deg u_t^1 + 1) + (\deg u_t^2 + 1) + \dots + (\deg u_t^{|S_1|} + 1).$$

Summing yields

$$(\delta + 1)n \geq \sum_{x \in M[S_1]} \deg x + (\delta + 1)|S_1|,$$

where $M[S_1] = \sum_{u \in S_1} M[u]$.

Similarly,

$$(\delta + 1)n \geq \sum_{x \in M[S_2]} \deg x + (\delta + 1)|S_2|.$$

Thus

$$\begin{aligned} 2(\delta + 1)n &\geq \sum_{x \in M[S_1]} \deg x + \sum_{x \in M[S_2]} \deg x + (\delta + 1)|S| \\ &= \sum_{x \in M[S_1]} \deg x + \sum_{x \in M[S_2]} \deg x + (\delta + 1)\left(\left\lfloor \frac{d-1}{3} \right\rfloor + 1\right). \end{aligned}$$

Hence

$$\begin{aligned} \sum_{x \in M[S_1]} \deg x + \sum_{x \in M[S_2]} \deg x &\leq 2(\delta + 1)n - (\delta + 1)\left(\left\lfloor \frac{d-1}{3} \right\rfloor + 1\right) \\ &= (\delta + 1)\left(2n - \left\lfloor \frac{d-1}{3} \right\rfloor - 1\right). \end{aligned}$$

Now for $u \in V(G)$, $D(u) \leq (n - 1)d \leq (n - 1)^2$. It follows that

$$\begin{aligned} \sum_{v \in M} D'(v) &= \sum_{v \in M} \deg v D(v) \\ &= \sum_{v \in M[S_1]} \deg v D(v) + \sum_{v \in M[S_2]} \deg v D(v) \\ &\leq (n - 1)^2 \left(\sum_{v \in M[S_1]} \deg v + \sum_{v \in M[S_2]} \deg v \right) \\ &\leq (n - 1)^2 (\delta + 1) \left(2n - \left\lfloor \frac{d-1}{3} \right\rfloor - 1 \right) \\ &= O(n^3), \end{aligned}$$

as required and so Claim 1 is proved.

Let C be a maximum set of disjoint pairs of vertices from $V - M$ which lie at a distance at least 3, that is, if $\{a, b\} \in C$, then $d(a, b) \geq 3$. If $\{a, b\} \in C$ we say a and b are partners. Finally, let K be the remaining vertices of G , that is, $K = V - M - \{x : x \in \{a, b\} \in C\}$. Let $|K| = k$, and $|C| = c$. Then

$$n = (\delta + 1)\left(\left\lfloor \frac{d-1}{3} \right\rfloor + 1\right) + 2c + k. \tag{2.2}$$

FACT 2.4. Let $\{a, b\} \in C$. Then $\deg a + \deg b \leq n - (d/3)(\delta + 1) + O(1)$.

PROOF OF FACT 2.4. Note that $N[a] \cap N[b] = \emptyset$, since $d(a, b) \geq 3$. Also, each of the two vertices can be adjacent to at most $2\delta + 1$ vertices on M . Thus,

$$\begin{aligned} n &\geq \deg a + 1 + \deg b + 1 + |M| - 2(2\delta + 1) \\ &= \deg a + \deg b + (\delta + 1) \left(\left\lfloor \frac{d-1}{3} \right\rfloor + 1 \right) - 4\delta, \end{aligned}$$

and rearranging the terms completes the proof of Fact 2.4.

Now consider two cases.

Case 1: $k \leq 1$. For $x \in K$, $D(x) \leq (n-1)^2$, so $D'(x) \leq (n-1)^3$. Thus $\sum_{x \in K} D'(x) = O(n^3)$.

CLAIM 2. If $\{a, b\} \in C$, then

$$D'(a) + D'(b) \leq \frac{1}{2} dn \left(n - \frac{d}{3}(\delta + 1) \right) + O(n^2).$$

PROOF OF CLAIM 2. By Proposition 2.2,

$$D(a) \leq d \left(n - \frac{d}{6}(\delta + 1) - \deg a \right) + O(n).$$

It follows that

$$D'(a) \leq \deg a \left(d \left(n - \frac{d}{6}(\delta + 1) - \deg a \right) \right) + O(n^2).$$

Similarly,

$$D'(b) \leq \deg b \left(d \left(n - \frac{d}{6}(\delta + 1) - \deg b \right) \right) + O(n^2).$$

Thus,

$$\begin{aligned} D'(a) + D'(b) &\leq \deg a \left(d \left(n - \frac{d}{6}(\delta + 1) - \deg a \right) \right) \\ &\quad + \deg b \left(d \left(n - \frac{d}{6}(\delta + 1) - \deg b \right) \right) + O(n^2) \\ &= d \left((\deg a + \deg b) \left(n - \frac{d}{6}(\delta + 1) \right) - ((\deg a)^2 + (\deg b)^2) \right) + O(n^2) \\ &\leq d \left((\deg a + \deg b) \left(n - \frac{d}{6}(\delta + 1) \right) - \frac{1}{2}(\deg a + \deg b)^2 \right) + O(n^2). \end{aligned}$$

Denote $\deg a + \deg b$ by x and let

$$f(x) = d \left(x \left(n - \frac{d}{6}(\delta + 1) \right) - \frac{1}{2}x^2 \right).$$

Then by Fact 2.4, $x \leq n - (d/3)(\delta + 1) + O(1)$. A simple differentiation shows that f is increasing for all $x \leq n - (d/6)(\delta + 1)$. Hence f attains its maximum for $x = n - (d/3)(\delta + 1) + O(1)$, to give

$$\begin{aligned} D'(a) + D'(b) &\leq f\left(n - \frac{d}{3}(\delta + 1) + O(1)\right) \\ &= \frac{1}{2} dn\left(n - \frac{d}{3}(\delta + 1)\right) + O(n^2), \end{aligned}$$

and Claim 2 is proved.

From (2.2),

$$c = \frac{1}{2}\left(n - (\delta + 1)\left(\left\lfloor \frac{d-1}{3} \right\rfloor + 1\right) - k\right).$$

Hence, since $k \leq 1$,

$$c = \frac{1}{2}\left(n - \frac{d}{3}(\delta + 1)\right) + O(1).$$

This, in conjunction with Claim 2, yields

$$\begin{aligned} \sum_{\{a,b\} \in C} (D'(a) + D'(b)) &\leq c\left(\frac{1}{2} dn\left(n - \frac{d}{3}(\delta + 1)\right) + O(n^2)\right) \\ &= \left(\frac{1}{2}\left(n - \frac{d}{3}(\delta + 1)\right) + O(1)\right)\left(\frac{1}{2} dn\left(n - \frac{d}{3}(\delta + 1)\right) + O(n^2)\right) \\ &= \frac{1}{4} dn\left(n - \frac{d}{3}(\delta + 1)\right)^2 + O(n^3). \end{aligned}$$

Hence

$$\begin{aligned} D'(G) &= \sum_{\{a,b\} \in C} (D'(a) + D'(b)) + \sum_{x \in K} D'(x) + \sum_{v \in M} D'(v) \\ &\leq \frac{1}{4} dn\left(n - \frac{d}{3}(\delta + 1)\right)^2 + O(n^3) + O(n^3) + O(n^3), \end{aligned}$$

and so the theorem is proved for Case 1.

Case 2: $k \geq 2$. Now the pairs of vertices in C will be partitioned further. Fix a vertex $x \in K$. For each pair $\{a, b\} \in C$, choose the vertex closer to x ; if $d(a, x) = d(b, x)$ arbitrarily choose one of the vertices. Let A be the set of all these vertices closer to x , and B be the set of partners of these vertices in A , so $|A| = |B| = c$. Furthermore, let $A_1(B_1)$ be the set of vertices $w \in A(B)$ whose partner is at a distance at most 9 from w . Let $c_1 = |A_1| = |B_1|$.

CLAIM 3. For all $u, v \in A \cup K$, $d(u, v) \leq 8$.

PROOF OF CLAIM 3. Since C is a maximum set of pairs of vertices of distance at least 3, any two vertices of K must be at a distance of at most 2. We show that $d(a, x) \leq 4$ for all $a \in A$. Suppose, to the contrary, that there exists a vertex $a \in A$ for which $d(a, x) \geq 5$.

Let b be the partner of a . By definition of A , $d(x, b) \geq 5$. Now consider another vertex $x' \in K$, $x \neq x'$. Since $d(x, x') \leq 2$,

$$5 \leq d(b, x) \leq d(b, x') + d(x, x') \leq d(b, x') + 2,$$

which implies that $d(b, x') \geq 3$. This contradicts the maximality of C since $\{a, b\}$ will be replaced by $\{a, x\}$ and $\{b, x'\}$. Hence $d(a, x) \leq 4$, for each $a \in A$. Thus for $u, v \in A$, $d(u, v) \leq d(u, x) + d(x, v) \leq 8$.

CLAIM 4. For all $x \in K$,

$$D'(x) \leq d\left(n - \frac{d}{3}(\delta + 1) - c\right)\left(n - c - c_1 - k - \frac{d}{6}(\delta + 1)\right) + O(n^2).$$

PROOF OF CLAIM 4. By Claim 3, all $c + k$ vertices in $A \cup K$ lie within a distance of 8 from each vertex $x \in K$. This implies that all the c_1 vertices in B_1 lie within a distance of $9 + 8$ from x . Thus, as in Proposition 2.2,

$$\begin{aligned} D(x) &\leq 8(c + k) + 17c_1 + 18 + 19 + 20(\delta - 1) + 21 + 22 + 23(\delta - 1) \\ &\quad + \dots + d\left(n - c - k - c_1 - \frac{d}{3}(\delta + 1)\right) \\ &= d\left(n - c - c_1 - k - \frac{d}{6}(\delta + 1)\right) + O(n). \end{aligned}$$

In order to find a bound on the degree of x we use a counting argument. Note that x can have at most $2\delta + 1$ neighbours in M . By definition of A and B , x cannot be adjacent to two vertices, w and z , where $w \in A$ is a partner of $z \in B$, since $d(w, z) \geq 3$. Thus, x is adjacent to at most c vertices in $A \cup B$. It follows that

$$\begin{aligned} n &\geq \deg x + |M| - (2\delta + 1) + |A \cup B| - c \\ &= \deg x + (\delta + 1)\left(\left\lfloor \frac{d-1}{3} \right\rfloor + 1\right) - (2\delta + 1) + c \\ &= \deg x + \frac{d}{3}(\delta + 1) + c + O(1). \end{aligned}$$

Hence $\deg x \leq n - (d/3)(\delta + 1) - c + O(1)$. Therefore,

$$\begin{aligned} D'(x) &= \deg x D(x) \\ &\leq d\left(n - \frac{d}{3}(\delta + 1) - c\right)\left(n - c - c_1 - k - \frac{d}{6}(\delta + 1)\right) + O(n^2), \end{aligned}$$

and this proves Claim 4.

We now turn to finding an upper bound on the contribution of the pairs in C to the degree distance. We abuse notation and write $\{a, b\} \in A_1 \cup B_1$ if a and b are partners, that is, $\{a, b\} \in C$, with $a \in A_1$ and $b \in B_1$. Note that

$$\sum_{\{a,b\} \in C} (D'(a) + D'(b)) = \sum_{\{a,b\} \in A_1 \cup B_1} (D'(a) + D'(b)) + \sum_{\{a,b\} \in (A-A_1) \cup (B-B_1)} (D'(a) + D'(b)).$$

We first consider the set $A_1 \cup B_1$.

CLAIM 5. *Let $\{a, b\} \in C$. If $d(a, b) \leq 9$, that is, if $\{a, b\} \in A_1 \cup B_1$, then*

$$D'(a) + D'(b) \leq d\left(n - \frac{d}{3}(\delta + 1)\right)\left(n - c - c_1 - k - \frac{d}{6}(\delta + 1)\right) + O(n^2).$$

PROOF OF CLAIM 5. We first show that any two vertices in $A \cup K \cup B_1$ lie within a distance of 26 from each other. By Claim 3, any two vertices in $A \cup K$ lie within a distance of 8 from each other. Now assume that $b, v \in B_1$, and let a and u be the partners of b and v in A_1 , respectively. Then $d(b, v) \leq d(b, a) + d(a, u) + d(u, v) \leq 9 + 8 + 9 = 26$. Thus any two vertices in B_1 are within a distance of 26 from each other. Now let $a \in A \cup K$ and $b \in B_1$, and let u be the partner of b in $A_1 \subseteq A$. Then $d(a, b) \leq d(a, u) + d(u, b) \leq 8 + 9 < 26$. Hence any two vertices in $A \cup K \cup B_1$ lie within a distance of 26 from each other.

Now let $w \in A_1 \cup B_1$. Since w is in $A \cup K \cup B_1$, all the $c + k + c_1 - 1$ vertices in $A \cup K \cup B_1$ lie within a distance of 26 from w . It follows, as in Proposition 2.2, that

$$\begin{aligned} D(w) &\leq 26(c + k + c_1 - 1) + 27 + 28 + 29(\delta - 1) + 30 + 31 + 32(\delta - 1) + \dots \\ &\quad + d\left(n - c - c_1 - k - \frac{d}{3}(\delta + 1)\right) \\ &= d\left(n - c - c_1 - k - \frac{d}{6}(\delta + 1)\right) + O(n). \end{aligned}$$

Thus, if $\{a, b\}$ is a pair in $A_1 \cup B_1$, then

$$\begin{aligned} D'(a) + D'(b) &\leq \deg a \left(d\left(n - c - c_1 - k - \frac{d}{6}(\delta + 1)\right) + O(n)\right) \\ &\quad + \deg b \left(d\left(n - c - c_1 - k - \frac{d}{6}(\delta + 1)\right) + O(n)\right) \\ &= (\deg a + \deg b) \left(d\left(n - c - c_1 - k - \frac{d}{6}(\delta + 1)\right) + O(n)\right). \end{aligned}$$

By Fact 2.4, $\deg a + \deg b \leq n - (d/3)(\delta + 1) + O(1)$. Therefore,

$$\begin{aligned} D'(a) + D'(b) &\leq \left(n - \frac{d}{3}(\delta + 1) + O(1)\right) \left(d\left(n - c - c_1 - k - \frac{d}{6}(\delta + 1)\right) + O(n)\right) \\ &= d\left(n - \frac{d}{3}(\delta + 1)\right) \left(n - c - c_1 - k - \frac{d}{6}(\delta + 1)\right) + O(n^2), \end{aligned}$$

and Claim 5 is proved.

Now consider pairs $\{a, b\}$ of vertices in C which are not in $A_1 \cup B_1$.

CLAIM 6. *Let $\{a, b\} \in C$. If $d(a, b) \geq 10$, that is, if $\{a, b\} \in (A - A_1) \cup (B - B_1)$, then*

$$\begin{aligned} D'(a) + D'(b) &\leq d(c + k) \left(n - c - c_1 - k - \frac{d}{6}(\delta + 1)\right) \\ &\quad + cd \left(n - \frac{d}{6}(\delta + 1) - c\right) + O(n^2). \end{aligned}$$

PROOF OF CLAIM 6. We consider vertices from $A - A_1$ and from $B - B_1$ separately. Let $a \in A - A_1$. Then as in Claim 5, all the $c + k - 1$ vertices in $A \cup K$ lie at a distance of 8 from a and all the c_1 vertices in B_1 lie within a distance of $9 + 8 = 17$ from a . Thus, as in Proposition 2.2,

$$\begin{aligned} D(a) &\leq 8(c + k - 1) + 17c_1 + 18 + 19 + 20(\delta - 1) + 21 + 22 + 23(\delta - 1) \\ &\quad + \cdots + d\left(n - c - c_1 - k - \frac{d}{3}(\delta + 1)\right) \\ &= d\left(n - c - c_1 - k - \frac{d}{6}(\delta + 1)\right) + O(n). \end{aligned}$$

We now find a bound on the degree of a . By definition of C , a cannot be adjacent to both w and u , where $w \in A$ is a partner of $u \in B$, since $d(w, u) \geq 3$. Hence a is adjacent to at most $c - 1$ vertices in $A \cup B$. Further, a is adjacent to at most $2\delta + 1$ vertices in M and has at most k neighbours in K . Thus,

$$\deg a \leq c - 1 + 2\delta + 1 + k = c + 2\delta + k.$$

It follows that

$$\begin{aligned} D'(a) &= \deg a D(a) \\ &\leq (c + k + 2\delta) \left(d\left(n - c - c_1 - k - \frac{d}{6}(\delta + 1)\right) + O(n^2) \right) \\ &= d(c + k) \left(n - c - c_1 - k - \frac{d}{6}(\delta + 1) \right) + O(n^2). \end{aligned} \tag{2.3}$$

Now let $b \in B - B_1$. By Proposition 2.2,

$$D(b) \leq d\left(n - \frac{d}{6}(\delta + 1) - \deg b\right) + O(n),$$

and so

$$D'(b) \leq \deg b \left(d\left(n - \frac{d}{6}(\delta + 1) - \deg b\right) \right) + O(n^2). \tag{2.4}$$

We first maximise

$$\deg b \left(d\left(n - \frac{d}{6}(\delta + 1) - \deg b\right) \right)$$

with respect to $\deg b$. Let

$$f(x) := x \left(d\left(n - \frac{d}{6}(\delta + 1) - x\right) \right),$$

where $x = \deg b$. A simple differentiation shows that f is increasing for $x \leq \frac{1}{2}(n - (d/6)(\delta + 1))$. We find an upper bound on x , that is, on $\deg b$. Note that as above, b can be adjacent to at most $c - 1$ vertices in $A \cup B$, and has at most $2\delta + 1$ neighbours in M . We show that b cannot be adjacent to any vertex in K . Suppose to the contrary

that $y \in K$ and $d(b, y) = 1$. Recall that a is the partner of b and $d(a, b) \geq 10$. By Claim 3, $d(a, y) \leq 8$. Hence $10 \leq d(a, b) \leq d(b, y) + d(y, a) \leq 1 + 8$, a contradiction. Thus, b cannot be adjacent to any vertex in K . We conclude that

$$\deg b \leq c - 1 + 2\delta + 1 = c + 2\delta.$$

We look at two cases separately. First assume that $\deg b = c + j$, where $j \in \{1, 2, \dots, 2\delta\}$. Then

$$\begin{aligned} f(\deg b) &= f(c + j) \\ &= (c + j) \left(d \left(n - \frac{d}{6}(\delta + 1) - (c + j) \right) \right) \\ &= cd \left(n - \frac{d}{6}(\delta + 1) - c \right) + O(n^2). \end{aligned} \tag{2.5}$$

Second, assume that $\deg b \leq c$. From (2.2), and since $k \geq 2$ and $\lfloor (d-1)/3 \rfloor + 1 \geq d/3$,

$$c = \frac{1}{2} \left(n - (\delta + 1) \left(\left\lfloor \frac{d-1}{3} \right\rfloor + 1 \right) - k \right) \leq \frac{1}{2} \left(n - \frac{d}{3}(\delta + 1) - 2 \right).$$

Notice that

$$\frac{1}{2} \left(n - \frac{d}{3}(\delta + 1) - 2 \right) \leq \frac{1}{2} \left(n - \frac{d}{6}(\delta + 1) \right),$$

and so f is increasing in $[1, c]$. Therefore,

$$f(\deg b) \leq f(c) = cd \left(n - \frac{d}{6}(\delta + 1) - c \right),$$

for this case. Comparing this with (2.5), we get that

$$f(\deg b) \leq cd \left(n - \frac{d}{6}(\delta + 1) - c \right) + O(n^2).$$

Thus, from (2.4),

$$D'(b) \leq cd \left(n - \frac{d}{6}(\delta + 1) - c \right) + O(n^2).$$

Combining this with (2.3),

$$\begin{aligned} D'(a) + D'(b) &\leq d(c + k) \left(n - c - c_1 - k - \frac{d}{6}(\delta + 1) \right) \\ &\quad + cd \left(n - \frac{d}{6}(\delta + 1) - c \right) + O(n^2), \end{aligned}$$

and Claim 6 is proved.

Using Claims 1 and 4–6 we bound $D'(G)$ as follows. Note that

$$\begin{aligned}
 D'(G) &= \sum_{u \in M} D'(u) + \sum_{x \in K} D'(x) + \sum_{\{a,b\} \in C} (D'(a) + D'(b)) \\
 &\leq dk \left(n - \frac{d}{3}(\delta + 1) - c \right) \left(n - c - c_1 - k - \frac{d}{6}(\delta + 1) \right) \\
 &\quad + c_1 \left(d \left(n - \frac{d}{3}(\delta + 1) \right) \left(n - c - c_1 - k - \frac{d}{6}(\delta + 1) \right) \right) \\
 &\quad + (c - c_1) \left(d(c + k) \left(n - c - c_1 - k - \frac{d}{6}(\delta + 1) \right) \right) \\
 &\quad + cd \left(n - \frac{d}{6}(\delta + 1) - c \right) + O(n^3) \\
 &= dk \left(n - \frac{d}{3}(\delta + 1) - c \right) \left(n - c - c_1 - k - \frac{d}{6}(\delta + 1) \right) \\
 &\quad + c_1 \left(d \left(n - \frac{d}{3}(\delta + 1) \right) \left(n - c - c_1 - k - \frac{d}{6}(\delta + 1) \right) \right) \\
 &\quad + d(c - c_1) \left((c + k) \left(n - c - k - \frac{d}{6}(\delta + 1) \right) \right) \\
 &\quad - c_1(c + k) + c \left(n - \frac{d}{6}(\delta + 1) - c \right) + O(n^3).
 \end{aligned}$$

For easy calculation in maximising this term, we note that $c - c_1 \geq 0$, and that by (2.2), $n - c - k - (d/6)(\delta + 1) \geq 0$. Hence the last term in the previous inequalities,

$$d(c - c_1) \left((c + k) \left(n - c - k - \frac{d}{6}(\delta + 1) \right) - c_1(c + k) + c \left(n - \frac{d}{6}(\delta + 1) - c \right) \right),$$

is at most

$$d(c - c_1) \left((c + k + 1) \left(n - c - k - \frac{d}{6}(\delta + 1) \right) - c_1(c + k) + c \left(n - \frac{d}{6}(\delta + 1) - c \right) \right).$$

It follows that

$$\begin{aligned}
 D'(G) &\leq dk \left(n - \frac{d}{3}(\delta + 1) - c \right) \left(n - c - c_1 - k - \frac{d}{6}(\delta + 1) \right) \\
 &\quad + c_1 \left(d \left(n - \frac{d}{3}(\delta + 1) \right) \left(n - c - c_1 - k - \frac{d}{6}(\delta + 1) \right) \right) \\
 &\quad + d(c - c_1) \left((c + k + 1) \left(n - c - k - \frac{d}{6}(\delta + 1) \right) - c_1(c + k) \right) \\
 &\quad + c \left(n - \frac{d}{6}(\delta + 1) - c \right) + O(n^3).
 \end{aligned}$$

Let $g(n, d, c, c_1)$ be the function

$$\begin{aligned} g(n, d, c, c_1) := & dk\left(n - \frac{d}{3}(\delta + 1) - c\right)\left(n - c - c_1 - k - \frac{d}{6}(\delta + 1)\right) \\ & + c_1\left(d\left(n - \frac{d}{3}(\delta + 1)\right)\left(n - c - c_1 - k - \frac{d}{6}(\delta + 1)\right)\right) \\ & + d(c - c_1)\left((c + k + 1)\left(n - c - k - \frac{d}{6}(\delta + 1)\right) - c_1(c + k)\right. \\ & \left. + c\left(n - \frac{d}{6}(\delta + 1) - c\right)\right). \end{aligned}$$

We first maximise g subject to c_1 , keeping the other variables fixed. It is easy to verify, using (2.2), that the derivative

$$\frac{dg}{dc_1} = -dk\left(n - \frac{d}{3}(\delta + 1)\right) - dc\left(n - \frac{d}{3}(\delta + 1) - 2c + c_1\right) - d\left(c + \frac{d}{6}(\delta + 1)\right)$$

is negative. Therefore, g is decreasing in c_1 . Thus, in conjunction with (2.2),

$$\begin{aligned} g(n, d, c, c_1) &\leq g(n, d, c, 0) \\ &= dk\left(n - \frac{d}{3}(\delta + 1) - c\right)\left(n - c - k - \frac{d}{6}(\delta + 1)\right) \\ &\quad + dc\left((c + k + 1)\left(n - c - k - \frac{d}{6}(\delta + 1)\right) + c\left(n - \frac{d}{6}(\delta + 1) - c\right)\right) \\ &= d\left(n - \frac{d}{3}(\delta + 1) - 2c\right)\left(n - \frac{d}{3}(\delta + 1) - c\right) \\ &\quad \times \left(n - c - \left(n - \frac{d}{3}(\delta + 1) - 2c\right) - \frac{d}{6}(\delta + 1)\right) \\ &\quad + dc\left(\left(c + \left(n - \frac{d}{3}(\delta + 1) - 2c\right) + 1\right)\right. \\ &\quad \left.\times \left(n - c - \left(n - \frac{d}{3}(\delta + 1) - 2c\right) - \frac{d}{6}(\delta + 1)\right)\right) \\ &\quad + dc\left(c\left(n - \frac{d}{6}(\delta + 1) - c\right)\right) + O(n^3) \\ &= d\left(n - \frac{d}{3}(\delta + 1) - 2c\right)\left(n - \frac{d}{3}(\delta + 1) - c\right)\left(c + \frac{d}{6}(\delta + 1)\right) \\ &\quad + dc\left(\left(n - \frac{d}{3}(\delta + 1) - c + 1\right)\left(c + \frac{d}{6}(\delta + 1)\right)\right) \\ &\quad + dc\left(c\left(n - \frac{d}{6}(\delta + 1) - c\right)\right) + O(n^3) \\ &= d\left(\left(n - \frac{d}{3}(\delta + 1) - c\right)^2\left(c + \frac{d}{6}(\delta + 1)\right)\right. \\ &\quad \left.+ c^2\left(n - \frac{d}{6}(\delta + 1) - c\right)\right) + O(n^3). \end{aligned}$$

A simple differentiation with respect to c shows that the function

$$\left(n - \frac{d}{3}(\delta + 1) - c\right)^2 \left(c + \frac{d}{6}(\delta + 1)\right) + c^2 \left(n - \frac{d}{6}(\delta + 1) - c\right)$$

attains its maximum for $c = \frac{1}{2}(n - (d/3)(\delta + 1))$ to give

$$\left(n - \frac{d}{3}(\delta + 1) - c\right)^2 \left(c + \frac{d}{6}(\delta + 1)\right) + c^2 \left(n - \frac{d}{6}(\delta + 1) - c\right) \leq \frac{n}{4} \left(n - \frac{d}{3}(\delta + 1)\right)^2.$$

Hence

$$g(n, d, c, c_1) \leq \frac{1}{4} dn \left(n - \frac{d}{3}(\delta + 1)\right)^2 + O(n^3),$$

and so

$$D'(G) \leq g(n, d, c, c_1) + O(n^3) \leq \frac{1}{4} dn \left(n - \frac{d}{3}(\delta + 1)\right)^2 + O(n^3),$$

and Case 2 of Theorem 2.3 is proved.

To see that the bound is asymptotically sharp, consider the graph $G_{n,d,\delta}$, $d \equiv 1 \pmod{3}$, constructed as follows. First, let H be the graph with diameter $d - 2$ obtained as follows: $V(H) = V_0 \cup V_1 \cup \dots \cup V_{d-2}$, where

$$|V_i| = \begin{cases} 1 & \text{if } i \equiv 0 \text{ or } 2 \pmod{3}, \\ \delta - 1 & \text{otherwise} \end{cases}$$

and two distinct vertices $v \in V_i, v' \in V_j$ are joined by an edge if and only if $|j - i| \leq 1$. Let the only vertex in V_0 be v_0 and the only vertex in V_{d-2} be v_{d-2} . Now let H_1 be the complete graph on $\lceil \frac{1}{2}(n - \frac{1}{3}(d - 1)(\delta + 1)) \rceil$ vertices and H_2 the complete graph on $\lfloor \frac{1}{2}(n - \frac{1}{3}(d - 1)(\delta + 1)) \rfloor$ vertices. The graph $G_{n,d,\delta}$ is obtained by joining the vertex v_0 in H to every vertex in H_1 and joining the vertex v_{d-2} in H to every vertex in H_2 . Then $G_{n,d,\delta}$ has diameter d , minimum degree δ and degree distance at least $(1/4)dn(n - (d/3)(\delta + 1))^2$, as desired. \square

Finally, the result below gives a strengthening of the bound in [3] and completely settles a conjecture of Tomescu [13].

COROLLARY 2.5. *Let G be a connected graph of order n and minimum degree δ . Then*

$$D'(G) \leq \frac{n^4}{9(\delta + 1)} + O(n^3).$$

Moreover for a fixed δ , this inequality is asymptotically tight.

PROOF. Let d be the diameter of G . By the theorem above,

$$D'(G) \leq \frac{1}{4} dn \left(n - \frac{d}{3}(\delta + 1)\right)^2 + O(n^3).$$

The term $\frac{1}{4} dn(n - (d/3)(\delta + 1))^2$ is maximised, with respect to d , for $d = n/(\delta + 1)$, to give

$$\frac{1}{4} dn\left(n - \frac{d}{3}(\delta + 1)\right)^2 \leq \frac{n^4}{9(\delta + 1)}.$$

Hence $D'(G) \leq n^4/(9(\delta + 1)) + O(n^3)$, as desired.

To see that the bound is asymptotically best possible, consider the graph $G_{n,d,\delta}$ constructed above. Note that

$$D'(G_{n,n/(\delta+1),\delta}) > \frac{n^4}{9(\delta + 1)},$$

as claimed. □

3. Open problems

Since the extremal graph in Corollary 2.5 has cut vertices, it would be interesting to determine a best upper bound on the degree distance in terms of order and vertex connectivity. As reported in [4], the determination of the maximum degree distance among graphs of given order n and size m seems a difficult problem. At present the problem has only been solved for two special cases, unicyclic graphs (see Hou and Chang [7]) and bicyclic graphs (see Ilić *et al.* [8]). Lastly, it would be interesting to find a proof that is not so lengthy, elaborate, and delicate as the one presented in this paper.

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