BOUNDS FOR DEGREE DISTANCE OF A GRAPH

SALMA KANWAL and IOAN TOMESCU

Communicated by Vasile Brînzănescu

Let G be a simple connected graph with vertex set $V(G)$, then the degree distance of G, $D'(G)$, is defined as

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

where $d(x)$ and $d(x,y)$ are the degree of x and the distance between x and y, respectively. In this paper, lower and upper bounds on $D'(G)$ are obtained in terms of various graphical parameters like first Zagreb index, order, size, diameter, radius, minimum degree, and graphs for which these bounds are attained are characterized.

AMS 2010 Subject Classification: Primary 05C12.

Key words: degree distance, first Zagreb index, eccentricity, diameter, regular graph, perfect matching.

1. INTRODUCTION AND NOTATION

In the last few years, a large number of mathematical investigations were reported on graph invariants originating from chemistry, and which have chemical applications (see [5, 6, 10, 14]). Quite a few of these graph invariants are based on vertex degrees and the distances between vertices. In this paper an invariant of connected graphs called the degree distance is considered. Let G be a connected graph of order n and $V(G)$ be its vertex set. We denote the degree of a vertex $x \in V(G)$ by $d(x)$ and the distance between vertices $x, y \in V(G)$ by $d(x,y)$. The expression $\sum_{x \in V(G)} d^2(x)$ is known as first Zagreb index of G, denoted by $Zg(G)$ [9]. The degree distance of G is defined as

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

The degree distance was first considered by Dobrynin and Kochetova [7] and by Gutman [8], who used a different name for it. The degree distance of a vertex $x \in V(G)$ is given by $D'(x) = d(x) \sum\limits_{y \in V(G)} d(x,y)$; we get $D'(G) =$

$\sum_{x \in V(G)} D'(x)$. Another molecular descriptor is the molecular topological index of G, denoted by $MTI(G)$ [13] and is defined by $MTI(G) = Zg(G) + D'(G)$.

The eccentricity $ecc(x)$ of a vertex x is $ecc(x) = \max_{y \in V(G)} d(x, y)$. If $diam(G)$ and $rad(G)$ denote the diameter and radius of a connected graph G respectively, then $diam(G) = \max_{x \in V(G)} ecc(x)$ and $rad(G) = \min_{x \in V(G)} ecc(x)$. Let $N_i(x) = \{y : d(x, y) = i\}$ for every $0 \le i \le ecc(x)$. The minimum degree and maximum degree of G are denoted by $\delta(G)$ and $\Delta(G)$, respectively. A perfect matching of a graph G is a subset M of the edge set of G such that
(a) every two edges of M have no common end;
(b) every vertex of G is incident to an edge of M.

Note that if G has a perfect matching then its order is even. As usual, we denote by K_n and $K_{a,b}$ the complete graph on n vertices and the complete bipartite graph on $a + b$ vertices with parts of size a and b.

In the mathematical literature $D'(G)$ was investigated by many people. In [17] it was shown that for $n \ge 2$ in the class of connected graphs of order n, minimum of $D'(G)$ equals $3n^2 - 7n + 4$ and the unique extremal graph is $K_{1,n-1}$, thus solving a conjecture proposed by Dobrynin and Kochetova [7]. In [2, 17, 18] several properties of the degree distance of connected graphs of fixed order and size were determined. In [15] and [16] it was shown that in the class of connected unicyclic graphs of order n the unique graph having minimum degree distance is $K_{1,n-1} + e$. An ordering of unicyclic graphs by their degree distance was deduced in [3] and unicyclic graphs with maximum degree distance were studied in [11]. In [20], authors presented an ordering of connected graphs having small degree distances, by introducing six new members in the list consisting of three graphs having minimum degree distance [19]. In [12], n-vertex unicyclic graphs with girth k, having minimum and maximum degree distance were characterized and was proved that the graph B_n, obtained from two triangles linked by a path, is the unique graph having the maximum degree distance among bicyclic graphs of order n.

In [4], Dankelmann, Gutman, Mukwembi and Swart gave an asymptotically sharp upper bound $D'(G) \le \frac{1}{4}nd(n-d)^2 + O(n^{\frac{7}{2}})$ for graphs of order n and diameter d and as a corollary they obtained the bound $D'(G) \le \frac{1}{27}n^4 + O(n^{\frac{7}{2}})$ for graphs of order n; this essentially proves a conjecture proposed by Tomescu [17]. In [21] Zhou and Trinajstić reported some properties of the reverse degree distance, including its bounds for connected (molecular) graphs, expressed in terms of other indices like first Zagreb index and Wiener index. For a connected graph of order n, size m and diameter d, since reverse degree distance ${}^rD'(G)$ and degree distance are related by

$${}^rD'(G) = 2(n-1)md - D'(G),$$

properties given in [21] give us some further information about relationship of degree distance with other indices.

In this paper, we present upper and lower bounds for the degree distance of simple connected graphs in terms of different graph invariants like first Zagreb index, radius, diameter and minimum degree, and characterize graphs for which these bounds are best possible.

2. BOUNDS ON DEGREE DISTANCE

LEMMA 2.1. *Let G be a connected graph of order n and $x \in V(G)$ such that $ecc(x) = p$. Then:*

$$D'(x) \geq d(x)(2n - d(x) + \frac{p^2 - 3p}{2} - 1); \tag{1}$$

$$D'(x) \leq d(x)(d(x) + p(n - d(x)) - \frac{p^2 - p}{2} - 1). \tag{2}$$

Equality holds in (1) if and only if:

$$p = 1 or p = 2 or p \geq 3 and |N_3(x)| = \ldots = |N_p(x)| = 1.$$

Equality holds in (2) if and only if: $p = 1$ or $p = 2$ or $p \geq 3$ and $|N_2(x)| = \ldots = |N_{p-1}(x)| = 1$.

Proof. For $p = 1$ and $p = 2$ we have $D'(x) = (n-1)^2$ and $D'(x) = d(x)(2n - 2 - d(x))$, respectively, and both (1) and (2) are equalities.

Let $p \geq 3$. The minimum value of $D'(x)$ is reached only for $|N_2(x)| = n - d(x) - p + 1$ and $|N_i(x)| = 1$ for every $3 \leq i \leq p$, thus giving $D'(x) \geq d(x)(d(x) + 2(n - d(x) - p + 1) + 3 + 4 + \ldots + p) = d(x)(2n - d(x) + \frac{p^2-3p}{2} - 1)$.

The maximum value is attained only for $|N_p(x)| = n - d(x) - p + 1$ and $|N_i(x)| = 1$ for every $2 \leq i \leq p - 1$.

In this case $D'(x) = d(x)(d(x) + 2 + 3 + \ldots + (p-1) + p(n - p - d(x) + 1)) = d(x)(d(x) + p(n - d(x)) - \frac{p^2-p}{2} - 1)$. □

Note that inequality (1) was used in [19, 20]. Since in a shortest path of length $ecc(x)$ starting from x there are $ecc(x) + 1$ vertices, it follows that $ecc(x) + 1 + d(x) - 1 \leq n$, or

$$ecc(x) + d(x) \leq n \tag{3}$$

holds for every vertex $x \in V(G)$. We need the following result.

LEMMA 2.2. *For any connected graph G of order n, we have*

$$diam(G) + \Delta(G) \leq n + 1. \tag{4}$$

Proof. Let $x \in V(G)$ such that $\Delta(G) = d(x)$. Let $diam(G) = d$ so there exists at least one diametral path P in G of length d. We have the following three possibilities for x:

(a) x is an end of P.

(b) x lies on P but is not an end.

(c) x does not lie on P.

(a) When x is an end of the diametral path P, then $ecc(x) = d$ and since in a shortest path of length d starting from x there are $d+1$ vertices, it follows that $d + 1 + \Delta(G) - 1 \leq n$ or $d + \Delta(G) \leq n$. So we are done in this case.

(b) In this case x lies on P but is not an end of P, so x is adjacent to exactly two vertices on P as otherwise diameter d will decrease, so $\Delta(G) \leq n - (d+1) + 2$, or $\Delta(G) + d \leq n + 1$, as desired.

(c) When x does not lie on P then it can only be adjacent to at most 3 (consecutive) vertices on P, so $\Delta(G) \leq n - (d + 1 - 3) - 1$, or $\Delta(G) + d \leq n + 1$. $\square$

THEOREM 2.3. *Let G be a connected graph of order n, size m and diameter equal to d. We have*

$$D'(G) \leq (1-d)Zg(G) + 2mnd - (d^2 - d + 2)m. \tag{5}$$

Equality holds if and only if G is K_n or a graph of diameter 2.

Proof. Denote

$$\varphi(z) = -\frac{z^2}{2} + z(n - d(x) + \frac{1}{2}) - 1. \tag{6}$$

This function is strictly increasing for $z \in [1, n - d(x) + \frac{1}{2}]$. For integer values of z it takes two equal maximum values for $z = n - d(x)$ and $z = n - d(x) + 1$. Lemma 2.2 implies that for every vertex x we have $d + d(x) \leq d + \Delta(G) \leq n + 1$, or $d \leq n - d(x) + 1$ for all $x \in V(G)$. Since $ecc(x) \leq d$ for every $x \in V(G)$ this gives us $\varphi(ecc(x)) \leq \varphi(d)$ for every vertex $x \in V(G)$.

From (2) we get

$$D'(x) \leq d(x)(d(x) + d(n - d(x)) - \frac{d^2 - d}{2} - 1). \tag{7}$$

Finally, from (7) we deduce

$$D'(G) = \sum_{x \in V(G)} D'(x) \leq \sum_{x \in V(G)} d^2(x)(1-d) + \sum_{x \in V(G)} d(x)(nd - \frac{d^2 - d}{2} - 1),$$

which implies (5) since $\sum_{x \in V(G)} d(x) = 2m$. Suppose that equality holds in (5). Since (7) is an equality for every $x \in V(G)$ it follows that vertices of G have equal eccentricities $ecc(x) = d$ and by Lemma 2.1, if $d \geq 3$ then $|N_2(x)| = \ldots = |N_{d-1}(x)| = 1$ for every $x \in V(G)$.

If $d \geq 4$ consider a shortest path $x_1, x_2, \ldots, x_5$ in G. In this case $d(x_3, x_1) = d(x_3, x_5) = 2$, hence $|N_2(x_3)| \geq 2$, a contradiction. It follows that $1 \leq d \leq 3$. Suppose that $d = 3$ and let x_1, x_2, x_3, x_4 be a shortest path of length 3 in G.

Since $N_2(x_1) = \{x_3\}$, it follows that $ecc(x_2) = 2$, a contradiction. The remaining cases are $d = 1$, when G is K_n or $d = 2$, when G is a graph of diameter 2.

If $d = 1$ or 2 (7) is an equality for every $x \in V(G)$, which implies that (5) is also an equality. □

Corollary 2.4. *Let G be a connected graph of order n, size m and diameter d. Then*

$$D'(G) \leq 2mnd - (d-1)\frac{4m^2}{n} - (d^2 - d + 2)m. \tag{8}$$

Equality holds if and only if G is K_n or a regular graph of diameter 2.

Proof. Since (5) holds, by the Cauchy- Schwarz inequality we have $nZg(G) = n\sum_{x \in V(G)} d^2(x) \geq 4m^2$,*i.e.*, $Zg(G) \geq \frac{4m^2}{n}$. Since $1 - d \leq 0$ this implies $(1-d)Zg(G) \leq (1-d)\frac{4m^2}{n}$ and (8) is proved.

Suppose that equality holds in (8). In this case the equality in the Cauchy-Schwarz inequality holds if and only if G is regular. But from Theorem 2.3 G is K_n, which is regular, or a graph of diameter 2 which must be also regular. □

Theorem 2.5. *If G is a connected graph of order n, size m and minimum degree $\delta(G) = \delta$, then*

$$D'(G) \leq m(n^2 + n + 2) + n\delta(\frac{\delta^2}{2} - n\delta + \frac{\delta}{2}). \tag{9}$$

Equality holds if and only if G is K_n or n is even and G is deduced from K_n by deleting the edges of a perfect matching.

Proof. The maximum value of $\varphi(z)$ defined by (6) for integer values of z is equal to

$$\varphi(n - d(x)) = \frac{n^2}{2} + \frac{n}{2} - 1 + \frac{d^2(x)}{2} - nd(x) - \frac{d(x)}{2}.$$

From (2) and (3) we get

$$D'(x) \leq d(x)(\frac{n^2}{2} + \frac{n}{2} - 1 + \frac{d^2(x)}{2} - nd(x) + \frac{d(x)}{2}). \tag{10}$$

Since the function

$$\psi(z) = \frac{z^3}{2} - z^2(n - \frac{1}{2})$$

is strictly decreasing for $z \in [1, n-1]$, it follows that

$$d(x)(\frac{d^2(x)}{2} - nd(x) + \frac{d(x)}{2}) \leq \delta(\frac{\delta^2}{2} - n\delta + \frac{\delta}{2})$$

for every $x \in V(G)$. Finally, from (10) we deduce

$$D'(G) = \sum D'(x) \leq (\frac{n^2}{2} + \frac{n}{2} - 1) \sum_{x \in V(G)} d(x) + n\delta(\frac{\delta^2}{2} - n\delta + \frac{\delta}{2})$$

$$= m(n^2 + n - 2) + n\delta(\frac{\delta^2}{2} - n\delta + \frac{\delta}{2}).$$

Suppose that equality holds in (9). In this case $d(x) = \delta$ for every $x \in V(G)$ *i.e.*, G is δ-regular and $ecc(x) = n - d(x)$, or $ecc(x) + d(x) = n$ for every vertex $x \in V(G)$. It follows that vertices of G have equal eccentricities $ecc(x) = p = n - \delta$ and by Lemma 2.1 if $p \geq 3$ then $|N_2(x)| = \ldots = |N_{p-1}(x)| = 1$ for every $x \in V(G)$.

If $p \geq 4$ consider a shortest path $x_1, x_2, \ldots, x_5$ in G. In this case $d(x_3, x_1) = d(x_3, x_5) = 2$, hence $|N_2(x_3)| \geq 2$, a contradiction. It follows that $1 \leq p \leq 3$. Suppose that $p = 3$ and let x_1, x_2, x_3, x_4 be a shortest path of length 3 in G.

Since $N_2(x_1) = \{x_3\}$ it follows that $ecc(x_2) = 2 < p$, a contradiction. The remaining cases are $p = 1$, when G is K_n or $p = 2$. In the last case it follows that $d(x) = n - 2$ for every $x \in V(G)$, which implies that n is even and G is deduced from K_n by deleting the edges of a perfect matching. □

If G is a connected graph of order n, size m and diameter $d = 2$, then $D'(G) = 2m(2n-2) - Zg(G)$ and Corollary 2.4 yields

$$D'(G) \leq 2m(2n-2) - \frac{4m^2}{n}. \tag{11}$$

Equality holds in (11) if and only if G is a regular graph.

Since almost all graphs of order n have diameter equal to 2 as $n \to \infty$ [1], the following corollary holds.

COROLLARY 2.6. *For almost all connected graphs G of order n and size m the following inequality holds as $n \to \infty$: $D'(G) \leq 2m(2n-2) - \frac{4m^2}{n}$.*

THEOREM 2.7. *Let G be a connected graph of order n, size m and radius equal to r. We have*

$$D'(G) \geq m(2n - 2 + r^2 - r).$$

Equality holds if and only if G is K_n or n is even and G is obtained from K_n by deleting the edges of a perfect matching.

Proof. Since (3) holds it follows that $n - d(x) \geq ecc(x)$, and from (1) we deduce that $D'(x) \geq d(x)(n-1+(ecc(x)^2-ecc(x))/2) \geq d(x)(n-1+(r^2-r)/2)$, thus implying $D'(G) \geq m(2n-2+r^2-r)$.

Suppose that equality holds in (12). It follows that equality holds in (1), or $n - d(x) = ecc(x)$ and also $ecc(x) = r$ for every $x \in V(G)$, i. e., G is regular of degree $n-r$ and has diameter equal to r. Moreover, if $r \geq 3$ then $|N_3(x)| = \ldots = |N_r(x)| = 1$ holds for every $x \in V(G)$. We also have $|N_2(x)| = n - r - d(x) + 1 = 1$ for every $x \in V(G)$. By an argument similar to that used in the proof of Theorem 2.3 we deduce that $r \leq 3$. If $r = 3$ let x, u_1, u_2, u_3 be a shortest path in G. It follows that $N_2(x) = \{u_2\}, N_3(x) = \{u_3\}$. As above, we get $ecc(u_1) = 2$, a contradiction.

Finally, we have $r = 1$ or $r = 2$. For $r = 1$ G is K_n and for $r = 2$ G is $(n-2)$-regular, hence n is even and G may be obtained from K_n by deleting the edges of a perfect matching. □

Acknowledgments. This research was partially supported by Higher Education Commission of Pakistan.

REFERENCES

[1] B. Bollobás, *Modern Graph Theory.* Graduate Texts in Mathematics **184**, Springer − Verlag, New York, 1998.

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

[3] A. Chen, *Ordering unicyclic graphs by their degree distance.* J. of Fuzhou Univ. Nat. Sci. **32**, 664–668 (2004).

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

[5] J. Devillers and A.T. Balaban (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR.* Gordon and Breach, Amsterdam, 1999.

[6] M.V. Diudea, I. Gutman and L. Jäntschi, *Molecular Topology.* Nova, New York, 2001.

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

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

[9] I. Gutman and N. Trinajstić, *Graph theory and molecular orbitals III. Total π − electron energy of alternant hydrocarbons.* Chem. Phys. Lett. **17** (1972), 535–538.

[10] I. Gutman and B. Furtula (Eds.), *Novel Molecular Structure Descriptors − Theory and Applications.* **I–II**, Univ. Kragujevac, Kragujevac, 2010.

[11] Y. Hou and A. Chang, *The unicyclic graphs with maximum degree distance.* J. Math. Study **39** (2006), 18–24.

[12] A. Ilić, D. Stevanović, L. Feng, G. Yu and P. Dankelmann, *Degree distance of unicyclic and bicyclic graphs.* Discrete Appl. Math. **159** (2011), 779–788.

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

[14] R. Todeschini and V. Consonni, *Molecular Descriptors for Chemoinformatics.* Wiley-VCH, Weinheim, 2009.

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

[16] A.I. Tomescu, *Minimal graphs with respect to the degree distance.* Technical Report, University of Bucharest, 2008. Available online at:
http://sole.dimi.uniud.it/~alexandru.tomescu/files/dd-distance.pdf.

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

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

[19] I. Tomescu, *Ordering connected graphs having small degree distances.* Discrete Appl. Math. **158** (2010), 1714–1717.

[20] I. Tomescu and S. Kanwal, *Ordering connected graphs having small degree distances. II.* MATCH Commun. Math. Comput. Chem. **67** (2012), 425–437.

[21] B. Zhou and N. Trinajstić, *On reverse degree distance.* J. Math. Chem. **47** (2010), 268–275.

Received 7 November 2013

Lahore College For Women University,
Lahore – Pakistan
salma.kanwal055@gmail.com

Faculty of Mathematics and Computer Science,
University of Bucharest,
010014 Bucharest, Romania
ioan@fmi.unibuc.ro