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ONE–TWO DESCRIPTOR OF GRAPHS

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A b s t r a c t. *In a recent paper [Vukičević et al., J. Math. Chem.* **48** *(2010) 395-400] a novel molecular–graph–based structure descriptor, named one–two descriptor (OT), was introduced. OT is the sum of vertex contributions, such that each pendent vertex contributes 1, each vertex of degree two adjacent to a pendent vertex contributes 2, and each vertex of degree higher than two also contributes 2. Vertices of degree two, not adjacent to a pendent vertex, do not contribute to OT. Vukučević et al. established lower and upper bounds on OT for trees. We now give lower and upper bounds on OT for general graphs, and also characterize the extremal graphs. The bounds of Vukičević et al. for trees follows as a special case. Moreover, we give another upper bound on OT for trees.*

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1. *Introduction*

The molecular structure descriptor is the final result of a logical and mathematical procedure that transforms chemical information encoded within a symbolic representation of a molecule (= structural formula) into a number or into the result of some standardized experiment [6, 7]. Molecular descriptors were shown to be useful for modeling many physico–chemical properties in QSAR and QSPR studies [8, 1, 5, 4].

In the recent years a large number of novel graph–based molecular structure descriptors has been put forward, see [7, 2, 3] and the references cited therein. One of these is the *one–two descriptor* (OT), introduced in [9]. In [9] it was demonstrated that OT can be successfully applied for modeling physico–chemical properties of organic compounds. In addition, some of its mathematical properties were established, namely lower and upper bounds for trees and chemical trees. In the present work we report our studies of the mathematical properties of the OT index, focusing our attention to general graphs.

In [9] it was shown that OT is a good predictor of heat capacity at constant pressure, and of the total surface area of octane isomers. Also in [9], some mathematical properties of OT were established for trees. In the present paper we give lower and upper bounds on OT of a general connected graph, and characterize the graphs for which these bounds are the best possible. We show that the bounds reported in [9] are special cases of ours. In addition, we give another upper bound on OT for trees.

In this paper we are concerned with simple graphs, that is, graphs without multiple edges, directed edges, and loops. Let G be a connected graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and let m be the cardinality of its edge set $E(G)$. i. e., the number of edges. The number of (first) neighbors of a vertex $v_i \in V(G)$ is its degree, and is denoted by d_i.

The distance $d(i,j)$ between the vertices v_i and v_j of the graph G is equal to the length of (= number of edges in) a shortest path that connects v_i and v_j. The eccentricity e_i of a vertex v_i in a connected graph G is the maximum graph distance between v_i and any other vertex of G. The minimum eccentricity of a vertex is the radius of G and is denoted by r.

Let G be a connected graph with n vertices and m edges. Let $n_i = n_i(G)$ be the number of its vertices of degree i. The quantity $\nu = m - n + 1$ is called the cyclomatic number of G.

A pendent vertex is a vertex of degree one. An edge of a graph is said to be pendent if one of its end-vertices is pendent.

K_n and C_n denote, respectively, the complete graph and the cycle with n vertices.

The one–two descriptor of a graph G is defined as the sum of vertex contributions is such a way that each pendent vertex contributes 1, each vertex of degree two adjacent to a pendent vertex contributes 2, and each vertex of degree higher than two also contributes 2. Vertices of degree two, not adjacent to a pendent vertex, have zero contribution. The one–two descriptor of a graph G will be denoted by $OT(G)$. The example depicted in Fig. 1 should be self-explanatory.

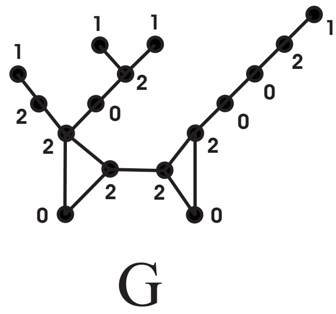

Fig. 1. The one–two descriptor is obtained by summing the vertex contributions, whose values are 1 (for pendent vertices), 2 (for vertices of degree greater than two, and for vertices of degree two adjacent to a pendent vertex), and 0 (for vertices of degree two, not adjacent to a pendent vertex). Thus, $OT(G) = 4 \times 1 + 7 \times 2 + 5 \times 0 = 18$.

2. *Bounds on one–two descriptor*

In this section we give lower and upper bounds on the one–two descriptor of general graphs. First we present a lower bound on OT for a connected graph.

Theorem 2.1 *Let G be a simple connected graph with n vertices and m edges. Then*

$$OT(G) \geq \begin{cases} 0 & \text{if } n = 1 \\ 1 & \text{if } n = 2 \\ 4 & \text{if } n = 3 \text{ and } m = 2 \\ 5 & \text{if } n = 4 \text{ and } m = 3 \\ 6 & \text{if } n \geq 5 \text{ and } m = n - 1 \\ 0 & \text{if } n \geq 3 \text{ and } m = n \\ 2\left\lceil \frac{3}{2} + \frac{1}{2}\sqrt{9 + 8m - 8n} \right\rceil & \text{if } n \geq 4 \text{ and } m > n\,. \end{cases}$$

P r o o f. If G is a tree $(m = n-1)$, the problem has been solved in [9]. If G is a unicyclic graph $(m = n)$, then it can be easily seen that $OT(C_n) = 0$. Moreover, C_n is the only unicyclic graph with zero OC-value. Hence, let us assume that $m > n$.

Denote by n_1 the number of vertices of degree 1, by n_2 the number of vertices of degree 2 and by k the number of vertices of degree greater than 2. Let G_1 be a graph obtained from the graph G by contraction of all vertices of degree 2. It holds $n(G_1) = n - n_2$ and $m(G_1) = m - n_2$. Further, let G_2 be a graph obtained from the graph G_1 by deleting all vertices of degree 1. Then $n(G_2) = n(G_1) - n_1 = n - n_1 - n_2 = k$ and $m(G_2) = m(G_1) - n_1 = m - n_1 - n_2 = m - n + k$. Hence,

$$\binom{k}{2} \geq m - n + k\ .$$

The latter inequality is equivalent to

$$k \leq \frac{3}{2} - \frac{1}{2}\sqrt{9 + 8m - 8n} \tag{1}$$

or

$$k \geq \frac{3}{2} + \frac{1}{2}\sqrt{9 + 8m - 8n}\ . \tag{2}$$

Since $m > n$, it follows that the right–hand side of (1) is negative. Therefore (1) does not hold. Further, since k is integer, from (2) follows that:

$$k \geq \left\lceil \frac{3}{2} + \frac{1}{2}\sqrt{9 + 8m - 8n} \right\rceil$$

which directly yields

$$OT(G) \geq 2\left\lceil \frac{3}{2} + \frac{1}{2}\sqrt{9 + 8m - 8n} \right\rceil .$$

We now prove that this bound is tight, i. e., for every $n < m \leq \binom{n}{2}$, the bound is obtainable.

For brevity denote $\left\lceil \frac{3}{2} + \frac{1}{2}\sqrt{9 + 8m - 8n} \right\rceil$ by x. Note that $\binom{x}{2} \geq m - n + x > x$. Hence, there is a supergraph G_3 with x vertices and $m - n + x$ edges, possessing the cycle C_x (just start with C_x and arbitrarily add $m - n$ edges). Let G_4 be a graph obtained from G_3 by replacing one of its edges with the path of length $n - x + 1$. Note that $n(G_4) = x + n - x = n$ and that $m(G_4) = m - n + x + n - x = m$. Further, only x vertices from G_3 contribute to $OT(G_4)$. Therefore,

$$OT(G_4) \leq 2\,x = 2\left\lceil \frac{3}{2} + \frac{1}{2}\sqrt{9 + 8m - 8n} \right\rceil .$$

This proves the Theorem. □

Now we discuss upper bounds on the one–two descriptor. ¿From the definition of one–two descriptor one can easily see that $OT(G) \leq 2n$ and that numerous graphs satisfy the relation $OT(G) = 2n$. For example, $OT(K_n) = 2n$ (provided $n \geq 4$) and $OT(K_n \setminus \{e\}) = 2n$ (provided $n \geq 5$), etc. So we have the following:

Theorem 2.2 *If* $3n \leq 2m \leq \binom{n}{2}$, *then there exists a graph* G *with* n *vertices and* m *edges, such that* $OT(G) = 2n$.

P r o o f. Let G_n be a graph with $n \geq 4$ vertices given by $V(G_n) = \{v_1,\ v_2, \ldots,\ v_n\}$ and

$$E(G_n) = \{v_1v_2, v_2v_3, \ldots, v_{n-1}v_n\} \cup \{v_nv_1\} \cup \{v_1v_{n/2+1}, v_2v_{n/2+2}, \ldots, v_{n/2}v_n\}$$

if n is even and

$$\begin{aligned} E(G_n) &= \{v_1v_2, v_2v_3, \ldots, v_{n-1}v_n\} \cup \{v_nv_1\} \\ &\cup \{v_1v_{(n-1)/2}, v_2v_{(n-1)/2+2}, \ldots, v_{(n-1)/2}v_{n-1}\} \cup \{v_2v_n\} \end{aligned}$$

if n is odd. It is sufficient to take G to be any supergraph of G_n. □

In view of the above theorem, we are interested to find the upper bound on $OT(G)$ when $2m < 3n$. Since $\nu = m - n + 1$, $2m < 3n$ implies that $2\nu < n+2$. We now give an upper bound on OT for graphs with $2\nu < n+2$. For this we define the following class of graphs:

Let $\Gamma(H, \nu)$ be the class of simple connected graphs $H = (V, E)$ with at least 6 vertices, cyclomatic number ν, and vertex degrees 1, 2, and 3, such that each vertex of degree 2 is adjacent to one pendent vertex and no vertex of degree 3 is adjacent to a pendent vertex. Then $n_3(H) = n_1(H) + 2(\nu - 1)$ and $n_1(H) = n_2(H)$. Then $OT(H) = (5n + 2\nu - 2)/3$. We will use T, U, and B to denote the sets of all trees, unicyclic, and bicyclic graphs, respectively. The three graphs depicted in Fig. 2 are in the class $\Gamma(H, \nu)$.

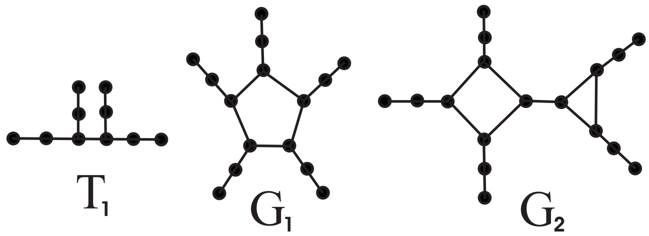

Fig. 2. A tree $T_1 \in \Gamma(T,0)$, a unicyclic graph $G_1 \in \Gamma(U,1)$, and a bicyclic graph $G_2 \in \Gamma(B,2)$

Theorem 2.3 *Let G be a connected graph of order n ($n \geq 6$) with $2\nu < n+2$. Then*

$$OT(G) \leq \left\lfloor \frac{5n+2\nu-2}{3} \right\rfloor \ . \tag{3}$$

Equality holds in (3) if and only if $G \in \Gamma(H,\nu)$.

P r o o f. Let G be a graph with maximal value of OT among all the graphs with $n \geq 6$ vertices and $m < 3n/2$ edges as $2\nu < n+2$. We show that G has no vertex of contribution 0.

Suppose the contrary, and let u be a vertex of contribution 0. This vertex is necessarily of degree 2. Let v_1 and v_2 be its neighbors. Denote by $NV = NV(G) \setminus \{u\}$ the set of all non-pendent vertices in G, different from u. We claim that all vertices in $NV \setminus \{v_i\}$ are adjacent to v_i, $i = 1,2$. Suppose the contrary, namely that the vertex $w \in NV \setminus \{v_i\}$ is not adjacent to v_i. Then the graph $G - u\,v_i + v_i\,w$ would have a greater value of OT, which is a contradiction.

We have to distinguish between three cases:

CASE 1: There are at least four vertices in NV.

We claim that the restriction $G[NV]$ of the graph G to the set NV is a complete graph. Suppose to the contrary that there are two vertices w_1 and w_2 that are not adjacent. Then the graph $G - u\,v_1 + w_1\,w_2$ has a greater value of OT, which is a contradiction.

Since, $n \geq 6$ and $m < 3n/2$, there is at least one pendent vertex. Denote it by w_3 and its only neighbor by w_4. The graph $G - w_3\,w_4 + u\,w_3$ has a greater value of OT, which is a contradiction.

CASE 2: The only vertices in NV are v_1 and v_2.

Since $n \geq 6$, it follows that there are at least three pendent vertices. Hence, without loss of generality, we may assume that v_1 is incident to at least two pendent vertices. Let w_5 be one of them. The graph $G - v_1\, w_5 + u\, w_5$ has a greater value of OT, which is a contradiction.

CASE 3: There are three vertices in NV.

Denote the third vertex in NV by v_3. If v_3 is adjacent to at least two pendent vertices, then denote one of them by w_6. The graph $G - v_3\, w_6 + u\, w_6$ has a greater value of OT, which is a contradiction. Otherwise, there is at least one pendent vertex adjacent to either v_1 or v_2. Denote it by w_7 and suppose without loss of generality that w_7 is adjacent to v_1. The graph $G - v_1\, w_7 + u\, w_7$ has a greater value of OT, which is a contradiction.

Hence, there are no vertices of contribution 0. Consequently, $n_1(G) \geq n_2(G)$.

Now we have

$$\sum_{i\geq 1} n_i(G) = n \qquad \text{and} \qquad \sum_{i\geq 1} i\, n_i(G) = 2m = 2(\nu + n - 1)$$

from which it follows

$$\begin{aligned} n_1(G) &= \sum_{i\geq 3}(i-3)n_i(G) + \sum_{i\geq 3} n_i(G) - 2\nu + 2 \\ &\geq n - n_1(G) - n_2(G) - 2\nu + 2 \quad \text{as } \sum_{i\geq 3}(i-3)n_i(G) \geq 0 \\ &\geq n - 2n_1(G) - 2\nu + 2 \quad \text{as } n_1(G) \geq n_2(G) \end{aligned}$$

that is,

$$n_1(G) \geq \frac{n - 2\nu + 2}{3}\ . \tag{4}$$

Using (4), we get

$$OT(G) \leq n_1(G) + 2\sum_{i\geq 2} n_i(G) = 2n - n_1(G) \leq \frac{5n + 2\nu - 2}{3}$$

as $\sum_{i\geq 1} n_i(G) = n$.

The first part of the proof is done.

Suppose now that equality holds in (3). Then all inequalities in the above argument must be equalities. So we must have $n_1(G) = n_2(G)$ and $n_i(G) = 0$ for $i \geq 4$. Hence $G \in \Gamma(H, \nu)$.

Conversely, let $G \in \Gamma(H,\nu)$. Then $n_3(G) = n_1(G) + 2(\nu - 1)$ and $n_1(G) = n_2(G)$, which implies $OT(G) = \lfloor (5n + 2\nu - 2)/3 \rfloor$. □

In [9] an upper bound was obtained in terms of n, but the extremal trees were not characterized. From the above theorem, we get the same upper bound on OT of trees, but also characterize the extremal trees.

Corollary 2.4 *Let T^* be a tree with n $(n > 1)$ vertices. Then*

$$OT(T^*) \leq \left\lfloor \frac{5n-2}{3} \right\rfloor \tag{5}$$

with equality in (5) if and only if $T^* \in \Gamma(T,0)$.

P r o o f. For a tree T^*, $\nu = 0$. By theorem 2.3, we get the result. □

Corollary 2.5 *Let G be a unicyclic graph with n $(n > 3)$ vertices. Then*

$$OT(G) \leq \left\lfloor \frac{5n}{3} \right\rfloor$$

with equality if and only if $G \in \Gamma(U,1)$.

P r o o f. For a unicyclic graph G, $\nu = 1$. By theorem 2.3, we get the result. □

Corollary 2.6 *Let G be a bicyclic graph with n $(n > 1)$ vertices. Then*

$$OT(G) \leq \left\lfloor \frac{5n+2}{3} \right\rfloor$$

with equality if and only if $G \in \Gamma(B,2)$.

P r o o f. For a bicyclic graph G, $\nu = 2$. By theorem 2.3, we get the result. □

In the considerations that follow we shall use the fact that the function f defined by

$$f(r) = \frac{(5n+1)2^{r-2} - 2n}{3 \cdot 2^{r-2} - 1}$$

is strictly increasing.

Denote by $T^*(n,r,p)$ a tree of order n with radius r and with p pendent vertices, such that $p = n_2(T^*)$ and $n = p + p + \frac{p}{2} + \frac{p}{2^2} + \cdots + \frac{p}{2^{r-3}} + \frac{p}{2^{r-2}} + 1 = p\left(3 - \frac{1}{2^{r-2}}\right) + 1$, where $n_2(T^*)$ is the number of vertices of degree 2. For example, $T^*(67,4,24)$ is depicted in Fig. 3.

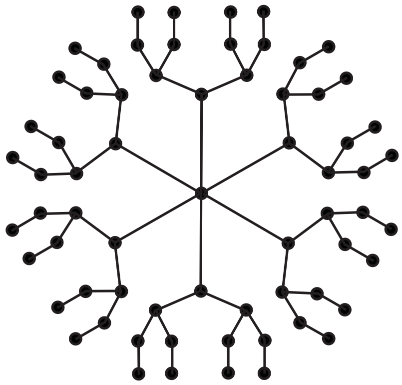

Fig. 3. The tree $T^*(67, 4, 24)$

Theorem 2.7 *Let T be a tree with n vertices and radius r. Then*

$$OT(T) \leq \frac{(5n+1)2^{r-2} - 2n}{3 \cdot 2^{r-2} - 1} \tag{6}$$

with equality in (6) if and only if $T \cong T^*(n, r, p)$.

P r o o f. Suppose the contrary. Let T be a tree with the smallest radius that contradicts the claim of the Theorem. We prove that T has no vertices of contribution 0. Suppose to the contrary that there is a vertex w_1 of degree 2. Let w_2 be a pendent vertex in T and w_3 its only neighbor. Let T' be the tree obtained by adding a pendent vertex w_4 to w_3. Let T'' be the tree obtained from T' by contraction of the vertex w_1 (i. e., by deleting w_1 and by adding the edge that connects its neighbors). It holds that

$$OT(T'') = OT(T') \geq OT(T) + 1 \geq \frac{(5n+1)2^{r-2} - 2n}{3 \cdot 2^{r-2} - 1} + 1$$

$n(T'') = n(T') - 1 = n(T) = n$ and $r(T'') \leq r(T') = r(T) = r$. On the other hand,

$$OT(T'') \leq \frac{(5n+1)2^{r(T')-2} - 2n}{3 \cdot 2^{r(T')-2} - 1} \leq \frac{(5n+1)2^{r-2} - 2n}{3 \cdot 2^{r-2} - 1} \,.$$

This is a contradiction.

Hence, there are no vertices of contribution 0. This means that each vertex of degree two is adjacent to a pendent vertex. Since T has radius

r, there exists a vertex v_i in $V(T)$ such that $d(i,j) \leq r$ for all $v_j \in V(T)$. Now, v_i, is the central vertex of T. Further, let p be the number of pendent vertices of T, that is, $n_1(T) = p$. There is a unique path from each pendent vertex to the central vertex v_i of T. We count the number of vertices along the paths from each pendent vertex to the central vertex (we count each vertex only once). In step 1, we count the p pendent vertices in T. In step 2, we count at most p vertices, the neighbors of the pendent vertices. In step 3, we count at most $p/2$ vertices, the second neighbors of the pendent vertices. In step 4, we count at most $p/2^2$ vertices, the third neighbors of the pendent vertices. ... In step $r-1$, we count at most $p/2^{r-3}$ vertices, the $(r-2)$-th neighbors of the pendent vertices. In step r, we count at most $p/2^{r-2}$ vertices, the $(r-1)$-th neighbors of the pendent vertices. Finally, in the $(r+1)$-th step we count the central vertex v_i, if not assigned previously. Thus we have

$$n \leq p + p + \frac{p}{2} + \frac{p}{2^2} + \cdots + \frac{p}{2^{r-3}} + \frac{p}{2^{r-2}} + 1 = p\left(3 - \frac{1}{2^{r-2}}\right) + 1$$

that is,

$$n_1(T) = p \geq \frac{(n-1)2^{r-2}}{3 \cdot 2^{r-2} - 1} \,. \tag{7}$$

Hence,

$$OT(T) \leq 1 \cdot n_1(T) + 2 \cdot \sum_{i \geq 2} n_i(T) = 2n - n_1(T) \,.$$

Substituting (7) into the above relation, we get the required result (6). By this the first part of the proof is done.

The equality holds in (6) if and only if the equality holds in (7), that is, if T is isomorphic to $T^*(n,r,p)$. Hence the theorem. □

Remark 2.8 *In some cases, but not always, the new bound (6) is better than the previous bound (5).*

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