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Degree Distance in Graphs with Forbidden Subgraphs

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Abstract

Let G be a simple, connected graph with minimum degree $\delta \geq 2$, order n, diameter $\mathrm{diam}(G) = d$ and degree distance $D'(G)$. We prove that

$$D'(G) \leq \begin{cases} \frac{1}{4}nd\left(n - \frac{1}{2}\delta d\right)^2 + O(n^3), & \text{if } G \text{ is triangle-free} \\ \frac{1}{4}nd\left(n - \frac{1}{5}(\delta^2 - \delta + 1)d\right)^2 + O(n^3), & \text{if } G \text{ is } C_4\text{-free.} \end{cases}$$

Although no construction has been found to show that the bounds are asymptotically tight, apart from improving known results in the literature, for triangle-free graphs the results confirm that an upper bound on the degree distance $\frac{1}{32}n^4 + O(n^3)$ conjectured by Dobrynin and Kochetova holds. This in conjunction with an infinite family of triangle-free graphs we construct in this paper that attain an upper bound on the degree distance, $\frac{1}{8}nd\left(n - \frac{1}{2}\delta d\right)^2 + O(n^3)$, give a guide for further research.

1 Introduction

Let $G = (V, E)$ be a simple, connected graph. The *degree* of a vertex $v \in V(G)$, $\deg_G(v)$ is the number of edges incident with v in G. The *minimum degree* of G, denoted $\delta(G)$, is defined as the smallest value of

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the degrees of vertices of G. The *distance* $d_G(u,v)$ is the length of a shortest path joining vertices u and v in G. The *eccentricity* of a vertex $v \in V(G)$, $ecc_G(v)$, is defined as $ecc_G(v) = \max\{d_G(u,v) : \; u \in V(G)\}$. The maximum eccentricity is the diameter, $\text{diam}(G)$. A triangle is a cycle of length 3 and a C_4 is a cycle of length 4. The *girth*, $g(G)$, is the length of the shortest cycle in G. G is triangle-free if its girth is at least 4 and C_4-free if it contains no cycle of length 4.

A *topological index* is a real number used for characterizing molecular graph and their fragments, predicting biological properties for chemical compound and other chemical applications [4, 11, 15, 21]. The oldest of such mathematical indices is the Weiner Index [21] introduced by Harold Weiner. The Weiner Index has been used to describe molecular branching and cyclicity as well as producing relationships with several physicochemical and thermodynamic parameters of chemical compounds such as the paraffin boiling point. Later, several authors came up with various topological indices that are crucial in analysing molecular graphs, such as the generalised Weiner Index [8], Szeged Index [10], Zagreb Index [1, 20], Eccentric Connectivity Index [16] Schultz Index of the first kind known as the degree distance [4, 7, 15] and the Schultz Index of the second kind which is commonly known as the Gutman Index, see for instance [7, 12]. Here we focus on the degree distance or Schultz Index of the first kind which was introduced at the same time by Dobrynin and Kochetova [4] and Gutman [7].

The degree distance of a graph G denoted by $D'(G)$ is given as

$$\begin{aligned} D'(G) &= \sum_{v \in V(G)} \deg_G(v) D(v) = \sum_{\{u,v\}} (\deg_G(u) + \deg_G(v)) d_G(u,v) \\ &= \sum_{v \in V(G)} D'(v), \end{aligned}$$

where $D(v)$ is the total distance or status of v. In other representation, $D(v) = \sum\limits_{u \in V(G)} d_G(u,v)$ and $D'(v) = \deg_G(v) D(v)$.

The degree distance is also called the degree analog of the Weiner Index [4]. In [4], the degree distance has been related to the Weiner Index where it is noted that adding an edge to any existing graph reduce the Weiner Index whereas this property is not valid for the degree distance. Hence the degree distance is a more sensitive weighted version of the Weiner Index than the Weiner Index. Based on different parameters and in different classes of graphs, the degree distance has been studied [2–5, 11, 13, 17–19].

For graphs in general, Dobrynin and Kochetova [4], conjectured that $D'G \leq \frac{1}{32}n^4 + O(n^3)$. Later, Tomescu [17] disproved this bound by giving an infinite family of graphs satisfying $D'(G) = \frac{1}{27}n^4 + O(n^3)$ but he did not manage to prove the bound. So, in the same paper [17], Tomescu conjectured that $D'G \leq \frac{1}{27}n^4 + O(n^3)$. In [2], it was indicated that the aforementioned conjecture by Tomescu was challenging to solve. Later the bound $D'G \leq \frac{1}{27}n^4 + O(n^{\frac{7}{2}})$ appeared in [3] thereby partially settling Tomescu's conjecture. Megan Jane Morgan *et al.* [13] finally settled Tomescu's conjecture by proving the bound $D'G \leq \frac{1}{27}n^4 + O(n^3)$. The same bound was also confirmed following a corollary to the following theorem by Mukwembi and Munyira [14]:

Theorem 1. *Let G be a simple, connected graph of order n, minimum degree δ, diameter d and degree distance $D'(G)$. Then*

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

and the bound is asymptotically sharp.

In graph theory, it is natural to ask on whether or not a given result can be strengthened by putting some relaxation on the properties of a graph. Here, we strengthen Theorem 1 for triangle-free graphs and C_4-free graphs. We mention here that although the bound $D'G \leq \frac{1}{32}n^4 + O(n^3)$ by Dobrynin and Kochetova [4] was disproved for graphs in general, one of the corollaries in this paper shows that exactly their bound holds for triangle-free graphs with $\delta \geq 2$. Corollaries in this paper also strengthen the results in [3, 13]

We use the following notation, apart from those already defined: We denote the vertex set of a graph G by $V(G)$ and the corresponding edge set by, $E(G)$. The *open-neighbourhood*, $N_G(v)$, of a vertex v in G is given by $N_G(v) = \{u \in V(G) :\ d_G(u,v) = 1\}$. The *closed-neighbourhood*, $N_G[v]$, is given by $N_G[v] = \{v\} \cup N_G(v)$. The i^{th} distance layer, N_i, from a vertex $v \in V(G)$ is given as $N_i = \{u \in V(G) :\ d_G(u,v) = i\}$. $G - \{e\}$ is the graph G minus an edge. Similarly, for a subgraph, H, $V(G) - V(H)$ denotes the set of vertices in G which are not in H. Where there is no ambiguity, we drop the argument G.

2 Main results

We start by introducing the following lemma which is an engine in the establishment of the results of this paper.

Lemma 1. *Let G be a simple, connected triangle-free graph of order n, diameter d and minimum degree $\delta \geq 2$. Let u, v be any vertices of G.*

(1) Then $d \leq \frac{2}{\delta}(n - \deg(v)) + \frac{3}{2}$

(2) If $d(u,v) \neq 2$, then $\deg(u) + \deg(v) \leq n - \frac{\delta d}{2} + O(1)$.

(3) $D(v) \leq d\left(n - \deg(v) - \frac{1}{4}d\delta)\right) + O(n)$

More so, these bounds are asymptotically sharp for each $\delta \geq 3$.

Proof. Let $P : v_0, v_1, \ldots, v_d$ be a diametric path of G. Let $S \subset V(P)$ be the set

$$S := \Big\{v_i : i \equiv 0 \text{ or } 1 \text{ (mode 4) } 1 \leq i \leq d\Big\}.$$

For each $u \in S$, choose any δ neighbours $u_1, u_2, \ldots, u_\delta$ of u and denote the set $\{u_1, u_2, \ldots, u_\delta\}$ by $M(u)$. Let $M = \cup_{u \in S} M(u)$. Then

$$|M| \geq \frac{(d+1)\delta}{2}.$$

Let v be any vertex of G. Then $|N(v) \cap M| \leq 2\delta$, since G is a triangle-free graph and P is a diametrical path. Thus

$$n \quad \geq \quad |M| + |N(v)| - |M \cap N(v)| \geq \frac{1}{2}\delta(d+1) + \deg(v) - 2\delta.$$

Hence (1) holds.

To prove (2), consider arbitrary vertices u, v, such that $d(u,v) \neq 2$, then $N(u) \cap N(v) = \emptyset$. It follows that

$$\begin{aligned} n &\geq |M| + |N(u)| + |N(v)| - |M \cap N(v)| - |M \cap N(v')| \\ &\geq \frac{\delta(d+1)}{2} + \deg(u) + \deg(v) - 2(2\delta). \end{aligned}$$

Therefore (2) is true.

We now settle (3). Let $ecc(v) = e$ and N_i be the i^{th} distance layer from v such that $k_i = |N_i|$. Further, let $u \in N_G(v)$ be one of the neighbours of v. Note that for adjacent vertices x and y; $2 \leq i \leq e-3$, if $x \in N_i$ and $y \in N_{i+1}$, then $N[x] \subseteq N_{i-1} \cup N_i \cup N_{i+1}$ and $N[y] \subseteq N_i \cup N_{i+1} \cup N_{i+2}$. This in conjunction with the fact that G is a triangle-free graph, imply that

$$k_{i-1} + k_i + k_{i+1} + k_{i+2} \geq 2\delta.$$

Now

$$D(v) = 1k_1 + 2k_2 + 3k_3 + \cdots + ek_e. \tag{1}$$

Consider $e = 4q+s,\ q \in \mathbb{Z}^+,\ s = 0,1,2,3$. Subject to $k_1 = \deg(v), k_2 \geq \deg(u)-1, k_i \geq 1, k_3+k_4+k_5+k_6 \geq 2\delta, k_7+k_8+k_9+k_{10} \geq 2\delta, \cdots, k_{e-5-s} + k_{e-4-s} + k_{e-3-s} + k_{e-2-s} \geq 2\delta, k_{e-1-s} + k_{e-s} + k_{e+1-s} + k_{e+2-s} \geq 2\delta$, where $e+2+s \leq e-1$, equation (1) is maximised for $k_1 = \deg(v)$,

$$k_2 = \deg(u) - 1, k_3 = 1 = k_4, k_5 = \delta - 1, k_6 = \delta - 1, k_7 = 1 = k_8,$$

$$k_9 = \delta - 1 = k_{10} \cdots, k_{e-5-s} = 1 = k_{e-4-s}, k_{e-3-s} = \delta - 1 = k_{e-2-s},$$

$k_{e-1-s} = 1 = k_{e-s} k_{e+1-s} = k_{e+2-s} = \delta - 1$ and
$k_e = n - \deg(v) - \frac{1}{2}(e-6)\delta - 1$, since $\deg(u) \geq \delta$. Thus

$$\begin{aligned} D(v) \leq\ & \deg(v) + 2(\deg(u)-1) + 3 + 4 + 5(\delta-1) + 6(\delta-1) + \\ & 7 + 8 + 9(\delta-1) + 10(\delta-1) \cdots + (e-5-s) + (e-4-s) + \\ & (e-3-s)(\deg(u)-1) + (e-2-s)(\delta-1) + (e-1-s) + \\ & (e-s) + (e+1-s)(\delta-1) + (e+2-s)(\delta-1) + \\ & e(n - \deg(v) - \frac{1}{2}(e-6)\delta - 1) \end{aligned}$$

$$= \frac{1}{2}(\delta-1)\sum_{r=1}^{e-1} r + e(n-\deg(v) - \frac{1}{2}(e-6)\delta - 1) + O(n)$$
$$= e(n-\deg(v) - \frac{1}{4}e\delta) + O(n).$$

For $e = d$ the result follows. Now for $e \leq d-1$, the function

$$f(x) = x(n - \deg(v) - \frac{1}{4}x\delta + 1)$$

is increasing for all $x \leq \frac{2}{\delta}(n - \deg(v))$. So by application of Lemma 1, item (1) and since $e \leq d-1$, item (3) is established. ■

To see that the bounds in Lemma 1 are asymptotically tight, for $d \equiv 0$ *mod* 4 take a chain of $\frac{1}{4}d$ components of complete birpartite graphs, where each interior component is $K_{\delta,\delta} - e$ and the ends components are each $K_{\delta,\delta+1} - e$. We now prove the main result of this paper.

Theorem 2. *Let G be a simple, connected, triangle-free graph of with minimum degree $\delta \geq 2$, order n, diameter d and degree distance $D'(G)$. Then $D'(G) \leq \frac{1}{4}dn\left(n - \frac{\delta d}{2}\right)^2 + O(n^3)$.*

Proof. Let $S, M(u)$ and M be as defined in the proof of Lemma 1. Also, define $M[u]$ by $M[u] = M(u) \cup \{u\}$. We partition S as $S = S_1 \cup S_2 \cup S_3 \cup S_4$, where

$$\begin{aligned} S_1 &= \{v_i \mid i \equiv 0 \pmod 8, 0 \leq i \leq d\}, \\ S_2 &= \{v_i \mid i \equiv 1 \pmod 8, 1 \leq i \leq d\}, \\ S_3 &= \{v_i \mid i \equiv 4 \pmod 8, 4 \leq i \leq d\}, \\ S_4 &= \{v_i \mid i \equiv 5 \pmod 8, 5 \leq i \leq d\}. \end{aligned}$$

It follow that

$$M = (\cup_{v\in S_1} M[v]) \cup (\cup_{v\in S_2} M[v]) \cup (\cup_{v\in S_3} M[v]) \cup (\cup_{v\in S_4} M[v]).$$

By our construction of $S_i,\ i = 1,2,3,4$, for each $u, v \in S_i$, $u \neq v$, 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 $S_1 = \{w_1, w_2, \ldots, w_{|S_1|}\}$. For each $w_j \in S_1$, let
$M(w_j) = \{w_1^j, w_2^j, \ldots, w_\delta^j\}$, where $w_1^j, w_2^j, \ldots, w_\delta^j$ are neighbours of w_j.

Since $d_G(w, w') \geq 8$ for any $w, w' \in S_1$, then

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

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

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

Summing we get

$$(\delta + 1)n \geq \sum_{x \in \left(\cup_{u \in S_1} M[u]\right)} \deg(x) + (\delta + 1)|S_1|.$$

That is,

$$\sum_{x \in \left(\cup_{u \in S_1} M[u]\right)} \deg(x) \leq (\delta + 1)n - (\delta + 1)|S_1|. \tag{2}$$

Similarly,

$$\sum_{x \in \left(\cup_{u \in S_i} M[u]\right)} \deg(x) \leq (\delta + 1)(n - |S_i|), \ i = 2, 3, 4. \tag{3}$$

Let $M[S_i] = \sum_{u \in S_i} M[u]$. Then

$$4(\delta + 1)n - (\delta + 1)\left(|S_1| + |S_2| + |S_3| + |S_4|\right) \geq \sum_{x \in \bigcup_{x \in M[S_i]}} \deg(x).$$

Therefore

$$\sum_{x \in M} \deg(x) \leq 4(\delta + 1)n - \frac{1}{2}(d + 1)(\delta + 1),$$

since $|S| \geq \frac{1}{2}(d+1)$. This in conjunction with $D(u) \leq (n-1)^2, \forall u \in V(G)$

yield

$$\begin{aligned}\sum_{v\in M} D'(v) &= \sum_{v\in M}\deg(v)D(v)\\ &\le (n-1)^2\sum_{v\in M}\deg(v)\\ &\le (n-1)^2\left(4(\delta+1)n-\frac{1}{2}(d+1)(\delta+1)\right).\end{aligned}$$

Consequently,

$$\sum_{v\in M} D'(v)\le O(n^3). \tag{4}$$

Let C be a maximum set of disjoint pairs of vertices from $V(G)-M$ such that for all $\{a,b\}\in C,\ d(a,b)\neq 2$. If $\{a,b\}\in C$, we say a and b are *partners*. Also Let

$$K = V(G)-M-\{x : x\in\{a,b\}\in C\}.$$

Set $|K|=k$ and $|C|=c$. Then

$$n = |M|+2c+k. \tag{5}$$

We consider two cases:

Consider first $k\le 1$. Note that $D(x)\le (n-1)^2$. So

$$\sum_{x\in K} D'(x) = \sum_{x\in K}\deg(x)D(x) = O(n^3).$$

We now show that $\forall\{a,b\}\in C,\ D'(a)+D'(b)\le \frac{1}{2}nd\left(n-\frac{1}{2}\delta d\right)+O(n^2)$. Following Lemma 1, item(3) for all $x\in\{a,b\}\in C$,

$$\begin{aligned}D'(x) &= \deg(x)D(x)\le \deg(x)\left[d\left(n-\frac{1}{4}\delta d-\deg(x)\right)\right]\\ &\quad +O(n^2),\ \text{since}\ \deg(x)=O(n).\end{aligned}$$

Thus

$$\begin{aligned}
D'(a)+D'(b) &\le d\left[x\left(n-\frac{1}{4}\delta d\right)-\left((\deg(a))^2+(\deg(b))^2\right)\right] \\
&\quad +O(n^2) \\
&\le d\left[x\left(n-\frac{1}{4}\delta d\right)-\frac{1}{2}\left((\deg(a)+\deg(b))^2\right)\right] \\
&\quad +O(n^2),
\end{aligned}$$

where $x=\deg(a)+\deg(b)$. Let $f(x)=d\left[x(n-\frac{1}{4}\delta d)-\frac{1}{2}x^2\right]$. Then $f(x)$ is increasing for $x\le n-\frac{\delta d}{4}$. Thus by Lemma 1, item(2), $f(x)$ attains it's maximum value for $x=n-\frac{1}{2}\delta d+O(1)$. That is,

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

Since $|M|\ge\frac{1}{2}(d+1)\delta$, we have $c=\frac{1}{2}(n-\frac{1}{2}\delta d)+O(1)$. Hence

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

Finally,

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

Consider $k\ge 2$.

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 a 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 1. For all $u, v \in A \cup K$, $d(u,v) \leq 8$.

Proof of Claim 1: Note by our choice of C and K that $d(x,x') = 2$, $\forall x, x' \in K$. We show that $d(a,x) \leq 4$, $\forall a \in A$. 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 $d(x,x') = 2$, we have

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

That is, $d(b,x') \geq 3$. 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 $a \in A$. Therefore, $u, v \in A$, $d(u,v) \leq d(u,x) + d(x,v) \leq 8$ as needed.

Claim 2. For all $x \in K$,

$$D'(x) \leq d\left(n - \frac{\delta d}{2} - c\right)\left(n - c - c_1 - k - \frac{\delta d}{4}\right) + O(n^2).$$

Proof of Claim 2: By Claim 1, 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 the proof of Lemma 1 item (3),

$$\begin{aligned} D(x) &\leq 8(c+k) + 17c_1 + 18 + 19 + 20(\delta-1) + 21(\delta-1) + 22 + 23 + \\ &\quad 24(\delta-1) + 25(\delta-1)\cdots + d\left(n - c - k - c_1 - \frac{\delta d}{2}\right) \\ &= d\left(n - c - c_1 - k - \frac{\delta d}{4}\right) + O(n). \end{aligned}$$

Recall that x has at most 2δ 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 $d(w,z) \neq 2$ and G is triangle-free. Thus, x is adjacent to at most c vertices in $A \cup B$. It follows that

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

$$= \quad \deg x + \frac{1}{2}\delta d + c + O(1).$$

Hence $\deg x \leq n - \frac{1}{2}\delta - c + O(1)$. Therefore,

$$\begin{aligned} D'(x) &= \deg x D(x) \\ &\leq d\left(n - \frac{\delta d}{2} - c\right)\left(n - c - c_1 - k - \frac{\delta d}{4}\right) + O(n^2), \end{aligned}$$

and this proves Claim 2.

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

$$D'(a) + D'(b) \leq d\left(n - \frac{\delta d}{2}\right)\left(n - c - c_1 - k - \frac{\delta d}{4}\right) + O(n^2).$$

Proof of Claim 3: 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 1, 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 the proof of Lemma 1 item (3), that

$$\begin{aligned} D(w) &\le 26(c+k+c_1-1)+27+28+29(\delta-1)+30(\delta-1)+31+ \\ &\quad 32+33(\delta-1)+\cdots\ +\ d\left(n-c-c_1-k-\frac{\delta d}{2}\right) \\ &= d\left(n-c-c_1-k-\frac{\delta d}{4}\right)+O(n). \end{aligned}$$

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

$$\begin{aligned} D'(a)+D'(b) &\le \deg a\left(d\left(n-c-c_1-k-\frac{\delta d}{4}\right)+O(n)\right) \\ &\quad +\ \deg b\left(d\left(n-c-c_1-k-\frac{\delta d}{4}\right)+O(n)\right) \\ &= (\deg a+\deg b)\left(d\left(n-c-c_1-k-\frac{\delta d}{4}\right)+O(n)\right). \end{aligned}$$

By Lemma 1 item (2), $\deg a+\deg b \le n-\frac{\delta d}{2}+O(1)$. Therefore,

$$\begin{aligned} D'(a)+D'(b) &\le \left(n-\frac{\delta d}{2}+O(1)\right)\left(d\left(n-c-c_1-k-\frac{\delta d}{4}\right)\right) \\ &\quad +O(n^2) \\ &= d\left(n-\frac{\delta d}{2}\right)\left(n-c-c_1-k-\frac{\delta d}{4}\right)+O(n^2), \end{aligned}$$

and Claim 3 is proven.

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

Claim 4. Let $\{a,b\} \in C$. If $d(a,b) \ge 10$, that is, if $\{a,b\} \in (A-A_1) \cup (B-B_1)$, then

$$D'(a)+D'(b) \le d(c+k)\left(n-c-c_1-k-\frac{\delta d}{4}\right)+cd\left(n-\frac{\delta d}{4}-c\right)+O(n^2).$$

Proof of Claim 4: We consider vertices from $A-A_1$ and from $B-B_1$ separately. Let $a \in A-A_1$. Then as in Claim 3, 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 the proof of Lemma 1 item

(3),

$$\begin{aligned} D(a) &\leq 8(c+k-1)+17c_1+18+19+20(\delta-1)+21(\delta-1)+22+ \\ &\quad 23+24(\delta-1)+25(\delta-1)+\cdots \ + \ d\left(n-c-c_1-k-\frac{\delta d}{2}\right) \\ &= d\left(n-c-c_1-k-\frac{\delta d}{4}\right)+O(n). \end{aligned}$$

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 $d(w,u) \neq 2$ and G is triangle-free. Hence a is adjacent to at most $c-1$ vertices in $A \cup B$. Further, a is adjacent to at most 2δ vertices in M and has at most k neighbours in K. Thus,

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

It follows that

$$\begin{aligned} D'(a) &= \deg a D(a) \\ &\leq (c+k+2\delta-1)\left(d\left(n-c-c_1-k-\frac{\delta d}{4}\right)+O(n^2)\right) \\ &= d(c+k)\left(n-c-c_1-k-\frac{\delta d}{4}\right)+O(n^2). \end{aligned} \tag{6}$$

Now let $b \in B - B_1$. By Lemma 1 item (3), we have

$$D(b) \leq d\left(n-\frac{\delta d}{4}-\deg b\right)+O(n),$$

and so

$$D'(b) \leq \deg b\left(d\left(n-\frac{\delta d}{4}-\deg b\right)\right)+O(n^2). \tag{7}$$

We first maximize $d \deg b\left(n-\frac{\delta d}{4}-\deg b\right))$ with respect to $\deg b$. Let

$$f(x) := xd\left(n-\frac{\delta d}{4}-x\right),$$

where $x = \deg b$.

A simple differentiation shows that f is increasing for $x \leq \frac{1}{2}\left(n - \frac{\delta d}{4}\right)$. 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 2δ 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 1, $d(a, y) \leq 8$. Hence

$$10 \leq d(a, b) \leq d(b, y) + d(y, a) \leq 1 + 8, \text{ a contradiction.}$$

Thus, b cannot be adjacent to any vertex in K. We conclude that

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

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

$$\begin{aligned} f(\deg b) &= f(c + j) = d(c + j)\left(n - \frac{\delta d}{4} - (c + j)\right) \\ &= cd\left(n - \frac{\delta d}{4} - c\right) + O(n^2). \end{aligned} \tag{8}$$

Second, assume that $\deg b \leq c$. Now

$$c = \frac{1}{2}(n - |M| - k) \leq \frac{1}{2}\left(n - \frac{\delta d}{2} - 2\right).$$

Notice that

$$\frac{1}{2}\left(n - \frac{\delta d}{2} - 2\right) \leq \frac{1}{2}\left(n - \frac{\delta d}{4}\right),$$

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

$$f(\deg b) \leq f(c) = cd\left(n - \frac{\delta d}{4} - c\right),$$

for this case. Comparing this with (8), we get that

$$f(\deg b) \leq cd\left(n - \frac{\delta d}{4} - c\right) + O(n^2).$$

Thus, from (7), we have

$$D'(b) \leq cd\left(n - \frac{\delta d}{4} - c\right) + O(n^2).$$

Combining this with (6), we get

$$D'(a)+D'(b) \leq d(c+k)\left(n - c - c_1 - k - \frac{\delta d}{4}\right) + cd\left(n - \frac{\delta d}{4} - c\right) + O(n^2),$$

and Claim 4 is proven.

By recalling that $\sum_{u \in M} D'(u) = O(n^3)$ and using Claims 2, 3, and 4 we bound $D'(G)$ as follows. Note that

$$\begin{aligned} D'(G) &= \sum_{u\in M} D'(u) + \sum_{x \in K} D'(x) + \sum_{\{a,b\}\in C} (D'(a) + D'(b)) \\ &\leq dk\left(n - \frac{\delta d}{2} - c\right)\left(n - c - c_1 - k - \frac{\delta d}{4}\right) \\ &\quad + c_1\left(d\left(n - \frac{\delta d}{2}\right)\left(n - c - c_1 - k - \frac{\delta d}{4}\right)\right) + (c - c_1) \\ &\quad \left(d(c+k)\left(n - c - c_1 - k - \frac{\delta d}{4}\right) + \left(n - \frac{\delta d}{4} - c\right)\right) \\ &\quad + O(n^3) \\ &= dk\left(n - \frac{\delta d}{2} - c\right)\left(n - c - c_1 - k - \frac{\delta d}{4}\right) \\ &\quad + c_1\left(d\left(n - \frac{\delta d}{2}\right)\left(n - c - c_1 - k - \frac{\delta d}{4}\right)\right) + d(c - c_1) \\ &\quad \left((c+k)\left(n - c - k - \frac{\delta d}{4}\right) - c_1(c+k) + c\left(n - \frac{\delta d}{4} - c\right)\right) \\ &\quad + O(n^3). \end{aligned}$$

For easy calculation in maximizing this term, we note that $c - c_1 \geq 0$. In addition, from $n = |M| + 2|C| + |K|$, we see that $n - c - k - \frac{\delta d}{4} \geq 0$. Hence the last term in the previous inequalities

$$d(c - c_1)\left((c + k)\left(n - c - k - \frac{\delta d}{4}\right) - c_1(c + k) + c\left(n - \frac{\delta d}{4} - c\right)\right)$$

is at most

$$d(c - c_1)\left((c + k + 1)\left(n - c - k - \frac{\delta d}{4}\right) - c_1(c + k) + c\left(n - \frac{\delta d}{4} - c\right)\right).$$

It follows that

$$\begin{aligned} D'(G) \leq\; & dk\left(n - \frac{\delta d}{2} - c\right)\left(n - c - c_1 - k - \frac{\delta d}{4}\right) \\ & + c_1\left(d\left(n - \frac{\delta d}{2}\right)\left(n - c - c_1 - k - \frac{\delta d}{4}\right)\right) \\ & + d(c - c_1)\left((c + k + 1)\left(n - c - k - \frac{\delta d}{4}\right) - c_1(c + k)\right. \\ & \left. + c\left(n - \frac{\delta d}{4} - c\right)\right) + O(n^3). \end{aligned}$$

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

$$\begin{aligned} g(n, d, c, c_1) :=\; & dk\left(n - \frac{\delta d}{2} - c\right)\left(n - c - c_1 - k - \frac{\delta d}{4}\right) \\ & + c_1\left(d\left(n - \frac{\delta d}{2}\right)\left(n - c - c_1 - k - \frac{\delta d}{4}\right)\right) \\ & + d(c - c_1)\left((c + k + 1)\left(n - c - k - \frac{\delta d}{4}\right)\right. \\ & \left. - c_1(c + k) + c\left(n - \frac{\delta d}{4} - c\right)\right). \end{aligned}$$

We first maximize g subject to c_1, keeping the other variables fixed. Following equation 5, it is easy to verify, that the derivative

$$\frac{dg}{dc_1} = -dk\left(n - \frac{\delta d}{2}\right) - dc\left(n - \frac{\delta d}{2} - 2c + c_1\right) - d\left(c + \frac{\delta d}{4}\right)$$

is negative. Therefore, g is decreasing in c_1. Thus,

$$\begin{aligned}
g(n,d,c,c_1) &\le g(n,d,c,0)\\
&= dk\left(n-\frac{\delta d}{2}-c\right)\left(n-c-k-\frac{\delta d}{4}\right)\\
&\quad + dc\left((c+k+1)\left(n-c-k-\frac{\delta d}{4}\right)\right.\\
&\quad\quad \left. + c\left(n-\frac{\delta d}{4}-c\right)\right)\\
&= d\,(w)\left(n-\frac{\delta d}{2}-c\right)\left(n-c-(w)-\frac{\delta d}{4}\right)\\
&\quad + dc\left((c+(w)+1)\left(n-c-(w)-\frac{\delta d}{4}\right)\right)\\
&\quad + dc\left(c\left(n-\frac{\delta d}{4}-c\right)\right)+O(n^3)\\
&= d\left(n-\frac{\delta d}{2}-2c\right)\left(n-\frac{\delta d}{2}-c\right)\left(c+\frac{\delta d}{4}\right)\\
&\quad + dc\left(\left(n-\frac{\delta d}{2}-c+1\right)\left(c+\frac{\delta d}{4}\right)\right)\\
&\quad + dc\left(c\left(n-\frac{\delta d}{4}-c\right)\right)+O(n^3)\\
&= d\left(\left(n-\frac{\delta d}{2}-c\right)^2\left(c+\frac{\delta d}{4}\right)+c^2\left(n-\frac{\delta d}{4}-c\right)\right)\\
&\quad + O(n^3),
\end{aligned}$$

where $w = n - \frac{\delta d}{2} - 2c$. A simple differentiation with respect to c shows that the function

$$\left(n-\frac{\delta d}{2}-c\right)^2\left(c+\frac{\delta d}{4}\right)+c^2\left(n-\frac{\delta d}{4}-c\right)$$

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

$$\left(n-\frac{\delta d}{2}-c\right)^2\left(c+\frac{\delta d}{4}\right)+c^2\left(n-\frac{\delta d}{4}-c\right)\le \frac{n}{4}\left(n-\frac{\delta d}{2}\right)^2.$$

Hence

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

and so

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

and Case 2 of Theorem 2 is proven.

Thus the result follows by Case 1 and Case 2. ■

We mention here that no construction has been found that yields sharpness or asymptotic sharpness of the bound in Theorem 2. This implies that Theorem 2 can be improved or researchers can try to look for graphs that yields asymptotic tightness on the bound. In view of this, here we construct an infinite family $G_{n,d,\delta}$ for $d \equiv 3 \ mod \ 4$, such that each graph in the family attains an upper bound on the degree distance, $\frac{1}{8}dn\left(n - \frac{\delta d}{2}\right)^2 + O(n^3)$, apart from the additive term $O(n^3)$. We are not sure whether or not this aforementioned bound is the asymptotic tight one and so, researchers can also try to find a proof for the bound. Let G' be a graph with $V(G') = V_0 \cup V_1 \cup V_2 \cup ...V_{d-4}$, where

$$|V_i| = \begin{cases} 1 & \text{if} \quad i \equiv \ 0 \text{ or } 3 \ mod \ 4 \\ \delta - 1 & \text{otherwise} \end{cases}$$

and two distinct $u \in V_i$ and $v \in V_j$ are joined by an if and only if $|i - j| = 1$. Let v_0 be the only vertex in V_0 and v_{d-4} be the only vertex in V_{d-4}. Let $G_1 = K_{p_1,q_1}$ be the complete birpartite graph with $p_1 = q_1 = \lceil \frac{1}{4}\left(n - \frac{1}{2}(d-5)\delta\right) \rceil$ and $G_2 = K_{p_2,q_2}$ be the complete birpartite graph with $p_2 = q_2 = \lfloor \frac{1}{4}\left(n - \frac{1}{2}(d-5)\delta\right) \rfloor$. Form $G_{n,d,\delta}$ by taking G' and join v_0 to every vertex in just one of the partite set of K_{p_1,q_1} and join v_{d-4} to every vertex in just one of the partite set of K_{p_2,q_2}.

The following corollary confirms that the conjectured bound $D'G \leq \frac{1}{32}n^4 + O(n^3)$ holds for triangle-free graphs of minimum degree $\delta \geq 2$.

Corollary 1. Let G be a simple, connected, triangle-free graph as defined in Theorem 2. Then $D'(G) \leq \frac{1}{16\delta}n^4 + O(n^3)$.

Proof. The bound in Theorem 2 is maximised with respect to d if $d = \frac{n}{\delta}$. Hence the result. Since $\delta \geq 2$, an upper bound by Dobrynin and Kochetova is confirmed for triangle-free graphs. ■

We now extend the results to C_4-free graphs. Similar to Lemma 1, the following lemma is crucial:

Lemma 2. *Let G be a connected C_4-free graph of order n, diameter d and minimum degree $\delta \geq 2$. Let u, v be any vertices of G.*

(1) Then $d \leq \frac{5}{\delta^2-\delta+1}(n - \deg(v) + 2\delta + 1) - 1$

(2) Then $\deg(u) + \deg(v) \leq n - \frac{1}{5}(\delta^2 - \delta + 1)d + O(1)$.

(3) $D(v) \leq d\left(n - \deg(v) - \frac{1}{10}d(\delta^2 - \delta + 1)\right) + O(n)$

Proof. Let $P : v_0, v_1, \ldots, v_d$ be a diametric path of G. Let $S \subset V(P)$ be the set

$$S := \left\{v_i : i \equiv 0 \text{ (mode 5) } 1 \leq i \leq d\right\}.$$

For each $u \in S$, choose any δ neighbours $u_1, u_2, \ldots, u_\delta$ of u and denote the set $\{u, u_1, u_2, \ldots, u_\delta\}$ by $M[u]$. For each $u_i \in M[u]$, $\forall u \in S$, take any $\delta - 2$ neighbours, say, $\{w_1^i, w_2^i, \cdots, w_{\delta-2}^i\}$ which are not in $M[u]$ and denote the set by $M(u_i)$. Note this is possible, since G is a C_4-free graph. By our construction of S and since G is a C_4-free graph, for $i \neq j$, $M(u_i) \cap M(u_j) = \emptyset$. More so, for any distinct pair of vertices $u, v \in S$, $M[u]$ and $M[v]$ are disjoint, and their neighbourhoods area also disjoint. Let $M = (\cup_{u \in S} M[u]) \cup \left(\cup_{u_i \in M[u]} M(u_i)\right)$. Then

$$|M| = |S|(\delta^2 - \delta + 1) \geq \frac{1}{5}(d + 1)(\delta^2 - \delta + 1).$$

Let v be any vertex of G. Then $|N(v) \cap M| \leq 2\delta + 1$, since G is a C_4-free graph and P is a diametrical path. Now

$$n \quad \geq \quad |M| + |N(v)| - |M \cap N(v)|.$$

Hence (1) holds.

To prove (2), consider arbitrary, distinct vertices $u, v \in V(G)$, $|N(u) \cap N(v)| \leq 1$, since G is a C_4-free graph. It follows that

$$n \geq \frac{1}{5}(\delta^2 - \delta + 1)(d+1) + \deg(u) + \deg(v) - 2(2\delta + 1) - 2.$$

Therefore (2) is true.

We now settle (3). Let $ecc(v) = e$ and N_i be the i^{th} distance layer from v such that $k_i = |N_i|$. Note that for a vertex $x \in N_i$, $3 \leq i \leq e-3$, if $x \in N_i$; $N[x] \subseteq N_{i-1} \cup N_i \cup N_{i+1}$ and $N^2(x) \subseteq N_{i-2} \cup N_{i+2}$. This in conjunction with the fact that G is a C_4-free graph, imply that

$$k_{i-2} + k_{i-1} + k_i + k_{i+1} + k_{i+2} \geq \delta^2 - \delta + 1.$$

Now

$$D(v) = 1k_1 + 2k_2 + 3k_3 + \cdots + ek_e. \tag{9}$$

Using similar arguments as in Lemma 1, item (3), maximising equation 9 subject to $k_1 = deg(v),\ k_2 \geq \deg(v)(\delta - 1) \quad k_i \geq 1, \quad$ and $k_{i-2} + k_{i-1} + k_i + k_{i+1} + k_{i+2} \geq \delta^2 - \delta + 1$, yields

$$\begin{aligned} D(v) &\leq \frac{1}{5}(\delta^2 - \delta + 1)\sum_{r=1}^{e-1} r + e(n - \deg(v) - \frac{1}{5}(e-2)(\delta^2 - \delta + 1) - 1) \\ &\quad +O(n) \\ &= e(n - \deg(v) - \frac{1}{10}e(\delta^2 - \delta + 1)) + O(n). \end{aligned}$$

For $e = d$ the result follows. Now for $e \leq d - 1$, the function

$$f(x) = x(n - \deg(v) - \frac{1}{10}x(\delta^2 - \delta + 1)),$$

is increasing for all $x \leq \frac{5}{\delta^2 - \delta + 1}(n - \deg(v))$. So, by an application of Lemma 2 item (1) and since $e \leq d - 1$, item (3) is established. ■

Bounds in Lemma 2 are nearly asymptotically sharp as revealed by a class of graphs by Erdős *et al.* [6] and are asymptotically tight for $\delta = 3$ as can be seen in C_4-free graphs constructed in [9].

Theorem 3. *Let G be a simple, connected, C_4-free graph of minimum degree $\delta \geq 2$, order n, diameter d and degree distance $D'(G)$. Then*

$$D'(G) \leq \frac{1}{4}dn\left(n - \frac{1}{5}(\delta^2 - \delta + 1)d\right)^2 + O(n^3).$$

Proof. Let S and M be as defined in the proof of Lemma 2. Then by partitioning S as $S = S_1 \cup S_2$, where

$$\begin{aligned} S_1 &= \{v_i \mid i \equiv 0 \pmod{10}, 0 \leq i \leq d\}, \\ S_2 &= \{v_i \mid i \equiv 5 \pmod{10}, 5 \leq i \leq d\}, \end{aligned}$$

It can easily be shown that

$$\sum_{v \in M} D'(v) \leq O(n^3). \tag{10}$$

Let C' be a maximal set of disjoint pair of vertices $\{a, b\}$ from $V(G) - M$ and $K' = V(G) - M - \{x : x \in \{a, b\} \in C'\}$. Set $|K'| = k'$ and $|C'| = c'$. Then

$$n = |M| + 2c' + k'. \tag{11}$$

Just as Theorem 2 has been proved using the choice of M, C and K in-conjunction with Lemma 1, here similar arguments establishes the proof following our choice of M, C' and K' together with the application of Lemma 2. ∎

We mention here that we are note sure whether or not Theorem 3 is almost asymptotically tight. So far the best family of C_4-free graphs we know are due to *Erdős et al.* [6] and they do not attain the bound. The results in this paper strengthens theorems in [3, 13] for all $\delta \geq 2$, apart from improving results in [14].

Similar arguments as used for C_4-free graphs can be used to obtain the upper bound on the degree distance for graphs of given girth g. It would be interesting if asymptotically sharp or almost asymptotically sharp upper bounds on the aforementioned topological index can be found for triangle-free graphs, C_4-free graphs or graphs of given girth. For triangle-free graphs if an upper bound $\frac{1}{8}dn\left(n-\frac{\delta d}{2}\right)^2+O(n^3)$ can be proved, then it is asymptotically sharp as revealed before.

References

[1] S. C. Basak, A. T. Balaban, G. D. Grunwald, B. D. Gute, Topological indices: their nature and mutual relatedness, *J. Chem. Inf. Comput. Sci.* **40** (2000) 891–898.

[2] O. Bucicovschi, S. M. Cioabă, The minimum degree distance of graphs of given order and size, *Discr. Appl. Math.* **156** (2008) 3518–3521.

[3] P. Dankelmann, I. Gutman, S. Mukwembi, H. C. Swart, On the degree distance of a graph, *Discr. Appl. Math.* **157** (2009) 2773–2777.

[4] A. A. Dobrynin, A. A. Kochetova, Degree distance of a graph: A degree analog of the Wiener index, *J. Chem. Inf. Comput. Sci.* **34** (1994) 1082–1086.

[5] M. Dragan, I. Tomescu, Bicyclic connected graphs having smallest degree distances, in: *2019 21st International Symposium on Symbolic and Numeric Algorithms for Scientific Computing (SYNASC)*, IEEE, 2019, pp. 105–108.

[6] P. Erdős, J. Pach, R. Pollack, Z. Tuza, Radius, diameter, and minimum degree, *J. Comb. Theory Ser. B* **47** (1989) 73–79.

[7] I. Gutman, Selected properties of the Schultz molecular topological index, *J. Chem. Inf. Comput. Sci.* **34** (1994) 1087–1089.

[8] I. Gutman, Ž. Tomović, Relation between distance-based topological indices, *J. Chem. Inf. Comput. Sci.* **40** (2000) 1333–1336.

[9] P. Mafuta, Bounds on the Leaf Number in Graphs of Girth 4 or 5, *J. Discr. Math. Sci. and Cryptogr.* **24** (2021) 1573–1582.

[10] T. Mansour, M. Schork, The vertex PI index and Szeged index of bridge graphs, *Discr. Appl. Math.* **157** (2009) 1600–1606.

[11] Y. Mao, Z. Wang, I. Gutman, A. Klobučar, Steiner degree distance, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 221–230.

[12] J. P. Mazorodze, P. Mafuta, S. Munyira, On the Gutman index and minimum degree of a triangle-free graph, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 231–240.

[13] M. J. Morgan, S. Mukwembi, H. C. Swart, On a conjecture by Tomescu, *Util. Math.* **102** (2017) 87–104.

[14] S. Mukwembi S. Munyira, Degree distance and minimum degree, *Bull. Aust. Math. Soc.* **87** (2013) 255–271.

[15] H. P. Schultz, Topological organic chemistry. 1. Graph theory and topological indices of alkanes, *J. Chem. Inf. Comput. Sci.* **29** (1989) 227–228.

[16] V. Sharma, R. Goswami, A. K. Madan, Eccentric connectivity index: A novel highly discriminating topological descriptor for structure-property and structure-activity studies, *J. Chem. Inf. Comput. Sci.* **37** (1997) 273–282.

[17] I. Tomescu, Some extremal properties of the degree distance of a graph, *Discr. Appl. Math.* **98** (1999) 159–163.

[18] A. I. Tomescu, Unicyclic and bicyclic graphs having minimum degree distance, *Discr. Appl. Math.* **156** (2008) 125–130.

[19] I. Tomescu, Properties of connected graphs having minimum degree distance, *Discr. Math.* **309** (2009) 2745–2748.

[20] T. Vetrík, S. Balachandran, General multiplicative Zagreb indices of trees, *Discr. Appl. Math.* **247** (2018) 341–351.

[21] H. Wiener, Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.* **69** (1947) 17–20.