MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **67** (2012) 425-437

ISSN 0340 - 6253

Ordering Connected Graphs Having Small Degree Distances. II [1]

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(Received April 4, 2011)

Abstract

The parameter $D'(G)$ of a connected graph G is called the degree distance of G and was introduced by Dobrynin and Kochetova and independently by Gutman as a weighted version of the Wiener index. It is defined by

$$D'(G) = \sum_{x \in V(G)} d(x) \sum_{y \in V(G)} d(x,y)\,,$$

where $d(x)$ and $d(x,y)$ are the degree of x and the distance between x and y, respectively.

In a previous paper [14] the first author found three graphs having smallest degree distances. Here the next six graphs of order n in this sequence are determined provided $n \geq 15$: two have diameter 2, three diameter 3 and one diameter 4.

1. INTRODUCTION

Let G be a simple connected undirected graph having $|V(G)| = n$ vertices and $|E(G)| = m$ edges. The distance $d(x,y)$ between vertices x and y is defined as the length of a shortest path between them. The maximum distance $\max\limits_{y \in V(G)} d(x,y)$ from x to any other vertex is called the eccentricity of x and is denoted by $ecc(x)$. The diameter of G, denoted by $diam(G)$ is the maximum of the eccentricities, *i.e*, $\max\limits_{x \in V(G)} ecc(x) = \max\limits_{x,y \in V(G)} d(x,y)$. If

[1] This research is partially supported by Higher Education Commission, Pakistan.

$ecc(x)$ is minimum then x is called a central vertex. $K_{1,n-1}$ is the star of order n, consisting of one vertex of degree $n-1$ and $n-1$ pendant vertices, $K_{1,n-1}+e$ is obtained from $K_{1,n-1}$ by joining two vertices of degree one by an edge and the bistar $BS(p,q)$ of order $n=p+q+2$ consist of two vertex disjoint stars $K_{1,p}$ and $K_{1,q}$ plus one edge joining the central vertices of $K_{1,p}$ and $K_{1,q}$, respectively.

Topological indices based on distances between vertices of a graph are widely used in mathematical chemistry [3, 4] because of their correlations with physical, chemical and thermodynamic parameters of chemical compounds.

By denoting $D(x) = \sum_{y\in V(G)} d(x,y)$ and $D(G) = \sum_{x\in V(G)} D(x)$, we have $W(G) = \frac{D(G)}{2}$, where $W(G)$ is the Wiener index, a well−known topological index in mathematical chemistry.

The new parameter $D'(G)$, called the degree distance of G, was introduced by Dobrynin and Kochetova [5] and Gutman [6] as a weighted version of the Wiener index. The degree distance $D'(x)$ of a vertex x is defined as $D'(x) = d(x)D(x)$, where $d(x)$ is the degree of x and the degree distance of G, denoted by $D'(G)$ is

$D'(G) = \sum_{x\in V(G)} D'(x) = \sum_{x\in V(G)} d(x)D(x) = \frac{1}{2} \sum_{x,y\in V(G)} d(x,y)(d(x)+d(y))$.

This parameter was intensively studied in the literature. In [10] it was shown that for $n \geq 2$ in the class of connected graphs of order n, the minimum of $D'(G)$ equals $3n^2-7n+4$ and the unique extremal graph is $K_{1,n-1}$ and a conjecture raised in [5] was disproved. *In* [14] *the next graphs of order* $n \geq 4$ *having smallest degree distances were found: they are* $BS(n-3,1)$ *and* $K_{1,n-1}+e$, *having* $D'(BS(n-3,1)) = 3n^2-3n-8$ *and* $D'(K_{1,n-1}+e) = 3n^2-3n-6$ *, where* $BS(n-3,1)$ *denotes the bistar consisting of vertex disjoint stars* $K_{1,n-3}$ *and* $K_{1,1}$ *with central vertices joined by an edge.* In [1] and [13] the authors reported several properties of connected graphs of fixed order and size. In [11, 12] the minimum degree distance of unicyclic and bicyclic graphs was obtained; in the case of unicyclic graphs the unique extremal graph is $K_{1,n-1}+e$. In [2] an asymptotically sharp upper bound of degree distance of graphs with given order and diameter was presented and in [8] the degree distance of partial Hamming graphs was obtained. In [7] the maximum degree distance among unicyclic graphs on n vertices was deduced and in [9] the unicyclic graphs of order n and girth k, having minimal and maximal degree distances respectively, were characterized. In this paper the list of three graphs having smallest degree distances deduced in [14] is completed up with six new members. In order to prove this ordering, which holds for the number of vertices greater than or equal to 15, we need some preliminary results which are included in the next section.

2. PRELIMINARY RESULTS

The technical results which follow will be useful in the main section. As in [14] , for parameters $m\,,n\,,p\,,t \in \mathbb{N}$, $t\,,m\,,n \geq 2$ and $n+t-1 \leq p \leq nt$, denote by $S_{p\,,m,\,t}(x_1,...,x_n)$, the symmetric function

$$S_{p,\,m,\,t}(x_1,...,x_n) = \sum_{i=1}^{n} x_i(m-x_i)\,.$$

This function is defined for $(x_1,...,x_n) \in D_1$, where D_1 is the set of all vectors $(x_1,...,x_n)$ with positive integer coordinates such that $1 \leq x_i \leq t$ for $1 \leq i \leq n$, $x_1 \geq x_2 \geq ... \geq x_n$ and $\sum\limits_{i=1}^{n} x_i = p$. Note that $S_{p,\,m,\,t}$ is strictly increasing in each variable on D_1 if $m \geq 2n-2$ and $t \leq n-2$. Consider the following transformation denoted by T_1 of vectors in D_1: If $1 \leq i < j \leq n$ and $x_i \leq t-1$ and $x_j \geq 2$ then $(x_1,...,x_n)$ is replaced by $(x_1,...,x_i+1,...,x_j-1,...,x_n)$. By reordering the components of this vector we get the vector $(x_1^*,...,x_n^*) \in D_1$, which will be denoted by $\mathbf{z}$. Since $i < j$ implies $x_i \geq x_j$ we deduce as in [14] that $S_{p,\,m,\,t}(x_1,...,x_n) - S_{p,\,m,\,t}(\mathbf{z}) = 2 + 2(x_i - x_j) > 0$. Eventually applying several times T_1 we deduce:

Lemma 2.1.(a) $S_{p,\,m,\,t}(x_1,...,x_n)$ is minimum over D_1 if and only if there is an index k, $1 \leq k \leq n$ such that $x_1 = ... = x_k = t$, $1 \leq x_{k+1} \leq t-1$ and $x_i = 1$ for every $k+2 \leq i \leq n$.

(b) Let $D_1^* = D_1 \setminus (t,...,t,x_{k+1},1,...,1)$, where $(t,...,t,x_{k+1},1,...,1)$ is the unique point of minimum of $S_{p,\,m,\,t}(x_1,...,x_n)$ over D_1. Then $S_{p,\,m,\,t}(x_1,...,x_n)$ is minimum over D_1^* if and only if

$(x_1,...,x_n) = (t,...,t,t-2,2,1,...,1)$ if $x_{k+1} = t-1$;

$(x_1,...,x_n) = (t,...,t,t-1,x_{k+1}+1,1,...,1)$ if $x_{k+1} \in \{1,2\}$;

$(x_1,...,x_n) \in \{(t,...,t,t-1,x_{k+1}+1,1,...,1),(t,...,t,x_{k+1}-1,2,1,...,1)\}$ if $3 \leq x_{k+1} \leq t-2$.

Note that the index k may be precisely determined; since $kt+n-k \leq p \leq kt+n-k+t-2$ it follows that $k(t-1) \leq p-n \leq k(t-1)+t-2$, which implies $k = \lfloor \frac{p-n}{t-1} \rfloor$.

We shall use the function $F(x_1,...,x_r,y_1,...,y_{n-r})$ (defined in [14]) for $n,r \in \mathbb{N}$, $n \geq 4$,

$5 \le r \le n-2$, α , $\beta \in \mathbb{R}$ such that $\beta \ge \alpha + 1 \ge 2n-1$ by

$$F(x_1, ..., x_r, y_1, ..., y_{n-r}) = \sum_{i=1}^{r} x_i(\alpha - x_i) + \sum_{j=1}^{n-r} y_j(\beta - y_j).$$

It is symmetric in the first r variables and in the last $n-r$ variables. This time F is defined on an extended domain D_2 , consisting of all vectors $(x_1, ..., x_r, y_1, ..., y_{n-r})$ having positive integer coordinates such that $x_1 \ge x_2 \ge ... \ge x_r$; $y_1 \ge y_2 \ge ... \ge y_{n-r}$; $2 \le x_i \le \gamma$ for $1 \le i \le r$; $1 \le y_j \le \gamma$ for $1 \le j \le n-r$ and $\sum_{i=1}^{r} x_i + \sum_{j=1}^{n-r} y_j = \delta$, where $\gamma \in \{n-2, n-3\}$, $\delta \in \{2n-2, 2n\}$. For $\alpha = 2n-2$ and $\beta = 2n-1$, F is strictly increasing in each variable on D_2 . Consider now the transformation T_2 of vectors in D_2 defined by :

If $y_1 \ge 2$ then $(x_1, ..., x_r, y_1, ..., y_{n-r})$ is replaced by $(x_1, ..., x_r + y_1 - 1, 1, y_2, ..., y_{n-r})$; reorder separately the first r components and the last $n-r$ components and we get $\mathbf{z} = (x_1^*, ..., x_r^*, y_1^*, ..., y_{n-r}^*) \in D_2$. From given conditions it follows that $x_r + y_1 - 1 \le 2n - 1 - \sum_{i=1}^{r-1} x_i - \sum_{j=2}^{n-r} y_j \le n - r + 2 \le n - 3 \le \gamma$ for any $r \ge 5$. As in [14] we get $F(x_1, ..., x_r, y_1, ..., y_{n-r}) - F(\mathbf{z}) = (y_1 - 1)(\beta - \alpha - 2 + 2x_r) > 0$.

Lemma 2.2. If $F(x_1, ..., x_r, y_1, ..., y_{n-r})$ is minimum over D_2 then $(x_1, ..., x_r) = (\delta - n - r + 2, 2, ..., 2)$ and $(y_1, ..., y_{n-r}) = (1, ..., 1)$.

Proof. Suppose that $\mathbf{z}^0 = (x_1^0, x_2^0, ..., x_r^0, y_1^0, ..., y_{n-r}^0)$ is a point of minimum for F in D_2 . Applying T_1 on the first r components and the last $n-r$ components and T_2 we deduce that $x_3^0 = ... = x_r^0 = 2$ and $y_1^0 = ... = y_{n-r}^0 = 1$. x_1^0 takes the greatest possible value, which is less than or equal to γ . Also $x_1^0 = \delta - n - r + 4 - x_2^0 \le \delta - n - r + 2$, which implies $x_1^0 = \min(\delta - n - r + 2, \gamma)$ and $x_2^0 = \delta - n - r + 4 - x_1^0$.

If $r \ge 5$ then $\delta - n - r + 2 \le \delta - n - 3 \le n - 3 \le \gamma$, thus implying $x_1^0 = \delta - n - r + 2$ and $x_2^0 = 2$. ■

Lemma 2.3. [14] Let G be a connected graph of order n and x be a vertex of G having eccentricity equal to e . Then $D'(x) = (n-1)^2$ for $e = 1$, $D'(x) = d(x)(2n - 2 - d(x))$ for $e = 2$ and $D'(x) \ge d(x)(2n - d(x) + \frac{e^2 - 3e}{2} - 1)$ for $e \ge 3$.

Six graphs $G_1 - G_6$ of order n are represented in $Figure\,1$. G_1 is the bistar $BS(n-4, 2)$. We will show that they are the next members completing the sequence $K_{1,n-1}$, $BS(n-3, 1)$, $K_{1,n-1} + e$ of graphs having smallest degree distances, provided $n \ge 15$.

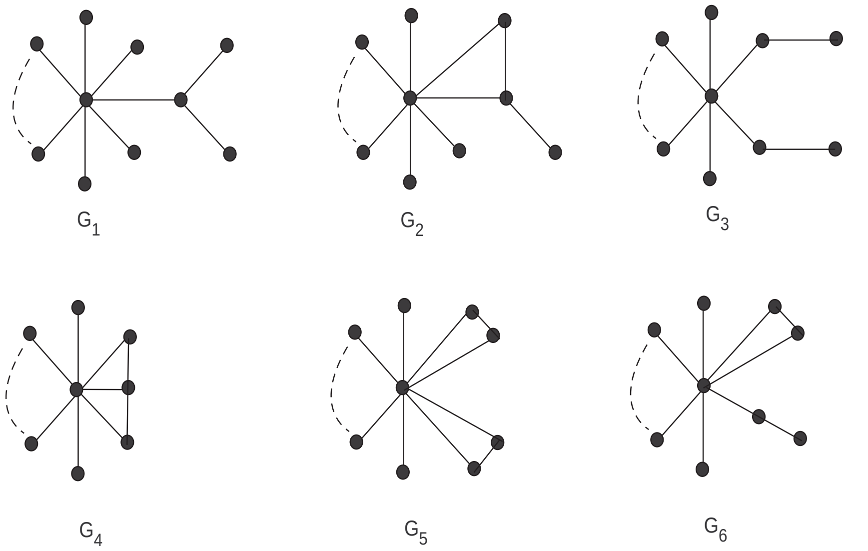

Figure 1: Six graphs of order n

By direct computations we deduce:

Lemma 2.4. For every $n \geq 5$ we have
$D'(G_1) = 3n^2+n-28\,;\; D'(G_2) = 3n^2+n-22\,;\; D'(G_3) = 3n^2+n-20\,;\; D'(G_4) = 3n^2+n-18$ and $D'(G_5) = D'(G_6) = 3n^2 + n - 16\,.$

3. MAIN RESULTS

We shall prove that unique graphs G of order n having $D'(G) \leq 3n^2 + n - 16$ are graphs $K_{1,n-1}, BS(n-3,1)\,, K_{1,n-1} + e$ and graphs $G_1 - G_6$ from $Figure\,1$ for $n \geq 15\,.$
This will be done by considering the cases when $diam(G) = 2, 3, 4$ or $diam(G) \geq 5\,.$

Lemma 3.1. All graphs G of order $n \geq 11$ and diameter 2 having $D'(G) \leq 3n^2 + n - 16$ are $K_{1,n-1}\,, K_{1,n-1} + e\,, G_4$ and $G_5\,.$

Proof. Let G be a graph of diameter 2 with $D'(G) \leq 3n^2 + n - 16\,.$ It follows that every vertex x of G has $ecc(x) = 1$(or equivalently, $d(x) = n-1$) or $ecc(x) = 2\,.$ If r denotes the number of vertices having eccentricity 1, by Lemma 2.3 we get

$$D'(G) = r(n-1)^2 + \sum_{x \in V(G); ecc(x)=2} d(x)(2n-2-d(x)),$$

where the sum has $n-r$ terms. Suppose $r=0$. If $x \in V(G)$ has $d(x)=1$ then the unique vertex y which is adjacent to x has $ecc(y)=1$, which contradicts the hypothesis. It follows that $2 \leq d(x) \leq n-2$ for every $x \in V(G)$, which implies that $d(x)(2n-2-d(x)) \geq 2(2n-4)$. In this case $D'(G) \geq 2n(2n-4) > 3n^2+n-16$ for every $n \geq 7$, which contradicts the hypothesis.

Hence G has $r \geq 1$ vertices of degree $n-1$. The function $d(x)(2n-2-d(x))$ is strictly increasing for $d(x)=1,...,n-1$ having a maximum equal to $(n-1)^2$.

If $r \geq 2$ it follows that all vertices x have $d(x) \geq 2$, which implies

$D'(G) \geq 2(n-1)^2 + 2(n-2)(2n-4) > 3n^2+n-16$ for every $n \geq 5$, a contradiction.

This implies that $r=1$ and G has a unique vertex z of degree $n-1$, hence G is deduced from $K_{1,n-1}$ eventually adding some new edges. If we add at most two edges we get $K_{1,n-1}$, $K_{1,n-1}+e$, G_4 and G_5 from $Figure\,1$.

We shall prove that if we add at least three edges then the resulting graph G will have $D'(G) > 3n^2+n-16$ for $n \geq 11$. Suppose that G is obtained from $K_{1,n-1}$ by adding exactly three edges, hence G has size $m=n+2$. If $x_1,...,x_{n-1}$ denote the degrees of the vertices adjacent to z, we obtain $x_i \geq 1$ for $1 \leq i \leq n-1$, $\sum_{i=1}^{n-1} x_i = n+5$ and

$$D'(G) = (n-1)^2 + \sum_{i=1}^{n-1} x_i(2n-2-x_i).$$

By Lemma 2.1 the minimum of the sum $S_{n+5,2n-2,n-2}$ in D_1 is reached for $x_1=7, x_2 = ... = x_{n-1} = 1$, which implies $D'(G) \geq (n-1)^2 + 7(2n-9) + (n-2)(2n-3) = = 3n^2+5n-56 > 3n^2+n-16$ for $n \geq 11$. Since $S_{p,2n-2,n-2}$ is strictly increasing in $p \geq n+5$ the proof is done. ■

Lemma 3.2. The set of graphs G of order $n \geq 15$, diameter 3 and $D'(G) \leq 3n^2+n-16$ contains only four members: $BS(n-3,1), G_1, G_2$ and G_6.

Proof. Let G be a connected graph of order $n \geq 15$, size $m \geq n-1$, diameter 3 and $D'(G) \leq 3n^2+n-16$. Since $diam(G)=3$ it follows that $d(x) \leq n-2$ for every $x \in V(G)$. We shall divide the proof in three cases: A. $m=n-1$; B. $m=n$ and C. $m \geq n+1$.

A. Consider first the case when $m=n-1$, i.e., G is a tree. Since G has diameter 3 it follows that G is a bistar $BS(r, n-2-r)$, where $1 \leq r \leq (n-3)/2$. By direct computation we obtain

$$D'(G) = 3n^2 - 7n + 4 - 4(r^2 - rn + 2r).$$

It results that $D'(G)$ is strictly increasing in $r \leq (n-3)/2$; for $r = 3$ we get $D'(G) = 3n^2 + 5n - 56 > 3n^2 + n - 16$ for every $n \geq 11$.

For $r = 1$, the resulting graph is $BS(n-3, 1)$ and for $r = 2$ we get G_1 from *Figure* 1. It remains to consider the case when $m \geq n$.

B. Suppose that $m = n$ and there is a vertex x such that $d(x) = n - 2$. There exist a vertex w which is not adjacent to x and two edges which are not incident to x. Since $diam(G) = 3$ we have only three possibilities to build such a graph, getting graphs G_2, G_6 and a graph, say F, deduced by making w adjacent to two vertices which are adjacent to x. By Lemma 2.4 we have $D'(G_2), D'(G_6) \leq 3n^2 + n - 16$ and by direct computation $D'(F) = 3n^2 + 2n - 24 > 3n^2 + n - 16$ for every $n \geq 9$.

Suppose that $m = n$ and $d(x) \leq n - 3$ for every vertex $x \in V(G)$. In this case we shall prove that $D'(G) > 3n^2 + n - 16$. Let $p \geq 0$ denote as above the number of vertices x of G having $ecc(x) = 2$; it results $n \geq p + 2$. We consider first the case when $p \geq 5$. By Lemma 2.3 we deduce that

$$D'(G) \geq \sum_{i=1}^{p} x_i(2n - 2 - x_i) + \sum_{j=1}^{n-p} y_j(2n - 1 - y_j),$$

where $x_1, ..., x_p$ and $y_1, ..., y_{n-p}$ are the degrees of vertices of eccentricity 2 and 3, respectively. Since $m = n$ we have $\sum_{i=1}^{p} x_i + \sum_{j=1}^{p} y_j = 2n$. From the hypothesis it follows that $x_i \leq n-3$ for $1 \leq i \leq p$ and $y_j \leq n-3$ for $1 \leq j \leq n-p$. If u is a vertex of eccentricity 2 and $d(u) = 1$, then the vertex v adjacent to u must have $d(v) = n - 1$, which contradicts the property that $diam(G) = 3$. It follows that $x_i \geq 2$ for every $i = 1, ..., p$. Using Lemma 2.2 for $F(x_1, ..., x_p, y_1, ..., y_{n-p})$, where $\alpha = 2n - 2$ and $\beta = 2n - 1$, we find that F is minimum for $x_1 = n - p + 2, x_2 = ... = x_p = 2$ and $y_1 = ... = y_{n-p} = 1$, which implies that

$D'(G) \geq (n-p+2)(n+p-4) + 2(p-1)(2n-4) + (n-p)(2n-2) = 3n^2 + 2np - 8n - p^2$.

We have $3n^2 + 2np - 8n - p^2 > 3n^2 + n - 16$ if and only if $n(2p - 9) > p^2 - 16$. This inequality is satisfied for $p = 5$ and $n \geq 10$. If $p \geq 6$ we can use inequality $n \geq p + 2$; we get $n(2p-9) \geq (p+2)(2p-9) = 2p^2 - 5p - 18$ and $2p^2 - 5p - 18 > p^2 - 16$ for any $p \geq 6$. Consequently, for $p \geq 5$ we have deduced that $D'(G) > 3n^2 + n - 16$. It remains to prove this inequality for $0 \le p \le 4$. If $p = 0$, $D'(G) \ge \sum_{j=1}^{n} y_j(2n-1-y_j)$, where $1 \le y_j \le n-3$ for $1 \le j \le n$ and $\sum_{j=1}^{n} y_j = 2n$. Using Lemma 2.1 the minimum of $S_{2n,2n-1,n-3}$ is reached for $y_1 = n-3, y_2 = 5, y_3 = ... = y_n = 1$ and is equal to $(n-3)(n+2) + 5(2n-6) + (n-2)(2n-2) = 3n^2 + 3n - 32 > 3n^2 + n - 16$ for every $n \ge 9$. If $1 \le p \le 4$ we can write $\sum_{i=1}^{p} x_i(2n-2-x_i) + \sum_{j=1}^{n-p} y_j(2n-1-y_j)$

$= \sum_{i=1}^{p} x_i(2n-2-x_i) + \sum_{j=1}^{n-p} y_j(2n-2-y_j) + \sum_{j=1}^{n-p} y_j$

$\ge \sum_{i=1}^{p} x_i(2n-2-x_i) + \sum_{j=1}^{n-p} y_j(2n-2-y_j) + n - p$.

By redenoting $y_1 = x_{p+1}, ..., y_{n-p} = x_n$, we get $D'(G) \ge \sum_{i=1}^{n} x_i(2n-2-x_i) + n - p$, where $1 \le x_i \le n-3$ for $1 \le i \le n$ and $\sum_{i=1}^{n} x_i = 2n$. By Lemma 2.1 we obtain that the minimum of $S_{2n,2n-2,n-3}$ is reached for $(n-3, 5, 1, ..., 1)$. But this sequence of degrees is not graphical. From Lemma 2.1(b) it follows that the next minimum of this function is reached for $(n-4, 6, 1, ..., 1)$ or for $(n-3, 4, 2, 1, ..., 1)$. We have $S_{2n,2n-2,n-3}(n-4, 6, 1, ..., 1) = 3n^2 + 3n - 50 > S_{2n,2n-2,n-3}(n-3, 4, 2, 1, ..., 1) = 3n^2 + n - 26$ for every $n \ge 13$. Consequently, since $n - p \ge n - 4$, $D'(G) \ge 3n^2 + n - 26 + n - 4 = 3n^2 + 2n - 30 > 3n^2 + n - 16$ for every $n \ge 15$.

C. If $m = n + 1$ and there is a vertex x such that $d(x) = n - 2$, it follows that $ecc(x) = 2$ and $D'(x) = n(n-2)$ by Lemma 2.3. By denoting by $p \ge 1$ the number of vertices of eccentricity 2 of G, the number of vertices of eccentricity 3 will be $n - p$. Let $x_2, ..., x_p$ be the degrees of the vertices of eccentricity 2 of G which are different from x and $y_1, ..., y_{n-p}$ be the degrees of the vertices of eccentricity 3 of G, arranged in a decreasing order. One has $D'(G) \ge n(n-2) + \sum_{i=2}^{p} x_i(2n-2-x_i) + \sum_{j=1}^{n-p} y_j(2n-1-y_j) =$

$= n(n-2) + \sum_{i=2}^{p} x_i(2n-2-x_i) + \sum_{j=1}^{n-p} y_j(2n-2-y_j) + \sum_{j=1}^{n-p} y_j$

$\ge n(n-2) + \sum_{i=2}^{n} x_i(2n-2-x_i) + n - p$, by redenoting $y_1 = x_{p+1}, ..., y_{n-p} = x_n$.

We have $\sum_{i=2}^{n} x_i = n + 4$. By Lemma 2.1 the minimum of $S_{n+4,2n-2,n-2}(x_1, ..., x_{n-1})$ is reached for $(6, 1, ..., 1)$ and it is equal to $6(2n-8) + (n-2)(2n-3) = 2n^2 + 5n - 42$. The extremities of a diametral path in G have eccentricities equal to 3, which implies $n \ge p+2$, or $n - p \ge 2$. It follows that $D'(G) \ge n(n-2) + 2n^2 + 5n - 42 + 2 = 3n^2 + 3n - 40 > 3n^2 + n - 16$ for any $n \ge 13$. Because $S_{q,2n-2,n-2}(x_1, ..., x_{n-1})$ is increasing for $q \ge n + 4$, we deduce that $D'(G) > 3n^2 + n - 16$ for any $m \ge n + 1$ and $n \ge 13$ if there is a vertex x of degree

$n-2$.
Note that for $m=n+1$ and $d(x) \leq n-3$ for every vertex $x \in V(G)$, the minimum of $S_{2n+2,2n-2,n-3}$ over D_1 is reached for $(n-3,7,1,...,1)$ and is equal to $3n^2+5n-60$. In this case $D'(G) \geq 3n^2+6n-64$ since $n-p \geq n-4$ and $3n^2+6n-64 > 3n^2+n-16$ for every $n \geq 10$. Since $S_{q,2n-2,n-3}$ is increasing for $q \geq 2n+2$, it follows that for $m \geq n+2$ and $d(x) \leq n-3$ for every vertex $x \in V(G)$, $D'(G) > 3n^2+n-16$ holds, which concludes the proof. $\blacksquare$

Lemma 3.3. There exists a unique graph G of order $n \geq 13$ having $diam(G)=4$ and $D'(G) \leq 3n^2+n-16$, namely G_3.

Proof. Suppose G is a graph of diameter 4, order $n \geq 13$ and $D'(G) \leq 3n^2+n-16$. It follows that $d(x) \leq n-3$ for every $x \in V(G)$. We shall prove that if $m=n-1$, i.e, G is a tree, then $G=G_3$. In this case the center of G consists of a single vertex w since the diameter is even. Denote by $p \geq 2$ the number of vertices x having $ecc(x)=4$; it follows that $n-p-1$ vertices y have eccentricity $ecc(y)=3$, only w having eccentricity $ecc(w)=2$. All vertices x with $ecc(x)=4$ have $d(x)=1$. It results that $\sum\limits_{ecc(y)=3} d(y)=n-1$ since $d(w)=n-p-1$. Since $d(w) \geq 2$ it follows that $n \geq p+3$. If $p=2$ we deduce that $G=G_3$. Suppose that $p \geq 3$. Let $N_i(u)=\{v \in V(G) : d(u,v)=i\}$. If there is a vertex z of eccentricity 4 such that $|N_2(z)|=p$, by denoting by y the vertex of eccentricity 3 adjacent to z we obtain $d(y)=p+1$. It results that y is adjacent to all vertices of G of eccentricity 4 which would imply that $diam(G)=3$, a contradiction. Suppose that there exists a vertex z such that $ecc(z)=4$ and $|N_2(z)|=p-1$.
In this case there is a unique tree H illustrated in $Figure\,2$ having these properties, where $d(w)=n-p-1$ and $d(y)=p$. By direct computation we get $D'(H)=3n^2-7n+4np-4p^2-4$. We have $D'(H) > 3n^2+n-16$ if and only if $n(4p-8) > 4p^2-12$. For $p=3$ this inequality holds for every ≥ 7. Let $p \geq 4$. Since $n \geq p+3$ we deduce $n(4p-8) \geq 4p^2+4p-24 > 4p^2-12$ for any $p \geq 4$. The remaining situation is that when for every vertex z of eccentricity 4 we have $|N_2(z)| \leq p-2$. We need a more careful evaluation of the lower bound for $D'(z)$. Since $d(z)=1$ and $|N_3(z)|=n-p-2$ we get $|N_2(z)|=n-1-(1+n-p-2)-|N_4(z)|=p-|N_4(z)|$. Since $|N_2(z)| \leq p-2$ it follows that $|N_4(z)| \geq 2$. We can write $D'(G)=1+2|N_2(z)|+3(n-p-2)+4|N_4(z)|=1+2p+3(n-p-2)+2|N_4(z)| \geq 3n-p-1$ since $|N_4(z)| \geq 2$. Finally,

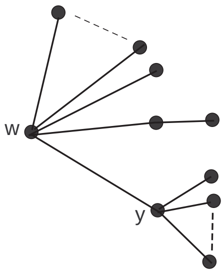

Figure 2: Tree H

$D'(G) \geq (n-p-1)(n+p-1) + \sum\limits_{ecc(y)=3} d(y)(2n-1-d(y)) + 3np - p^2 - p$. The minimum value of $\sum\limits_{ecc(y)=3} d(y)(2n-1-d(y))$ is realized, by Lemma 2.1 for $(p+1, \underbrace{1, ..., 1}_{n-p-2})$. But this sequence of degrees of vertices of eccentricity 3 cannot be realized by a tree of diameter 4 since a unique vertex has its degree greater than 1. By Lemma 2.1 the next minimum value of $S_{2n-2,2n-1,n-3}$ is realized for $(p, 2, \underbrace{1, ..., 1}_{n-p-3})$. It follows that

$D'(G) \geq (n-p-1)(n+p-1) + p(2n-1-p) + 2(2n-3) + (n-p-3)(2n-2) + 3np - p^2 - p = 3n^2 + 3np - 6n - 3p^2 + 1$.

$D'(G) > 3n^2 + n - 16$ holds if $n(3p-7) > 3p^2 - 17$. If $p \geq 3$ and $n \geq p+3$ the expression $n(3p-7)$ is greater than or equal to $3p^2 + 2p - 21$ and this polynomial is strictly greater than $3p^2 - 17$ for every $p \geq 3$.

Let now $m = n$. By Lemma 2.3 we deduce

$D'(G) \geq \sum\limits_{ecc(x)=2} d(x)(2n-2-d(x)) + \sum\limits_{ecc(y)=3} d(y)(2n-1-d(y)) + \sum\limits_{ecc(z)=4} d(z)(2n+1-d(z))$.

Let u, a, t, b, v be a shortest path of length 4 between two vertices of eccentricity 4. It follows that $ecc(a), ecc(b) \geq 3$ and $d(a), d(b) \geq 2$. Since $d(y)(2n-1-d(y)) = d(y)(2n-2-d(y)) + d(y)$ and $d(z)(2n+1-d(z)) = d(z)(2n-2-d(z)) + 3d(z)$, it results that $D'(G) \geq \sum\limits_{x \in V(G)} d(x)(2n-2-d(x)) + 10$, where $\sum\limits_{x \in V(G)} d(x) = 2n$. Since $diam(G) = 4$ we get $d(x) \leq n-3$ for any $x \in V(G)$. For $p = 2n, m = 2n-2$ and $t = n-3$, the minimum of $S_{2n,2n-2,n-3}(x_1, ..., x_n)$ in D_1 is realized for $x_1 = n-3, x_2 = 5, x_3 = ... = x_n = 1$. But the sequence $(n-3, 5, 1, ..., 1)$ is not graphical. By Lemma 2.1 the next minimum of $S_{2n,2n-2,n-3}$ is realized for $\mathbf{z}^1 = (n-4, 6, 1, ..., 1)$ or $\mathbf{z}^2 = (n-3, 4, 2, 1, ..., 1)$.

In the first case we get $D'(G) \geq 3n^2 + 3n - 40 > 3n^2 + n - 16$ for every $n \geq 13$ and in the second case $D'(G) = 3n^2 + n - 16$. Equality is reached only for $\mathbf{z}^2$, which has a unique graphical realization, having diameter 3, which contradicts the hypothesis. We can conclude that for $m = n$ for all graphs G of order n, size m and diameter 4 $D'(G)$ is strictly greater than $3n^2 + n - 16$.

Let $m = n + 1$. The minimum of $S_{2n+2,2n-2,n-3}$ is realized for $(n-3, 7, 1, ..., 1)$ and is equal to $3n^2 + 5n - 60$. We deduce $D'(G) \geq 3n^2 + 5n - 50 > 3n^2 + n - 16$ for $n \geq 9$. For $m \geq n + 2$, $S_{p,2n-2,n-3}$ being increasing in $p \geq 2n + 2$, the same conclusion holds. ■

lemma 3.4. Let G be a graph of order $n \geq 8$ and diameter $diam(G) \geq 5$. Then $D'(G) > 3n^2 + n - 16$.

Proof. If G has diameter at least 5 it follows that for every $x \in V(G)$ we have $ecc(x) \geq 3$ since otherwise, by triangle inequality, we obtain $diam(G) \leq 4$. The same conclusion holds if there exists a vertex x having $d(x) \geq n - 3$. It follows that $d(x) \leq n - 4$ for every $x \in V(G)$. Since $ecc(x) \geq 3$, by Lemma 2.3 we obtain that $D'(x) \geq d(x)(2n - 1 - d(x))$, which implies that $D'(G) \geq \sum_{x \in V(G)} d(x)(2n - 1 - d(x))$. Suppose that G has diameter 5 and it is a tree, hence $m = n - 1$. It follows that $D'(G) \geq S_{2n-2,2n-1,n-4}(x_1, ..., x_n)$, where $x_1, ..., x_n$ are the degrees of the vertices of G. By Lemma 2.1 it follows that the minimum of $S_{2n-2,2n-1,n-4}$ is reached in D_1 for $x_1 = n - 4, x_2 = 4$ and $x_3 = ... = x_n = 1$ and is equal to $(n-4)(n+3) + 4(2n-5) + (n-2)(2n-2) = 3n^2 + n - 28$. Note that $(n - 4, 4, 1, ..., 1)$ has a unique graphical realization which has diameter 3. If G has diameter 5, let u, v be two diametral vertices of G and u, x, w, t, y, v be a shortest path between them. It follows that $ecc(u) = ecc(v) = 5, ecc(x) \geq 4, ecc(y) \geq 4$ and $d(x), d(y) \geq 2$. This implies that $D'(u) \geq d(u)(2n + 4 - d(u))$ and the difference $d(u)(2n + 4 - d(u)) - d(u)(2n - 1 - d(u)) = 5d(u) \geq 5$. In a similar way we get $D'(x) \geq d(x)(2n + 1 - d(x))$ and $d(x)(2n + 1 - d(x)) - d(x)(2n - 1 - d(x)) = 2d(x) \geq 4$. It follows that we can write $D'(G) \geq 3n^2 + n - 28 + 2(5 + 4) = 3n^2 + n - 10 > 3n^2 + n - 16$ for every n.

The inequality $D'(G) \geq \min_{x_1 + ... + x_n = 2n-2} S_{2n-2,2n-1,n-4}(x_1, ..., x_n) + 18$ also holds if $diam(G) > 5$ and the constant 18 may be improved by a similar argument. Since $S_{p,2n-1,n-4}$ is strictly increasing in $p \geq 2n - 2$, it follows that $D'(G) > 3n^2 + n - 16$ for any connected graph G of order n, size $m \geq n - 1$ and diameter $diam(G) \geq 5$. ■

The main result of the paper can be concluded as follows:

Theorem 3.5. The connected graphs of order $n \geq 15$ having the smallest degree distances are (in this order): $K_{1,n-1}$, $BS(n-3,1)$, $K_{1,n-1}+e$, G_1, G_2, G_3, G_4, G_5, G_6 , the last two graphs having equal degree distances.

Note that the degree distance and the Wiener index of trees are connected by relation $D'(G) = 4W(G) - n(n-1)$ [6], which implies that the ordering of trees on n vertices with respect to the Wiener index is the same for the degree distance parameter. There are various transformations on trees and general graphs (see [9]) that decrease degree distance and/or Wiener index. On this way the first four extremal trees and unicyclic graphs having small degree distance could be also determined using this method.

Acknowledgement. The authors are indebted to the referee for his/her valuable comments. This work has been done while the first author was invited at Abdus Salam School of Mathematical Sciences, GC University, Lahore.

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