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# **On Average Eccentricity**

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#### Abstract

The average eccentricity has been used as a molecular descriptor since 1988. In this paper, we give lower and upper bounds for the average eccentricity in terms of the numbers of vertices and edges, give lower and upper bounds for average eccentricity of trees with fixed diameter, fixed number of pendent vertices and fixed matching number, respectively, and determine the *n*-vertex trees with the

first four smallest and the first |n/2| th-largest average eccentricities for  $n \ge 6$ .

## 1. Introduction

We consider simple graphs. Let G be a connected simple graph with vertex set V(G) and edge set E(G). The distance between vertices u and v in G, denoted by  $d_G(u,v)$ , is the length (number of edges) of a shortest path connecting u and v in G. The eccentricity of vertex u in G, denoted by  $e_G(u)$ , is the distance from u to a vertex farthest away from it in G. The average eccentricity of G is

$$avec(G) = \frac{1}{n} \sum_{u \in V(G)} e_G(u),$$

where n = |V(G)|. This concept was introduced by Skorobogatov and Dobryninin [1] in

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mathematical chemistry used as a molecular descriptor, see also [2]. It is named the eccentric mean by Buckley and Harray [3]. Dankelmann, Goddard and Swart [4] established an upper bound for the average eccentricity in terms of number of vertices and minimum degree, obtained Nordhaus-Gaddum results, and examined the change in the average eccentricity when a graph is replaced by a spanning subgraph. Several packages, such as Dragan and Cerius<sup>2</sup>, include the average eccentricity (AECC) among their molecular descriptors, thus making it available for various structure-property models. A recent application may be found in [5].

In this paper, we give lower and upper bounds for the average eccentricity in terms of the numbers of vertices and edges, give lower and upper bounds for average eccentricity of trees with fixed diameter, fixed number of pendent vertices and fixed matching number, respectively, and determine the *n*-vertex trees with the first four smallest and the first |n/2| th-largest average eccentricities for  $n \ge 6$ .

## 2. Preliminaries

For a connected graph G, the radius r(G) and the diameter D(G) are, respectively, the minimum and maximum eccentricity among the vertices of G [1]. For  $u \in V(G)$ , let  $d_G(u)$  be the degree of u in G. A connected graph is called a self-centered graph if all of its vertices have the same eccentricity. Evidently, a connected graph G is self-centered if and only if r(G) = D(G).

Let  $K_n$  be the complete graph with n vertices. Let  $K_{r,s}$  be the complete bipartite graph with r and s vertices in its bipartite sets, respectively. Let  $S_n$  and  $P_n$  be, respectively, the star and the path with n vertices. By direct calculation, the following formulae hold:  $avec(K_n) = 1$ ,  $avec(K_{r,s}) = 2$ ,  $avec(S_n) = 2 - \frac{1}{n}$ ,  $avec(C_n) = \left\lfloor \frac{n}{2} \right\rfloor$ , and

 $avec(P_n) = \left\lfloor \frac{3n-2}{4} \right\rfloor.$ 

For a graph G and a subset E' of its edge set  $(E^*)$  of the edge set of its complement, respectively), G - E'  $(G + E^*)$ , respectively) denotes the graph formed from G by deleting (adding, respectively) edges from E'  $(E^*)$ , respectively). For  $u \in V(G)$ , G - u denotes the graph formed from G by deleting the vertex u (and its incident edges).

We will use techniques developed in [7].

#### 3. Average eccentricity of connected graphs

In this section, we give various lower and upper bounds for average eccentricity of connected graphs in terms of other graph invariants.

If G is a connected graph, then  $r(G) \le avec(G) \le D(G)$  with either equality if and only if G is a self-centered graph.

**Proposition 3.1.** Let G be an n-vertex connected graph, and k the number of vertices of degree n-1 in G, where  $0 \le k \le n$ . Then

$$avec(G) \ge 2 - \frac{k}{n}$$

with equality if and only if all the vertices of degree less than n-1 have eccentricity two.

**Proof.** Note that there are k vertices with eccentricity one and n-k vertices with eccentricity two. Then the result follows easily.  $\Box$ 

Let  $G \lor H$  be the graph formed from vertex-disjoint graphs G and H by adding edges between each vertex in G and each vertex in H. Denote by G(n,m) the set of graphs  $K_a \lor H$  with *n* vertices and *m* edges, where  $a = a_{(n,m)} = \left\lfloor \frac{2n - 1 - \sqrt{(2n-1)^2 - 8m}}{2} \right\rfloor$ . Obviously, each vertex of H has eccentricity two in  $K_a \lor H$ . **Proposition 3.2.** Let G be an n-vertex connected graph with m edges, where  $\begin{vmatrix} 2\pi & 1 \end{vmatrix} = \sqrt{(2\pi - 1)^2 - 8\pi}$ 

$$n-1 \le m < \binom{n}{2}$$
. Let  $a = \left\lfloor \frac{2n-1-\sqrt{(2n-1)^2-8m}}{2} \right\rfloor$ . Then  
 $avec(G) \ge 2 - \frac{a}{n}$ 

with equality if and only if  $G \in G(n, m)$ .

**Proof.** Let k be the number of vertices of degree n-1 in G, where  $0 \le k \le n-1$ . By Propisition 3.1,  $avec(G) \ge 2 - \frac{k}{n}$  with equality if and only if all the vertices of degree less than n-1 have eccentricity two. If k = 0, then  $avec(G) \ge 2 > 2 - \frac{a}{n}$ . Suppose that  $k \ge 1$ . Since  $2m \ge k(n-1) + k(n-k)$  and a is the largest integer satisfying  $2m \ge a(n-1) + a(n-a)$ , we have  $avec(G) \ge 2 - \frac{k}{n} \ge 2 - \frac{a}{n}$  with equalities if and only if all the n-k vertices of degree less than n-1 have eccentricity two and k = a, i.e.,  $G \in G(n,m)$ .

Note that for  $n \ge 5$ , if G is an *n*-vertex unicyclic or bicyclic graph, then a = 1, and that G(n,n) contains exactly one (unicyclic) graph, formed by adding an edge to the *n*-vertex star, G(n, n+1) contains exactly two (bicyclic) graphs, formed by adding two edges to the *n*-vertex star. Thus, by Proposition 3.2, we have

**Corollary 3.3.** Let G be a unicyclic (bicyclic, respectively) graph with  $n \ge 5$  vertices. Then

$$avec(G) \ge 2 - \frac{1}{n}$$

with equality if and only if G is formed by adding one edge (two edges, respectively) to the *n*-vertex star.

Define  $K_n - ke$  as a graph formed by deleting k independent edges from the complete graph  $K_n$ , where  $k = 1, 2, ..., \lfloor n/2 \rfloor$ .

**Proposition 3.4.** Let G be a connected graph with  $n \ge 2$  vertices and m edges. Then  $avec(G) \le n - \frac{2m}{r}$ 

with equality if and only if  $G = K_n - ke$  for  $k = 0, 1, ..., \lfloor n/2 \rfloor$ , or  $G = P_4$ .

**Proof.** Let d(u;i) be the number of vertices that are of distance *i* from vertex *u* in *G*, where  $i = 1, 2, ..., e_G(u)$ . For  $u \in V(G)$ , it is easily seen that

$$n-1 = d_G(u) + \sum_{i=2}^{e_G(u)} d(u;i) \ge d_G(u) + \sum_{i=2}^{e_G(u)} 1 = d_G(u) + e_G(u) - 1,$$

and thus  $d_G(u) + e_G(u) \le n$ , with equality if and only if  $e_G(u) = 1$ , i.e.  $d_G(u) = n-1$  or  $e_G(u) \ge 2$  with  $d(u;2) = d(u;3) = \dots = d(u;e_G(u)) = 1$ . Then

$$avec(G) = \frac{1}{n} \sum_{u \in \mathcal{V}(G)} e_G(u) \le \frac{1}{n} \left[ \sum_{u \in \mathcal{V}(G)} \left( n - d_G(u) \right) \right] = n - \frac{1}{n} \sum_{u \in \mathcal{V}(G)} d_G(u) = n - \frac{2m}{n}.$$

Suppose that equality holds in the above inequality. Then  $e_G(u) = 1$ , i.e.,  $d_G(u) = n-1$  or  $e_G(u) \ge 2$  with  $d(u;2) = d(u;3) = \cdots = d(u;e_G(u)) = 1$  for every  $u \in V(G)$ . Suppose first that  $e_G(u) = 1$  for some  $u \in V(G)$ . Then  $d_G(u) = n-1$  and  $e_G(v) = 1$  or 2 for all  $v \ne u$ . If  $e_G(v) = 1$  for all  $v \ne u$ , then  $G = K_n$ . Suppose that there exists some vertex v with  $e_G(v) = 2$ . Then there exists a vertex  $w \in V(G)$  such that d(v,w) = 2. Since d(v;2) = d(w;2) = 1, the vertex w is unique for fixed v. Thus  $d_G(v) = d_G(w) = n-2$ , implying that  $G = K_n - ke$  for  $k = 1, \dots, \lfloor (n-1)/2 \rfloor$ . Now suppose that  $e_G(u) \ge 2$  with  $d(u;2) = d(u;3) = \cdots = d(u;e_G(u)) = 1$  for every  $u \in V(G)$ . If  $e_G(u) = 2$  for every  $u \in V(G)$ , then  $d_G(u) = n-2$  for every  $u \in V(G)$ , and thus n is even and  $G = K_n - \frac{n}{2}e$ . If  $e_G(u) \ge 3$  for some  $u \in V(G)$ , then D(G) = 3, otherwise, for a center x of a diametrical path,  $d(x;2) \ge 2$ , a contradiction, and thus  $G = P_4$ .

Conversely, it is easily checked that  $avec(G) = n - \frac{2m}{n}$  for  $G = K_n - ke$  with  $k = 0, 1, ..., \lfloor n/2 \rfloor$ , or  $G = P_4$ .  $\Box$ 

#### 4. Average eccentricity of trees

In this section, we give lower and upper bounds for average eccentricity of *n*-vertex trees with fixed diameter, fixed number of pendent vertices and fixed matching number, respectively. We also determine the *n*-vertex trees with the first four smallest and the first |n/2| th-largest average eccentricities for  $n \ge 6$ .

**Lemma 4.1.** Let u be a vertex of a tree Q with at least two vertices. For integer  $a \ge 1$ , let  $G_1$  be the tree obtained by attaching a star  $S_{a+1}$  at its center v to u of Q, and  $G_2$ the tree obtained by attaching a+1 pendent vertices to u of Q. Then  $avec(G_2) < avec(G_1)$ .

**Proof.** Let w be a pendent neighbor of v in  $G_1$  and a pendent neighbor of u in  $G_2$ outside Q. Note that  $e_{G_2}(x) \le e_{G_1}(x)$  for any  $x \in V(Q)$ ,  $e_{G_1}(u) \le e_{G_1}(v) < e_{G_1}(w)$ , and  $e_{G_2}(w) = e_{G_1}(v)$ . Then

$$n[avec(G_2) - avec(G_1)] = \sum_{x \in V(Q)} \left[ e_{G_2}(x) - e_{G_1}(x) \right] + (a+1)e_{G_2}(w) - a \cdot e_{G_1}(w) - e_{G_1}(v)$$
  
$$\leq (a+1)e_{G_1}(v) - a \cdot e_{G_1}(w) - e_{G_1}(v)$$
  
$$= a \left[ e_{G_1}(v) - e_{G_1}(w) \right] < 0,$$

and thus  $avec(G_2) < avec(G_1)$ .  $\Box$ 

For  $2 \le d \le n-1$ , let  $\mathbf{T}(n,d)$  be the set of *n*-vertex trees with diameter d,  $T_{(n,d)}$ be the set of *n*-vertex trees obtained from the path  $P_{d+1} = v_0 v_1 \dots v_d$  by attaching n-d-1pendent vertices to  $v_{\lfloor d/2 \rfloor}$  and/or  $v_{\lceil d/2 \rceil}$ , and let  $T^{(n,d)} = \left\{T_{n,d}^a : 1 \le a \le \lfloor (n+1-d)/2 \rfloor\right\}$ , where  $T_{n,d}^a$  is the *n*-vertex tree obtained by attaching a and n+1-a-d pendent vertices respectively to the two end vertices of the path  $P_{d-1}$ . In particular,  $T_{(n,2)} = T^{(n,2)} = \{S_n\}$  and  $T_{(n,n-1)} = T^{(n,n-1)} = \{P_n\}$ .

For  $4 \le d \le n-3$ , let  $T_{(n,d)}^1$  be the set of trees obtained from a tree in  $T_{(n-1,d)}$  by attaching a pendent vertex to a pendent vertex different from  $v_0$  and  $v_d$ . For  $4 \le d \le n-2$ , let  $T_{(n,d)}^2$  be the set of trees obtained from a tree in  $T_{(n-1,d)}$  by attaching a pendent vertex to  $v_{\lfloor d/2 \rfloor -1}$  or  $v_{\lfloor d/2 \rfloor +1}$ .

**Proposition 4.2.** Let  $G \in \mathbf{T}(n,d)$ , where  $2 \le d \le n-1$ . Then

$$\frac{1}{n} \left[ \left\lfloor \frac{3(d+1)^2 - 2(d+1)}{4} \right\rfloor + (n-d-1) \left( \left\lceil \frac{d}{2} \right\rceil + 1 \right) \right] \le avec(G) \le \frac{1}{n} \left[ \left\lfloor \frac{3(d+1)^2 - 2(d+1)}{4} \right\rfloor + (n-d-1)d \right]$$

with left equality if and only if  $G \in T_{(n,d)}$ , and right equality if and only if  $G \in T^{(n,d)}$ .

**Proof.** The cases d = 2 and n-1 are trivial. Suppose that  $3 \le d \le n-2$ .

Suppose first that *G* is a tree in  $\mathbf{T}(n,d)$  with the minimum average eccentricity. Let  $P(G) = v_0 v_1 \dots v_d$  be a diametrical path of *G*. By Lemma 4.1, all vertices outside P(G) are pendent. Suppose that there exists some  $v_k$  with  $k \neq \lfloor d/2 \rfloor, \lceil d/2 \rceil$ , such that  $d_G(v_k) \ge 3$ . Let  $u_1, u_2, \dots, u_t$  be all the pendent neighbors of  $v_k$  outside P(G). Let  $G' = G - \{v_k u_1, \dots, v_k u_t\} + \{v_{\lfloor d/2 \rfloor} u_1, \dots, v_{\lfloor d/2 \rfloor} u_t\}$ . Then  $G' \in \mathbf{T}(n,d)$ . Since  $e_G(v_k) > e_G(v_{\lfloor d/2 \rfloor})$ , we have -412-

$$avec(G) - avec(G') = \frac{1}{n} \left[ t \cdot \left( e_G(v_k) + 1 \right) - t \cdot \left( e_G(v_{\lfloor d/2 \rfloor}) + 1 \right) \right]$$
$$= \frac{t}{n} \left[ e_G(v_k) - e_G(v_{\lfloor d/2 \rfloor}) \right] > 0,$$

and then avec(G) > avec(G'), a contradiction. Thus  $G \in T_{(n,d)}$ .

Conversely, it is easily seen that  

$$avec(G) = \frac{1}{n} \left[ \left\lfloor \frac{3(d+1)^2 - 2(d+1)}{4} \right\rfloor + (n-d-1) \left( \left\lceil \frac{d}{2} \right\rceil + 1 \right) \right]$$
 for  $G \in T_{(n,d)}$ .

Now suppose that G is a tree in  $\mathbf{T}(n,d)$  with the maximum average eccentricity. Suppose that  $G \notin T^{(n,d)}$ . Let  $P(G) = v_0 v_1 \dots v_d$  be a diametrical path of G. Let y be a pendent vertex outside P(G), and x the neighbor of y, where  $x \neq v_1, v_{d-1}$ . Obviously,  $e_G(y) \leq d$ . Form a tree  $G_1 = G - \{xy\} + \{v_1y\} \in \mathbf{T}(n,d)$ . Note that  $e_{G_1}(y) = d$ . It is easily seen that

$$avec(G) - avec(G_1) = \frac{1}{n} \Big[ e_G(y) - e_{G_1}(y) \Big] \le \frac{1}{n} (d - d) = 0$$

with equality if and only if  $e_G(y) = d$ . If  $e_G(y) < d$ , then  $avec(G) < avec(G_1)$ , a contradiction. Then  $e_{\overline{G}}(y) = d$ , and thus x lies outside P(G). Repeating the above procedure to all pendent neighbors of x, we may finally obtain a tree  $G_2$  with diametrical path P(G) such that x is a pendent vertex in  $G_2$  and  $e_{\overline{G}_2}(x) < d$  and  $avec(G) = avec(G_2)$ . Obviously, x is not a neighbor of  $v_1$  or  $v_{d-1}$ . Repeating the above procedure to x of  $G_2$ , we have a tree in  $\mathbf{T}(n,d)$  with larger average eccentricity, a contradiction. Thus  $G \in T^{(n,d)}$ .

Conversely, it is easily seen that  $avec(G) = \frac{1}{n} \left[ \left\lfloor \frac{3(d+1)^2 - 2(d+1)}{4} \right\rfloor + (n-d-1)d \right]$ for  $G \in T^{(n,d)}$ .  $\Box$ 

By previous proposition, we may determine trees with the first a few smallest and

largest average eccentricities as follows.

**Proposition 4.3.** Among the n-vertex trees with  $n \ge 6$ ,  $S_n$ , n-vertex double-stars (trees in  $T_{(n,3)}$ ), the tree in  $T_{(n,4)}$ , and the trees in  $T_{(n,4)}^1 \cup T_{(n,4)}^2$  ( $T_{(6,4)}^1 = \emptyset$ ) are respectively the unique trees with the smallest, second-smallest, third-smallest and fourth-smallest average eccentricity, which are equal to  $2 - \frac{1}{n}$ ,  $3 - \frac{2}{n}$ ,  $3 + \frac{1}{n}$ , and  $3 + \frac{2}{n}$ , respectively.

**Proof.** Let f(d) be the expression of the lower bound in Proposition 4.2, where  $2 \le d \le n-1$ . Suppose that  $d \le n-2$ . If d is even, then

$$n[f(d+1) - f(d)] = \frac{3(d+2)^2 - 2(d+2)}{4} + (n-d-2)\left(\frac{d+2}{2} + 1\right)$$
$$-\frac{3d^2 - 2d - 1}{4} - (n-d-1)\left(\frac{d}{2} + 1\right)$$
$$= n-1 > 0.$$

and if d is odd, then

$$n[f(d+1) - f(d)] = \frac{3(d+2)^2 - 2(d+2) - 1}{4} + (n - d - 2)\left(\frac{d+1}{2} + 1\right)$$
$$-\frac{3(d+1)^2 - 2(d+1)}{4} - (n - d - 1)\left(\frac{d+1}{2} + 1\right)$$
$$= d > 0$$

It follows that f(d) is increasing for  $2 \le d \le n-1$ . Thus, for any  $T \in \mathbf{T}(n,d)$  with  $d \ge 5$ , we have by Proposition 4.2 that  $avec(T) \ge f(5) > f(4) > f(3) > f(2)$ . Note that  $T_{(n,2)} = \{S_n\}, T_{(n,3)}$  contains exactly all the  $\lfloor n/2 - 1 \rfloor$  double-stars and  $T_{(n,4)}$  contains the unique tree formed by attaching n-5 pendent vertices to the center of the path with five vertices. Now by Proposition 4.2, we have: Among the *n*-vertex trees with  $n \ge 6$ ,  $S_n$ , *n*-vertex double-stars, and the tree in  $T_{(n,4)}$  are respectively the unique trees with the smallest, second-smallest, and third-smallest average eccentricity, which are equal to  $2 - \frac{1}{n}, 3 - \frac{2}{n},$ and  $3 + \frac{1}{n}$ , respectively. Let *T* be an *n*-vertex tree different from  $S_n$ , *n*-vertex double-stars, or the tree in  $T_{(n,4)}$ . If  $d \ge 5$ , then by Proposition 4.2,  $avec(T) \ge f(d) \ge f(5) = 4 > 3 + \frac{2}{n}$ . Suppose that d = 4. Then there is exactly one vertex of eccentricity 2 in *T* and at least three vertices of eccentricity 4. Thus  $avec(T) \ge \frac{1}{n} [2 + 3 \times 4 + 3(n-4)] = 3 + \frac{2}{n}$  with equality if and only if  $T \in T_{(n,4)}^1 \cup T_{(n,4)}^2$ . It follows that among the *n*-vertex trees with  $n \ge 6$ , the trees in  $T_{(n,4)}^1 \cup T_{(n,4)}^2$  are the unique trees with the fourth-smallest average eccentricity, which is equal to  $3 + \frac{2}{n}$ .

For  $n \ge 4$ , let  $T_n^i$  be the tree formed by attaching a pendent vertex  $v_{n-1}$  to vertex

$$v_i$$
 of the path  $P_{n-1} = v_0 v_1 \dots v_{n-2}$ , where  $1 \le i \le \left\lfloor \frac{n-2}{2} \right\rfloor$ . Since

$$avec(T_n^{i+1}) - avec(T_n^i) = \frac{1}{n} \left[ e_{T_n^{i+1}}(v_{n-1}) - e_{T_n^i}(v_{n-1}) \right] = \frac{1}{n} \left[ (n-1-i-1) - (n-1-i) \right] = -\frac{1}{n} < 0, \quad \text{we}$$
  
have  $avec(T_n^{i+1}) < avec(T_n^i)$ , where  $1 \le i \le \lfloor n/2 - 2 \rfloor$ .

**Proposition 4.4.** Among the n-vertex trees,  $P_n$  with  $n \ge 3$  is the unique graph with the largest average eccentricity, and  $T_n^i$  for  $1 \le i \le \lfloor n/2 - 1 \rfloor$  is the unique graph with the (i+1)th-largest average eccentricity, where

$$avec(P_{n}) = \begin{cases} \frac{3n-2}{4} & \text{if } n \text{ is even} \\ \frac{3n^{2}-2n-1}{4n} & \text{if } n \text{ is odd,} \end{cases}$$
$$avec(T_{n}^{i}) = \begin{cases} \frac{3(n-1)^{2}+2n-3-4i}{4n} & \text{if } n \text{ is even} \\ \frac{3(n-1)^{2}+2n-2-4i}{4n} & \text{if } n \text{ is odd.} \end{cases}$$

**Proof.** Let g(d) be the expression of the upper bound in Proposition 4.2, where  $2 \le d \le n-1$ . Suppose that  $d \le n-2$ . If d is even, then

$$n[g(d+1)-g(d)] = \frac{3(d+2)^2 - 2(d+2)}{4} + (n-d-2)(d+1)$$
$$-\frac{3(d+1)^2 - 2(d+1)}{4} - (n-d-1)d$$
$$= n - \frac{d}{2} > 0,$$

and if d is odd, then

$$n[g(d+1)-g(d)] = \frac{3(d+2)^2 - 2(d+2) - 1}{4} + (n-d-2)(d+1)$$
$$-\frac{3(d+1)^2 - 2(d+1) - 1}{4} - (n-d-1)d$$
$$= n - \frac{d+1}{2} > 0.$$

It follows that g(d) is increasing for  $2 \le d \le n-1$ . Thus, for any  $T \in \mathbf{T}(n,d)$  with  $d \le n-3$ , we have by Proposition 4.2 that  $avec(T) \le g(d) \le g(n-3) < g(n-2) < g(n-1)$ . Note that  $T^{(n,n-1)} = \{P_n\}$  and  $T^{(n,n-2)} = \{T_n^1\}$ . Then  $P_n$  for  $n \ge 3$  and  $T_n^1$  for  $n \ge 4$  are respectively the unique trees with the largest and the second-largest average eccentricity.

Suppose that  $2 \le i \le \lfloor n/2 - 1 \rfloor$ . Among the *n*-vertex trees, the (i+1)th-largest average eccentricity is achieved by the trees in  $\mathbf{T}(n, n-2) \setminus \bigcup_{i=1}^{i-1} T_n^i$  or in  $T^{(n,n-3)}$  with maximum

average eccentricity, and let  $T_1 \in \mathbf{T}(n, n-2) \setminus \bigcup_{j=1}^{i-1} T_n^j$ . Since  $avec(T_n^i) < avec(T_n^{i-1})$  for  $2 \le i \le \lfloor n/2 - 1 \rfloor$ , we have  $avec(T_1) \le avec(T_n^i)$  with equality if and only if  $T_1 = T_n^i$ . By direct calculation, we have

$$avec(T_n^i) = \begin{cases} \frac{3(n-1)^2 + 2n - 3 - 4i}{4n} & \text{if } n \text{ is even} \\ \frac{3(n-1)^2 + 2n - 2 - 4i}{4n} & \text{if } n \text{ is odd,} \end{cases}$$

and for  $T_2 \in T^{(n,n-3)}$ ,

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$$avec(T'_{n}) - avec(T_{2})$$

$$= \begin{cases} \frac{3(n-1)^{2} + 2n - 3 - 4i}{4n} - \frac{3(n-2)^{2} - 2(n-2) + 8(n-3)}{4n} & \text{if } n \text{ is even} \\ \frac{3(n-1)^{2} + 2n - 2 - 4i}{4n} - \frac{3(n-2)^{2} - 2(n-2) - 1 + 8(n-3)}{4n} & \text{if } n \text{ is odd} \end{cases}$$

$$= \begin{cases} \frac{2n - 4i + 8}{4n} & \text{if } n \text{ is even} \\ \frac{2n - 4i + 10}{4n} & \text{if } n \text{ is odd} \end{cases}$$

$$\geq \begin{cases} \frac{3}{n} & \text{if } n \text{ is even} \\ \frac{7}{2n} & \text{if } n \text{ is odd} \end{cases}$$

$$> 0.$$

Thus  $T = T_n^i$  is the unique *n*-vertex tree with the (i+1)th-largest average eccentricity. The result follows.  $\Box$ 

**Lemma 4.5.** Let *w* be a vertex of a connected graph *G*. For integers  $p, q \ge 1$ , let G(p,q) be the graph obtained from *G* by attaching pendent paths  $P = wu_1u_2...u_p$  and  $Q = wv_1v_2...v_q$  to vertex *w*. If  $p \ge q$ , then avec(G(p,q)) < avec(G(p+1,q-1)).

**Proof.** Obviously, G(p+1,q-1) is obtained from G(p,q) by deleting the edge  $v_{q-1}v_q$  and adding the edge  $u_pv_q$ .

**Case 1.**  $e_G(w) > p$ . Then  $e_{G(p,q)}(x) = e_{G(p+1,q-1)}(x)$  for  $x \neq v_q$ , and  $e_{G(p,q)}(v_q) = e_{G(p+1,q-1)}(v_q) - p - 1 + q < e_{G(p+1,q-1)}(v_q)$ . **Case 2.**  $q < e_G(w) \le p$ . Then  $e_{G(p,q)}(x) = e_{G(p+1,q-1)}(x) - 1 < e_{G(p+1,q-1)}(x)$  for

 $x \in V(G) \cup V(Q) \setminus \{v_q\}, \qquad e_{G(p,q)}(x) = e_{G(p+1,q-1)}(x) \quad \text{for} \quad x \in V(P) \setminus \{w\}, \quad \text{and} \\ e_{G(p,q)}(v_q) < e_{G(p+1,q-1)}(v_q).$ 

**Case 3.**  $e_G(w) \le q$ . Then  $\sum_{x \in V(P \cup Q)} e_{G(p+1,q-1)}(x) = \sum_{x \in V(P \cup Q)} e_{G(p+1,q-1)}(x)$  and  $e_{G(p,q)}(x) = e_{G(p+1,q-1)}(x) - 1 < e_{G(p+1,q-1)}(x)$  for  $x \in V(G) \setminus \{w\}$ .

Combing Cases 1-3, we have avec(G(p,q)) < avec(G(p+1,q-1)).  $\Box$ 

**Lemma 4.6.** Let G and G' be the trees shown in Fig. 1, where vertices x and y are connected by a path of length at least one (vertices in this path except x and y are of degree two), and x has a unique neighbor in N. In G, vertex x has at least one neighbor in M, and all of such neighbors are switched to be neighbors of y in G'. Suppose that  $\max\{d_G(x,u): u \in V(M)\} \le \max\{d_G(x,u): u \in V(N)\}$ . Then

(i) If  $e_G(x) > e_G(y)$ , then avec(G) > avec(G');

(ii) If  $e_G(x) = e_G(y)$ , then avec(G) = avec(G').



Fig. 1. Graphs G and G' in Lemma 4.6.

**Proof.** Let s be the number of neighbors of x of G in M. We know  $s \ge 1$ .

Suppose that  $e_G(x) > e_G(y)$ . Then  $\max\{d_G(x,u) : u \in V(N)\}$   $< \max\{d_G(y,u) : u \in V(Q)\}$ . Note that  $\max\{d_G(x,u) : u \in V(M)\}$  $\le \max\{d_G(x,u) : u \in V(N)\}$ . Then  $e_G(v) = e_{G'}(v)$  for  $v \in V(G) \setminus V(M)$ , and  $e_G(v) \ge e_{G'}(v) + 1$  for  $v \in V(M)$ . It is easily seen that -418-

$$avec(G') - avec(G) = \frac{1}{n} \sum_{x \in V(M)} [e_{G'}(v) - e_{G}(v)] \le -\frac{s}{n} < 0$$

and thus avec(G) > avec(G').

Suppose that  $e_G(x) = e_G(y)$ . Then  $\max\{d_G(x,u) : u \in V(N)\}\$ =  $\max\{d_G(y,u) : u \in V(Q)\}$ . Note that  $\max\{d_G(x,u) : u \in V(M)\}\$  $\leq \max\{d_G(x,u) : u \in V(N)\}$ . Then  $e_G(v) = e_G(v)$  for  $v \in V(G)$ , and thus avec(G) = avec(G').  $\Box$ 

Let  $T'_{n,p}$  be the set of *n*-vertex trees with *p* pendent vertices, where  $2 \le p \le n-1$ . A tree is starlike if it has exactly one vertex of degree at least 3. For integers *n* and *p* with  $3 \le p \le n-1$ , let  $k = \lfloor (n-1)/p \rfloor$  and r = n-1-kp, let  $T_1^{(n,p)}$  be the tree obtained by attaching p-r paths on *k* vertices and *r* paths on *k*+1 vertices to a common vertex, and if  $p \mid (n-2)$ , then let  $T_2^{(n,p)}(s)$  be the tree obtained by attaching respectively *s* paths and p-s paths on (n-2)/p vertices to the two end vertices of an edge, where  $1 \le s \le \lfloor p/2 \rfloor$ . So we can obtain

**Proposition 4.7.** Let  $G \in T'_{n,p}$ , where  $2 \le p \le n-2$ , let  $k = \lfloor (n-1)/p \rfloor$  and r = n-1-kp. Let

$$f(n,p) = \begin{cases} \frac{(3n-1)k+n-1}{2n} & \text{if } r=0, \\ \frac{(3n-1)(k+1)}{2n} & \text{if } r=1, \\ \frac{(3n+1)(k+1)}{2n} & \text{if } r \ge 2. \end{cases}$$

Then

$$f(n,p) \le avec(G) \le \frac{1}{n} \left[ \left\lfloor \frac{3(n-p+2)^2 - 2(n-p+2)}{4} \right\rfloor + (p-2)(n-p+1) \right]$$

with right equality if and only if  $G \in T^{(n,n+1-p)}$  and left equality if and only if  $G = T_1^{(n,p)}$  or  $G = T_2^{(n,p)}(s)$  with  $2 \le s \le \lfloor p/2 \rfloor$  if  $p \mid (n-2)$ , and  $G = T_1^{(n,p)}$  otherwise.

**Proof.** If 
$$G \in T^{(n,n+1-p)}$$
, then by direct calculation, we have  
 $avec(G) = \frac{1}{n} \left[ \left\lfloor \frac{3(n-p+2)^2 - 2(n-p+2)}{4} \right\rfloor + (p-2)(n-p+1) \right]$ . If  $G = T_1^{(n,p)}$  or

 $G = T_2^{(n,p)}(s) \text{ with } 2 \le s \le \lfloor p/2 \rfloor \text{ if } p \mid (n-2), \text{ and } G = T_1^{(n,p)} \text{ otherwise, then we can}$ also easily get  $avec(G) = \frac{(3n-1)k+n-1}{2n}$  if r = 0,  $avec(G) = \frac{(3n-1)(k+1)}{2n}$  if r = 1and  $avec(G) = \frac{(3n+1)(k+1)}{2n}$  if r = 2.

Let *d* be the diameter of *G*. From the proof of Proposition 4.3,  $g(d) = \frac{1}{n} \left[ \left\lfloor \frac{3(d+1)^2 - 2(d+1)}{4} \right\rfloor + (n-d-1)d \right]$  is increasing on *d*. Since  $d \le n-p+1$ , then by Proposition 4.2,  $avec(G) \le g(d) \le g(n-p+1)$  with equality if and only if  $G \in T^{(n,n+1-p)}$ .

Let G be a tree in  $G \in T'_{n,p}$  with the minimum average eccentricity. Let  $V_1(G) = \{x \in V(G) : d_G(x) \ge 3\}.$ 

**Case 1.**  $|V_1(G)| = 1$ . Then G is starlike. By Lemma 4.5,  $G = T_1^{(n,p)}$ .

**Case 2.**  $|V_1(G)| \ge 2$ .

Choose  $x, y \in V_1(G)$  such that all the internal vertices (if exist) of the path P connecting x and y have degree two. Suppose that  $e_G(x) \neq e_G(y)$ , say  $e_G(x) > e_G(y)$ . By Lemma 4.6 (1), we may get a tree in  $T'_{n,p}$  with smaller average eccentricity, a contradiction. Thus  $e_G(x) = e_G(y)$ . Suppose that  $|V_1(G)| \ge 3$ . Let  $z \in V_1(G) \setminus \{x, y\}$  such that  $\min\{d_G(x,z), d_G(y,z)\}$  is as small as possible, say  $\min\{d_G(x,z), d_G(y,z)\} = d_G(y,z)$ . As above,  $e_G(y) = e_G(z)$ . Since  $e_G(x) = e_G(y)$ , and we know that  $e_G(z) \ge d_G(y,z) + e_G(y)$ . This implies that  $d_G(y,z) \le 0$ , a contradiction. Thus  $|V_1(G)| = 2$ . Suppose that  $d_G(x,y) \ge 2$ , and  $x_1$  is the neighbor of x in P. We find that  $e_G(x) > e_G(x_1)$ . By Lemma 4.6 (1), we may get a tree in  $T'_{n,p}$  with smaller average eccentricity, a contradiction. Thus  $d_G(x,y) = 1$ .

Note that the longest pendent paths at x and y have the same length, say a If all pendent paths have equal lengths, then  $p \mid n-2$  and  $G = T_2^{(n,p)}(s)$  with  $1 \le s \le \lfloor p/2 \rfloor$ .

Suppose that  $p \mid n-2$  and there is a pendent path of length t < a. Making use of Lemma 4.6 (2), we may get a tree G' in  $T'_{n,p}$  with  $V_1(G') = \{y\}$  such that avec(G') = avec(G). Note that there are two pendent paths in G' at y with lengths a+1 and t, respectively. As in Case 1, we have  $G = T_1^{(n,p)}$ .  $\Box$ 

A matching M of the graph G is a subset of E(G) such that no two edges in Mshare a common vertex. The matching number of G is the maximum number of edges of a matching in G. If every vertex of G incidence an edge in M of G, then M is a perfect matching. For integers n and  $1 \le m \le \lfloor n/2 \rfloor$ , let U(n,m) be the set of the n-vertex trees with matching number m. Obviously,  $U(n,1) = \{S_n\}$ . For  $2 \le m \le \lfloor n/2 \rfloor$ , let  $U_{(n,m)}$  be the tree obtained by attaching m-1 paths on two vertices to the center of the star  $S_{n-2m+2}$ .

**Proposition 4.8.** Let  $T \in U(2m,m)$  with  $m \ge 3$ . Then  $avec(T) \ge \frac{7}{2} - \frac{1}{m}$  with equality if and only if  $T = U_{(2m,m)}$ .

**Proof.** Let  $T \in U(2m,m)$  with  $m \ge 3$ . Let d be the diameter of T.

Suppose first m = 3. Then d = 4,5. From the proof of Proposition 4.3, we know that  $f(d) = \frac{1}{n} \left[ \left\lfloor \frac{3(d+1)^2 - 2(d+1)}{4} \right\rfloor + (n-d-1) \left( \left\lceil \frac{d}{2} \right\rceil + 1 \right) \right]$  is increasing for  $2 \le d \le n-1$ . By Proposition 4.2,  $avec(T) \ge f(d) \ge f(4) = \frac{7}{2} - \frac{1}{3}$  with equality if and only if  $G \in T_{(6,4)}$ , i.e.,  $G = U_{(6,3)}$ .

Suppose that  $m \ge 4$  and the result holds for trees in U(2m-2,m-1). Let  $T \in U(2m,m)$  with a perfect matching M. Let u a pendent vertex of a diametrical path of T. Obviously, the unique neighbor v of u has degree two. Then  $uv \in M$  and  $T - u - v \in U(2m - 2, m - 1).$ By the induction hypothesis, we have  $\sum_{x=1}^{\infty} e_{T-u-v}(x) \ge 7(m-1)-2 \text{ with equality if and only if and } T-u-v = U_{(2m-2,m-1)}. \text{ Let } w$ be the neighbor of v different from Note that  $e_{\tau}(w) \ge 2$ . Then u.  $e_{\tau}(u) = e_{\tau}(v) + 1 \ge e_{\tau}(w) + 2 \ge 4$ . Then

$$avec(T) \ge \frac{1}{2m} \left[ \sum_{x \in T - u - v} e_{T - u - v}(x) + e_T(u) + e_T(v) \right] \ge \frac{1}{2m} \left[ \sum_{x \in T - u - v} e_{T - u - v}(x) + 4 + 3 \right]$$
$$\ge \frac{1}{2m} [7(m - 1) - 2 + 7] = \frac{7}{2} - \frac{1}{m}$$

with equalities if and only if  $e_{T-u-v}(x) = e_T(x)$  for all  $x \in V(T) \setminus \{u, v\}$ ,  $e_T(u) = 4$ ,  $e_T(v) = 3$ ,  $e_T(w) = 2$ , and  $T-u-v = T_{(2m-2,m-1)}$ , i.e.,  $T = U_{(2m,m)}$ .

**Proposition 4.9.** Let  $T \in U_{(n,m)}$  with  $2 \le m \le \lfloor n/2 \rfloor$ .

(i) If 
$$m = 2$$
, then  $avec(T) \ge 3 - \frac{2}{n}$  with equality if and only if  $T = U_{(n,2)}$ .

(ii) If 
$$m \ge 3$$
, then  $avec(T) \ge 3 + \frac{m-2}{n}$  with equality if and only if  $T = U_{(n,m)}$ .

(iii) If 
$$m = \left\lfloor \frac{n}{2} \right\rfloor$$
, then  $\operatorname{avec}(T) \le \left\lfloor \frac{3n-2}{4} \right\rfloor$  with equality if and only if  $T \in P_n$ .

(iv) If 
$$m < \lfloor \frac{n}{2} \rfloor$$
, then  
 $avec(T) \le \frac{1}{n} \left[ \frac{3(2m+1)^2 - 2(2m+1) - 1}{4} + 2(n-2m-1)m \right]$ 

with equality if and only if  $T \in T^{(n,2m)}$ .

**Proof.** Let *d* be the diameter of *T*. Suppose that m = 2. Then d = 3, 4. If d = 3, then  $T \in U(n,2)$ , and thus  $avec(T) = 3 - \frac{2}{n}$ . Suppose that d = 4. Then *T* may be obtained by attaching pendent vertices at the two end vertices of a path on three vertices. Thus  $avec(T) = 4 - \frac{4}{n} > 3 - \frac{2}{n}$ . Now (i) follows.

Suppose that  $m \ge 3$ . We prove the result (ii) by induction on n (for fixed m). If n = 2m, then by Proposition 4.8, the result holds. Suppose that n > 2m and the result holds for trees in U(n-1,m). Let  $T \in U(n,m)$ . Then there is a matching M with |M| = m and a pendent vertex u of T such that u is incident with any edge of M in T [6]. Thus  $T-u \in U(n-1,m)$ . By the induction hypothesis,

$$\sum_{x \in T-u} e_{T-u}(x) \ge 3(n-1) + m - 2$$

with equality if and only if  $T - u = U_{(n-1,m)}$ . Let v be the unique neighbor of u. Note that  $e_{\tau}(u) \ge e_{\tau}(v) + 1 \ge 3$ . Then

$$avec(T) \ge \frac{1}{n} \left[ \sum_{x \in T-u} e_{T-u}(x) + e_T(u) \right] \ge \frac{1}{n} \left[ 3(n-1) + m - 2 + 3 \right] = 3 + \frac{m-2}{n}$$

with equalities if and only if  $e_{T-u}(x) = e_T(x)$  for all  $x \in V(T) \setminus \{u\}$ ,  $e_T(u) = 3$ ,  $e_T(v) = 2$ and  $T-u = U_{(n-1,m)}$ , i.e.,  $T = U_{(n,m)}$ . The result (ii) follows.

Note that the matching number of  $P_n$  is  $\lfloor n/2 \rfloor$ . Then (iii) follows from Proposition 4.4.

Now we prove (iv). From the proof of Proposition 4.4,

$$g(d) = \frac{1}{n} \left[ \left\lfloor \frac{3(d+1)^2 - 2(d+1)}{4} \right\rfloor + (n-d-1)d \right]$$
 is increasing for  $2 \le d \le n-1$ . Since  $d \le 2m$ , we have by Proposition 4.2 that  $avec(T) \le g(d) \le g(2m)$ 
$$= \frac{1}{n} \left[ \frac{3(2m+1)^2 - 2(2m+1) - 1}{4} + 2(n-2m-1)m \right]$$
 with equalities if and only if  $T \in T^{(n,2m)}$ .

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### References

- V. A. Skorobogatov, A. A. Dobrynin, Metric analysis of graphs, *MATCH Comm. Math. Comp. Chem.* 23 (1988) 105–151.
- [2] E. V. Konstantinova, V. A. Skorobogatov, Molecular hypergraphs: The new representation of nonclassical molecular structures with polycentric delocalized bonds, *J. Chem. Inf. Comput. Sci.* 35 (1995) 472–478.
- [3] F. Buckley, F. Harary, Distance in Graphs, Addison-Wesley, Redwood, 1990.
- [4] P. Dankelmann, W. Goddard, C. S. Swart, The average eccentricity of a graph and its subgraphs, *Util. Math.* 65 (2004) 41-51.
- [5] M. Goodarzi, M. P. Freitas, N. Ghasemi, QSAR studies of bioactivities of 1-(azacyclyl)-3-arylsulfonyl-1H-pyrrolo[2,3-b]pyridines as 5-HT6 receptor ligands using physicochemical descriptors and MLR and ANN-modeling, *Europ. J. Med. Chem.* 45 (2010) 3911-3915.
- [6] R. A. Brualdi, J. L. Goldwasser, Permanent of the Laplacian matrix of trees and bipartite graphs, *Discr. Math.* 48 (1984) 1-21.
- [7] B. Zhou, Z. Du, On eccentric connectivity index, MATCH Commun. Math. Comput. Chem. 63 (2010) 181-198.