Degree Distance of a Graph: A Degree Analogue of the Wiener Index

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A novel graph invariant defined as $D'(G) = \sum_{v\in v(G)} \deg(v)\, D(v)$, where $D(v)$ is the sum of distances between v and all vertices of a graph G, is considered. Properties of the invariant are compared with properties of the Wiener index. A conjecture concerning decomposition of the Wiener index for graphs of cata-condensed benzenoid hydrocarbons is proposed.

INTRODUCTION

Topological indices and graph invariants based on the distances between vertices of a graph are widely used for characterizing molecular graphs and their fragments, establishing relationships between structure and properties of molecules, predicting biological activity of chemical compounds, and making other chemical applications.[1–12] A new graph invariant was proposed for describing edge induced subgraphs having the same vertices in a graph.[12] This invariant is constructed as follows.

By the distance $d_G(u,v)$ between vertices $v,u \in V(G)$ we mean the length of a simple path which joins the vertices v and u in the graph G and contains the minimal number of edges. The *distance of a vertex* v in G is the sum of the distances from v to all other vertices, $D_G(v) = \sum_{u\in V(G)} d_G(u,v)$. Consider the edge induced subgraphs marked by heavy lines in Figure 1. A location of a subgraph $F \subseteq G$ can be described by the invariant $D'(F) = {}^1/_2\sum_{e\in E(F)} D_G(e)$, where $D_G(e)$ is the distance of edge $e = (u,v)$ defined as $D_G(e) = D_G(u) + D_G(v)$. This invariant can be written in another form, namely, $D'(F) = {}^1/_2\sum_{v\in V(F)} \deg_F(v)\, D_G(v)$. Each subgraph of Figure 1 has a different value of this invariant.

In the present article we specialize F to the full graph G, considering some properties of the graph invariant

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

which is called the *degree distance of a graph G*. The vertex invariant $D'(v) = \deg(v)\, D_G(v)$ is called the *degree distance of a vertex v*.

The properties of the graph degree distance will be compared with properties of the Wiener index.[1–7] The Wiener index (or the Wiener number) is a well-known topological index, which equals the sum of distances between all pairs of vertices of a molecular graph

$$W(G) = {}^1/_2 \sum_{v\in V(G)} D_G(v)$$

This index was used to describe molecular branching and cyclicity and establish correlations with various physicochemical and thermodynamic parameters of chemical compounds. Among them are the boiling point, density, critical pressure, refractive indices, heats of isomerization and vaporization of various hydrocarbon species, etc. The Wiener index found interesting applications in polymer chemistry, in studies of crystals and in drug design.[1–8,13–20,25–30] Mathematical properties of this invariant were studied for classes of chemical and abstract graphs.[10–24,28–38] Since the degree distance is a weighted sum of the distances of vertices, it will be called also the degree analogue of the Wiener index. We assume throughout this paper that a graph has order p (number of vertices) and size q (number of edges).

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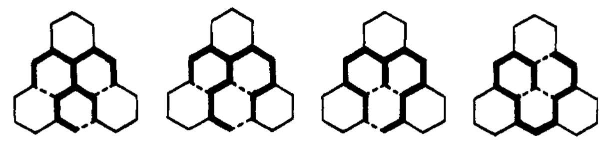

Figure 1. Edge induced subgraphs having the same vertices and distinct values of the invariant $D'(F)$.

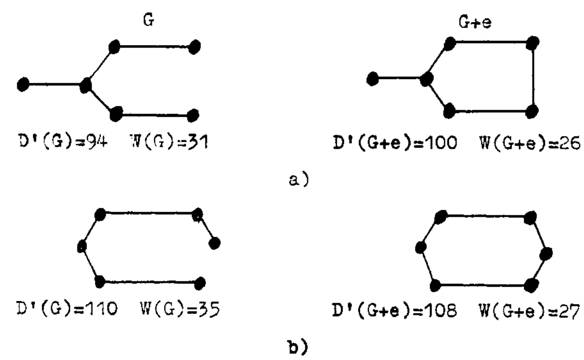

Figure 2. Nonmonotonic changes of the degree distance due to edge addition.

CHANGES OF THE INVARIANT DUE TO EDGE ADDITION

Clearly, if we add a new edge, then the lengths of the shortest paths between graph vertices cannot increase. Let $G + e$ be obtained from a graph G by adding a new edge. Then, the Wiener index is a strictly decreasing function; *i.e.* $W(G + e) < W(G)$. This property is not valid for its degree analogue. If changes of the distances are not essential, then $D'(G + e) > D'(G)$ (see Figure 2a). On the other hand, if we join the end vertices of the path P_6 (see Figure 2b), we obtain the converse inequality $D'(G + e) < D'(G)$.

The degree distance of a graph is a more sensitive invariant than the Wiener index. The set of graphs with the same values of an invariant is called the *class of invariant degeneracy*. Consider the sets of connected graphs with six vertices and different numbers of edges. The numbers of degeneracy classes for the Wiener index (N_W) and the degree distance ($N_{D'}$) are presented in the third and fourth columns of Table 1, where N is the number of graphs with q edges. The last four columns contain the minimal and maximal values of these invariants for corresponding classes. The graphs of Figure 3 illustrate various cases of the invariants' coincidence.

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Table 1. Sizes of Degeneracy Classes of the Wiener Index (N_W) and the Degree Distance ($N_{D'}$) and Its Extremal Values on Graphs with Order 6 (N is the Number of Graphs with q Edges)

q	N	N_W	$N_{D'}$	W_{min}	W_{max}	D'_{min}	D'_{max}
5	6	6	6	25	35	70	110
6	13	6	10	24	31	84	118
7	19	6	10	23	28	96	121
8	22	4	11	22	25	102	124
9	20	3	8	21	23	114	128
10	14	2	5	20	21	124	132
11	9	1	5	19	19	130	138
12	5	1	4	18	18	138	144
13	2	1	2	17	17	144	146

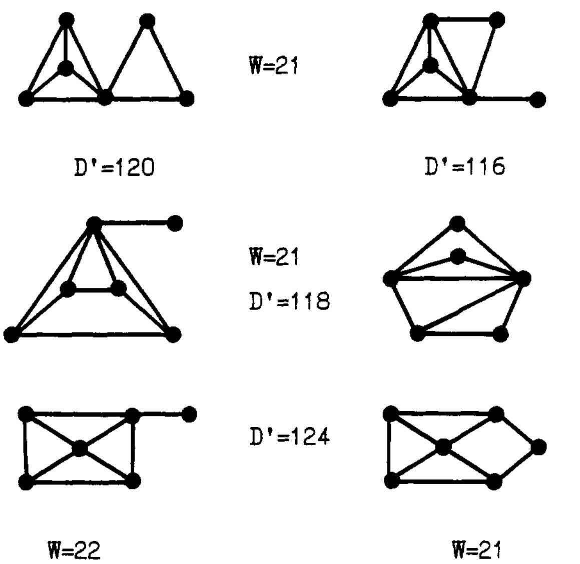

Figure 3. Examples of degeneracy for the Wiener index and its degree analogue.

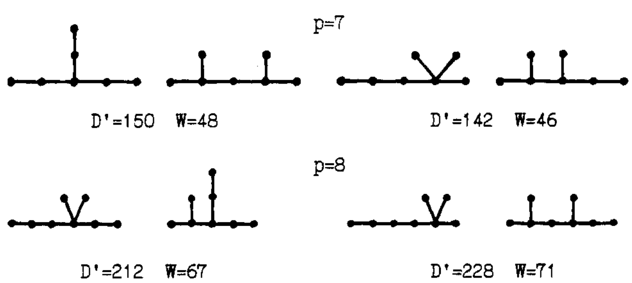

Figure 4. All trees of orders 7 and 8 with the same degree distance.

DEGREE DISTANCE OF TREES

Trees with the same degree distance have the minimal order 7. All such trees of orders 7 and 8 are shown in Figure 4. A degeneracy of the Wiener index implies a degeneracy of the degree distances for all trees with orders less than or equal to 10. Both degree sequences and distance of vertices are distinct for nonequivalent vertices for all trees of Figure 4. By nonequivalent vertices we mean those which belong to the distinct orbits of the automorphism group of a graph. Trees with the same degree distance for nonequivalent vertices have the minimal order 8. All trees of orders 8–10 with the pairs of such vertices are presented in Figure 5. Note that the minimal tree with the same distance of vertices has order 10 (see Figure 6a).

There are nonisomorphic trees with coinciding degree sequences and distances of vertices (see Figure 6b). Trees of order 9, shown in Figure 7, have the same degree sequences and different sequences of distances of vertices (see Table 2).

Trees of orders 9 and 10 from the maximal degeneracy classes of the degree distance are presented in Figure 8. Some pairs of these trees have the same degree sequences.

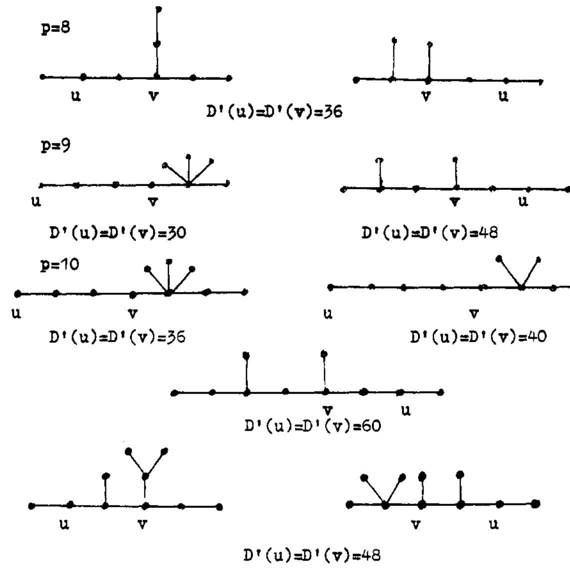

Figure 5. All trees of orders 8–10 having the nonequivalent vertices with the same degree distance.

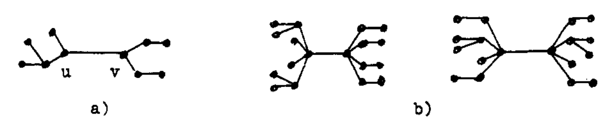

Figure 6. Nonisomorphic trees with coinciding degree sequences and degree distance of vertices.

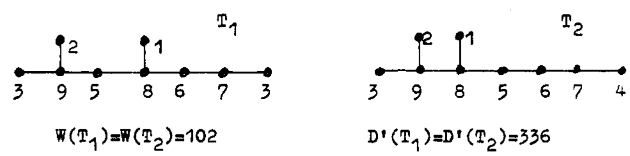

Figure 7. Trees with coinciding degree sequences and distinct degree distances of vertices.

Table 2. Degrees and the Degree Distance of Vertices for Trees in Figure 7

v	deg(v)	$D_{T_1}(v)$	$D'_{T_1}(v)$	$D_{T_2}(v)$	$D'_{T_2}(v)$
1	1	23	23	23	23
2	1	27	27	26	27
3	1	27	27	26	27
4	1	31	31	32	32
5	2	17	34	17	34
6	2	19	38	20	40
7	2	24	48	25	50
8	3	16	48	16	48
9	3	20	60	19	57
total		204	336	204	336

EXTREMAL VALUES OF THE DEGREE DISTANCE

It is well-known that the extremal values of the Wiener index are realized by a complete graph and a path. It would be interesting to establish the lower and upper bounds of the degree distance of a graph. Note that $2\delta \leqslant D'(G)/W(G) \leqslant 2\Delta$, where δ and Δ are the minimal and maximal degrees of vertices in G. The bounds coincide on regular graphs. We present the exact values of the invariant for some graphs.

1. If G is a regular graph of degree r, then $D'(G) = 2rW(G)$. The discriminating ability of the Wiener index and its degree analogue is the same for regular graphs.

2. Let K_p be a complete graph; then

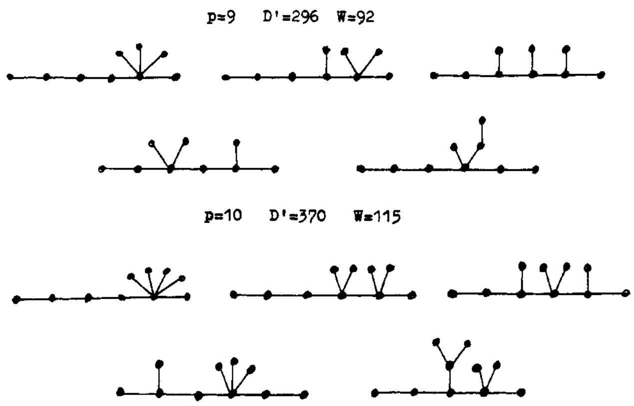

Figure 8. Maximal degeneracy classes of degree distances of trees of orders 9 and 10.

$$D'(K_p) = 2(p-1)W(K_p) = p(p-1)^2$$

3. Let P_p be a path; then

$$D'(P_p) = 4W(P_p) - p(p-1) = p(p-1)(2p-1)/3$$

4. Let $K_{1,p-1}$ be a star; then

$$D'(K_{1,p-1}) = 2W(K_{1,p-1}) + (p-1)(p-2) = (p-1)(3p-4)$$

5. Let K_{p_1,p_2} be a complete bipartite graph; then we have

$$D'(K_{p_1,p_2}) = p_1p_2(3p-4)$$

6. If G is a wheel on p vertices and $p \geq 4$, then

$$D'(G) = W(G) + (p-1)(5p-12) = (p-1)(7p-16)$$

7. If G is a graph with $d(G) = r(G) = 2$, where $d(G)$ and $r(G)$ are the diameter and radius of G, then

$$D'(G) = \sum_v \deg(v)(2p - \deg(v) - 2) = 4q(p-1) - \sum_v \deg^2(v)$$

The degree distance of a graph depends on both the diameter and degrees of its vertices. Suppose that G is obtained by joining a complete graph and a path as illustrated in Figure 9. If the diameter of G is equal to d, then we derive

$$D'(G) = (3d^4 - 2d^3(3p+4) + 3d^2(p^2 + 7p - 1) - d(15p^2 + 3p - 8) + 6p(p^2 - 1))/6$$

The last expression achieves the maximal value $D'(K_p)$ at $d = 1$ for $2 \leqslant p \leqslant 14$. If $p \geqslant 15$, then the maximal value of the function $D'(G)$ occurs at $d = p/2$ for even p and at $d = (p-1)/2$ for odd p. It is equal to $D'(G) = (3p^4 + 44p^3 - 36p^2 - 32p)/96$ for even p and $D'(G) = (3p^4 + 44p^3 - 42p^2 + 52p - 57)/96$ for odd p. We conjecture that the extremal values of the degree distance are realized by the star and the graph G.

GRAPHS HAVING THE SAME DEGREE DISTANCE OF VERTICES

In this section we consider graphs having nonequivalent vertices with the same degree distance.

Let u,v be arbitrary vertices of a graph G. We need a simple preliminary statement.

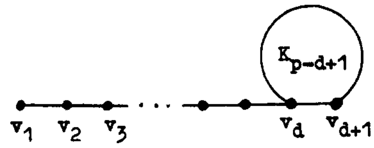

Figure 9. Graph with conjectural maximal degree distance.

Proposition 1. Let $D(u) \equiv D(v) \pmod n$, and the distance of v (or u) is not divisible by n. Then $D'(u) \equiv D'(v) \pmod n$ if and only if $\deg(u) \equiv \deg(v) \pmod n$.

Proof. Suppose that $D(v)$ is not divisible by n. We have $D'(u) - D'(v) = \deg(u)(D(u) - D(v)) + (\deg(u) - \deg(v))D(v)$. It is easy to see that if $D'(u) \equiv D'(v) \pmod n$, then $\deg(u) - \deg(v)$ is divisible by n, and conversely.

We apply the proposition 1 to determine vertices with coinciding degree distances in polyhexes and trees.

A polyhex is a connected system of congruent regular hexagons, where either any two hexagons share exactly one edge or they are disconnected. In a cata-condensed polyhex, no three hexagons share a common vertex and its hexagons can not form a closed ribbon. Every hexagon in an unbranched system is adjacent to at most two other hexagons. Molecular graphs of benzenoid hydrocarbons serve as examples of such polyhexes.[4,6,29]

Proposition 2. Let G be a cata-condensed polyhex and $u,v \in V(G)$. Then $D'(u) = D'(v)$ if and only if $D(u) = D(v)$ and $\deg(u) = \deg(v)$.

Proof. If v is an arbitrary vertex of a cata-condensed polyhex, then $D(v) \equiv 1 \pmod 4$.[21-23] Then for every pair of vertices v and u we have $D(v) \equiv D(u) \pmod 4$. Finally we note that a polyhex contains vertices with degree 2 or 3 only.

Among all trees we consider trees having a perfect matching.

Proposition 3. Let T be a tree of order $4k + 2$ with a perfect matching. If $D'(u) = D'(v)$ then $\deg(v)$ and $\deg(u)$ have the same parity.

Proof. If v is an arbitrary vertex of such a tree, then $D(v) \equiv 1 \pmod 2$; *i.e.* $D(v)$ is odd.[24] Hence, $D(v) \equiv D(u) \pmod 2$ for every $u,v \in V(T)$, and we can use proposition 1.

This result implies that all trees of order 10, shown in Figure 5, cannot have a perfect matching. If T is a tree of order $4k$ with a perfect matching, then $D(v) \equiv 0 \pmod 2$; *i.e.* $D(v)$ is even.[24] In this case proposition 3 is not valid. For example, the first tree of order 8, shown in Figure 5, has a perfect matching and vertices of degree 2 and 3 with the same invariant.

DECOMPOSITION CONJECTURE OF THE WIENER INDEX

Various types of decomposition of the Wiener index were used to establish well correlations between the biological activities of chemical compounds and the parts of this index.[25-27] We consider a relationship between the Wiener index and its degree analogue for cata-condensed polyhexes. The set of vertices of a cata-condensed polyhex with h rings can be divided into two disjoint subsets $V_2 = \{u|\deg(u) = 2\}$ and $V_3 = \{u|\deg(u) = 3\}$, where $|V_2| = 2(h+2)$ and $|V_3| = 2(h-1)$. It is easy to see that the Wiener index can be presented as follows

$$W(G) = {}^1/_2\Big(\sum_{u\in V_2, v\in V(G)} d(u,v) + \sum_{u\in V_3, v\in V(G)} d(u,v)\Big) = {}^1/_2(D_2(G) + D_3(G))$$

where $D_i(G)$ is a sum of distances for vertices having degree i in G.

Table 3. Decomposition of the Wiener Index for Unbranched Cata-Condensed Polyhexes

h	N	W	$D_2/2$	$D_3/2$	$D_{22}/2$	$D_{33}/2$	D_{23}
5	2	971	667	304	449	86	436
6	3	1565	1036	529	674	167	724
7	4	2391	1533	858	969	294	1128
8	9	3201	2034	1167	1272	405	1524
9	15	4571	2827	1744	1727	644	2200
10	28	6125	3724	2401	2240	917	2968
11	59	7799	4693	3106	2795	1208	3796
12	135	9905	5890	4015	3470	1595	4840
13	311	12523	7355	5168	4285	2098	6140
14	673	15253	8888	6365	5140	2617	7496
15	1659	18463	10673	7790	6127	3244	9092
16	4066	22369	12818	9551	7300	4033	11036

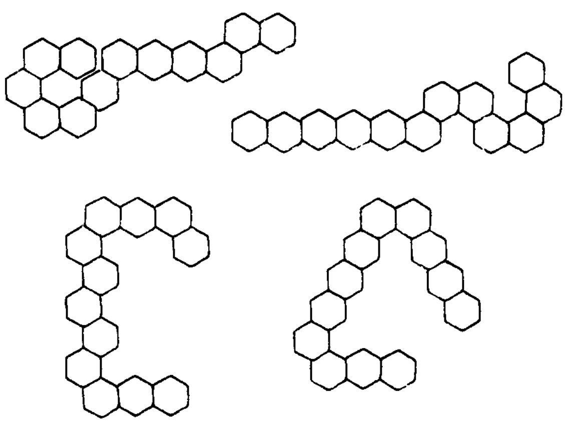

Figure 10. Configurations of some unbranched cata-condensed polyhexes with $W = 9905$.

Let G and H be arbitrary cata-condensed polyhexes. The first decomposition conjecture asserts that the parts D_2 and D_3 are equal for G and H.

Conjecture 1. If $W(G) = W(H)$, then $D_2(G) = D_2(H)$ and $D_3(G) = D_3(H)$.

Consider another decomposition of the Wiener index into three parts:

$$W(G) = {}^1/_2\Big(\sum_{u,v\in V_2} d(u,v) + \sum_{u\in V_2,v\in V_3} d(u,v) + \sum_{u\in V_3,v\in V_2} d(u,v) + \sum_{u,v\in V_3} d(u,v)\Big)$$

$$= {}^1/_2(D_{22}(G) + 2D_{23}(G) + D_{33}(G))$$

where $D_{ij}(G)$ is a sum of distances between vertices having degrees i and j. Now we propose the second decomposition conjecture.

Conjecture 2. If $W(G) = W(H)$, then $D_{22}(G) = D_{22}(H)$, $D_{23}(G) = D_{23}(H)$ and $D_{33}(G) = D_{33}(H)$.

It is obvious that conjecture 2 implies conjecture 1.

In order to verify these conjectures we calculate values of corresponding parts of the Wiener index for various classes of polyhexes having the same index. Obtained results support the conjectures. Numerical data for the maximal classes of unbranched polyhexes with the same Wiener index are presented in Table 3. Here h is the number of hexagons, and N is the number of graphs in each maximal class. These classes also contain polyhexes which cannot be embedded into a regular hexagonal lattice in the plane.[39] Configurations of some graphs with $W(G) = 9905$ are presented in Figure 10.

Table 4 shows analogous data for maximal classes of graphs without unbranched polyhexes for $h = 6$–8.[40,41]

Table 4. Decomposition of the Wiener Index for Branched Cata-Condensed Polyhexes

h	N	W	$D_2/2$	$D_3/2$	$D_{22}/2$	$D_{33}/2$	D_{23}
6	2	1381	944	437	628	121	632
7	5	2143	1409	734	907	232	1004
8	11	2977	1922	1055	1216	349	1412

If the decomposition conjectures are valid, then we can state the following result formulated as a new conjecture for the Wiener index and its degree analogue.

Conjecture 3. For arbitrary cata-condensed polyhexes, $D'(G) = D'(H)$ if and only if $W(G) = W(H)$.

We can write $D'(G) - D'(H) = (2\sum_{v\in V_2} D_G(v) + 3\sum_{v\in V_3} D_G(v) - 2\sum_{v\in V_2} D_H(v) - 3\sum_{v\in V_3} D_H(v)) = 4(W(G) - W(H)) + D_3(G) - D_3(H)$.

CHANGES OF THE INVARIANT DUE TO VERTEX DELETING

Let $G - v$ be obtained from a graph G by deleting the vertex v and all edges incident to v. We assume that a graph $G - v$ is always connected. It is clear that $d_G(u,w) \leq d_{G-v}(u,w)$ for arbitrary vertices u and w of G. We consider the simplest case when the last expression is an equality. The following result is obvious.

Proposition 4. Let v be a vertex of G such that $G - v$ is connected. Then $d_G(u,w) = d_{G-v}(u,w)$ for all vertices u,w of $G - v$ if and only if the vertex v and every pair of its neighbors form a cycle C_3 or belong to a cycle C_4.

Denote by $S(G)$ the set of vertices v with such a property.

Proposition 5. If $v \in S(G)$, then $W(G) = W(G-v) + D(v)$.

Proof. We have $2W(G) = \sum_{u\neq v} D(u) + D(v) = \sum_{u\neq v}(d_G(u,v) + \sum_{w\neq v} d(u,w)) + D(v) = \sum_{u,w\neq v} d_G(u,v) + \sum_{u\neq v} d_G(u,v) + D(v) = 2W(G-v) + 2D(v)$.

Corollary. If $v \in V(G)$, then $W(G-v)/W(G) \leq 1 - 1/p$.

Proof. By the proposition 5, $W(G-v)/W(G) = 1 - D(v)/W(G)$. Then, $2W(G) = \sum_{u,v} d(u,v) \leq \sum_u(\sum_v(d(u,w) + d(w,v))) = 2pD(w)$. We can choose the vertex w such that $D(w) = \min_v\{D(v)\}$. Hence, $W(G) \leq pD(w)$ and $W(G-v)/W(G) \leq 1 - D(w)/pD(w) = 1 - 1/p$.

We present the exact values of the ratio $W(G-v)/W(G)$ for some graphs. For a complete graph we have $W(K_p - v)/W(K_p) = 1 - 2/p$; for a star and for a path with the end vertex v the equalities $W(K_{1,p-1} - v)/W(K_{1,p-1}) = 1 - 2/(p-1) + 1/(p-1)^2$ and $W(P_p - v)/W(P_p) = 1 - 3/(p+1)$ hold.

Now we derive the similar results for the degree distance.

Proposition 6. If $v \in S(G)$, then

$$D'(G) = D'(G-v) + D'(v) + \sum_u \deg(u)\, d(v,u)$$

Proof. We have the equalities $D'(G) = \sum_{u\neq v} \deg(u)\, D(u) + \deg(v)\, D(v) = \sum_{u\neq v} \deg(u)(\sum_{w\neq v} d_G(u,w) + d_G(u,v)) + D'(v) = D'(G-v) + \sum_u \deg(u)\, d(v,u) + D'(v)$.

Corollary. If $v \in S(G)$, then $D'(G-v)/D'(G) \leq 1 - \delta/\Delta p$.

Proof. By proposition 6, we can write $D'(G-v)/D'(G) = 1 - D'(v)/D'(G) - \sum_u deg(u) d(v,u)/D'(G) \leq 1 - \delta D(v)/2\Delta W(G) - \delta \sum_u d(v,u)/2\Delta W(G) = 1 - \delta D(v)/\Delta W(G) \leq 1 - \delta/\Delta p$.

For regular graphs the bound is the same as in case of the Wiener index. For a star and for a path with the end vertex v we have

$D'(K_{1,p-1}-v)/D'(K_{1,p-1}) = 1-3/(3p-4)-1/(p-1)+4/(3p-4)(p-1)$ and $D'(P_p-v)/D'(P_p) = 1 - 1/(p+4) - 2/p + 2/p(p+4)$.

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