MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **65** (2011) 731-744

ISSN 0340 - 6253

Eccentric Connectivity Index of Chemical Trees

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(Received May 25, 2009)

Abstract

The eccentric connectivity index ξ^c is a distance–based molecular structure descriptor that was recently used for mathematical modeling of biological activities of diverse nature. We prove that the broom has maximum ξ^c among trees with a fixed maximum vertex degree, and characterize such trees with minimum ξ^c. In addition, we propose a simple linear algorithm for calculating ξ^c of trees.

1 Introduction

Let G be a simple connected graph with $n = |V|$ vertices. For a vertex $v \in V(G)$, $deg(v)$ denotes the degree of v. For vertices $v, u \in V$, the distance $d(v, u)$ is defined as the length of a shortest path between v and u in G. The eccentricity $\varepsilon(v)$ of a vertex v is the maximum distance from v to any other vertex.

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Sharma, Goswami and Madan [14] introduced a distance–based molecular structure descriptor, which they named "*eccentric connectivity index*" and which they defined as

$$\xi^c = \xi^c(G) = \sum_{v \in V(G)} deg(v) \cdot \varepsilon(v) \ .$$

The index ξ^c was successfully used for mathematical modeling of biological activities of diverse nature [2, 5, 10, 12, 13]. Some mathematical properties of ξ^c were recently reported in [22].

Chemical trees (trees with maximum vertex degree at most four) provide the graph representation of alkanes [7]. It is therefore a natural problem to study trees with bounded maximum degree.

Denote by $\Delta = \Delta(T)$ the maximum vertex degree of a tree T. The path P_n is the unique n-vertex tree with $\Delta = 2$, while the star S_n is the unique tree with $\Delta = n-1$. Therefore, we can assume that $3 \leq \Delta \leq n-2$.

For an arbitrary tree T on n vertices [22],

$$\left\lfloor \frac{3(n-1)^2+1}{2} \right\rfloor = \xi^c(P_n) \geq \xi^c(T) \geq \xi^c(S_n) = 3(n-1) \ .$$

2 Chemical trees with maximum eccentric connectivity index

The broom $B_{n,\Delta}$ is a tree consisting of a star $S_{\Delta+1}$ and a path of length $n-\Delta-1$ attached to a pendent vertex of the star. It is proven in [11] that among trees with maximum vertex degree equal to Δ, the broom $B_{n,\Delta}$ uniquely minimizes the largest eigenvalue of the adjacency matrix. Further, within the same class of trees, the broom has minimum Wiener index and Laplacian-energy like invariant [16]. In [18] and [21] it was demonstrated that the broom has minimum energy among trees with, respectively, fixed diameter and fixed number of pendent vertices.

Figure 1: *The broom* $B_{11,6}$.

The Δ-starlike tree $T(n_1, n_2, \ldots, n_\Delta)$ is a tree composed of the root v, and the paths P_{n_1}, P_{n_2}, ..., P_{n_Δ}, attached to v. The number of vertices of $T(n_1, n_2, \ldots, n_\Delta)$ is thus equal to $n_1+n_2+\cdots+n_\Delta+1$. Notice that the broom $B_{n,\Delta}$ is a Δ-starlike tree, $B_{n,\Delta} \cong T(n-\Delta, 1, 1, \ldots, 1)$.

Theorem 2.1 *Let w be a vertex of a nontrivial connected graph G. For nonnegative integers p and q, let $G(p,q)$ denote the graph obtained from G by attaching to the vertex w pendent paths $P = wv_1v_2\dots v_p$ and $Q = wu_1u_2\dots u_q$ of lengths p and q, respectively. If $p \geq q \geq 1$, then*

$$\xi^c(G(p,q)) < \xi^c(G(p+1,q-1)) \ .$$

Proof: The degrees of vertices u_{q-1} and v_p are changed, while all other vertices have the same degree in $G(p+1,q-1)$ as in $G(p,q)$. Since after this transformation the longer path has increased, the eccentricity of vertices from G are either the same or increased by one. We will consider three cases based on the longest path from the vertex w in the graph G. Denote by $deg'(v)$ and $\varepsilon'(v)$ the degree and eccentricity of vertex v in $G(p+1,q-1)$.

Case 1. The length of the longest path from the vertex w in G is greater than p. This means that the pendent vertex of G, most distant from w is the most distant vertex for all vertices of P and Q. It follows that $\varepsilon_{G(p+1,q-1)}(v) = \varepsilon_{G(p,q)}(v)$ for all vertices $w, v_1, v_2, \dots, v_p, u_1, u_2, \dots, u_{q-1}$, while the eccentricity of u_q increased by $p+1-q$.

$$\begin{aligned}
\xi^c(G(p+1,q-1)) - \xi^c(G(p,q)) &\geq \left[deg'(u_{q-1})\,\varepsilon'(u_{q-1}) + deg'(u_q)\,\varepsilon'\,(u_q) + deg'(v_p)\,\varepsilon'(v_p)\right] \\
&- \left[deg(u_{q-1})\,\varepsilon(u_{q-1}) + deg(u_q)\,\varepsilon(u_q) + deg(v_p)\,\varepsilon(v_p)\right] \\
&= -\varepsilon(u_{q-1}) + (p-q+1) + \varepsilon(v_p) > 0 \ .
\end{aligned}$$

Case 2. The length of the longest path from the vertex w in G is less than or equal to p and greater than q. This means that the pendent vertex of G that is most distant from w is the most distant vertex for all vertices of P, while for the vertices $w, u_1, u_2, \dots, u_q$ the most distant vertex is v_p. It follows that $\varepsilon_{G(p+1,q-1)}(v) = \varepsilon_{G(p,q)}(v)$ for vertices $v_1, v_2, \dots, v_p$, while $\varepsilon_{G(p+1,q-1)}(v) = \varepsilon_{G(p,q)}(v) + 1$ for vertices $w, u_1, u_2, \dots, u_{q-1}$. The eccentricity of u_q increased by at least 1.

$$\begin{aligned}
\xi^c(G(p+1,q-1)) - \xi^c(G(p,q)) &\geq deg'(w)\,\varepsilon'(w) + deg'(v_p)\,\varepsilon'(v_p) + \sum_{j=1}^{q} deg'(u_j)\,\varepsilon'(u_j) \\
&- deg(w)\,\varepsilon(w) - deg(v_p)\,\varepsilon(v_p) - \sum_{j=1}^{q} deg(u_j)\,\varepsilon(u_j) \\
&\geq q + [\varepsilon(u_{q-1}) + 1]\,[deg(u_{q-1}) - 1] - \varepsilon(u_{q-1})\,deg(u_{q-1}) + \varepsilon(v_p) \\
&> \varepsilon(v_p) - \varepsilon(u_{q-1}) > 0 \ .
\end{aligned}$$

Case 3. The length of the longest path from the vertex w in G is less than or equal to q. This means that the pendent vertex most distant from the vertices of P and Q is either v_p or u_q, depending on the position. Using the formula for eccentric connectivity index of a path, we have

$$\begin{aligned}\xi^c(G(p+1,q-1)) - \xi^c(G(p,q)) &> \xi^c(P_{p+q+1}) + [deg(w)-2]\,\varepsilon'(w)\\ &- \xi^c(P_{p+q+1}) - [deg(w)-2]\,\varepsilon(w)\\ &= deg(w) - 2 \geq 0\ .\end{aligned}$$

Since G is a nontrivial graph with at least one vertex, we have strict inequality.

This completes the proof. $\square$

Theorem 2.2 *Let $T \ncong B_{n,\Delta}$ be an arbitrary tree on n vertices with maximum vertex degree Δ. Then*

$$\xi^c(B_{n,\Delta}) > \xi^c(T)\ .$$

Proof: Fix a vertex v of degree Δ as a root and let $T_1, T_2, \ldots, T_\Delta$ be the trees attached at v. We can repeatedly apply the transformation described in Theorem 2.1 to any vertex of degree at least three with greatest eccentricity from the root in every tree T_i, as long as T_i does not become a path. When all trees $T_1, T_2, \ldots, T_\Delta$ turn into paths, we can again apply transformation from Theorem 2.1 at the vertex v as long as there exists at least two paths of length greater than one, further decreasing the eccentric connectivity index. Finally, we arrive at the broom $B_{n,\Delta}$ as the unique tree with maximum eccentric connectivity index. $\square$

By direct verification, it holds

$$\xi^c(BT_{n,\Delta}) = \left\lfloor \frac{3n^2 - 2\Delta n - 2n - \Delta^2 + 4\Delta}{2} \right\rfloor .$$

From the above proof, we also get that $B'_{n,\Delta} = T(n-\Delta-1, 2, 1, \ldots, 1)$ has the second minimal ξ^c among trees with maximum vertex degree Δ.

It was proven in [22] that the path P_n has maximum and the star S_n minimum ξ^c-value among connected graphs on n vertices. From Theorem 2.2 we know that the maximum eccentric connectivity index among trees on n vertices is achieved for one of the brooms $B_{n,\Delta}$. If $\Delta > 2$, we can apply the transformation from Theorem 2.1 at the vertex of degree Δ in $B_{n,\Delta}$ and obtain $B_{n,\Delta-1}$. Thus, it follows

$$EE(S_n) = EE(B_{n,n-1}) < EE(B_{n,n-2}) < \cdots < EE(B_{n,3}) < EE(B_{n,2}) = EE(P_n)\ .$$

Also, it follows that $B_{n,3}$ has the second maximum eccentric connectivity index among trees on n vertices.

3 The minimum eccentric connectivity index of trees with fixed radius

Vertices of minimum eccentricity form the center. A tree has exactly one or two adjacent center vertices; in this latter case one speaks of a bicenter. In what follows, if a tree has a bicenter, then our considerations apply to any of its center vertices.

For a tree T with radius $r(T)$,

$$d(T) = \begin{cases} 2\,r(T) - 1 & \text{if } T \text{ has a bicenter} \\ 2\,r(T) & \text{if } T \text{ has has a center.} \end{cases}$$

Let $T_{(n,d)}$ be the set of n-vertex trees obtained from the path $P_{d+1} = v_0 v_1 \dots v_d$ by attaching $n-d-1$ pendent vertices to $v_{\lfloor d/2 \rfloor}$ and/or $v_{\lceil d/2 \rceil}$, where $2 \leq d \leq n-2$. Zhou and Du in [22] proved that for arbitrary tree T on n vertices and diameter d,

$$\xi^c(T) \geq \xi(T^*)\ , \quad T^* \in T_{(n,d)}$$

with equality if and only if $T \in T_{(n,d)}$. Using the transformation from Theorem 2.1 and applying it to a center vertex, it follows that $\xi^c(T') < \xi^c(T'')$ for $T' \in T_{(n,2r-1)}$ and $T'' \in T_{(n,2r)}$.

Corollary 3.1 *Let T be an arbitrary tree on n vertices with radius r. Then*

$$\xi^c(T) \leq 3r(2r-1) + 2 + (n-2r)(2r+1)$$

with equality if and only if $T \in T_{(n,2r-1)}$.

4 The maximum eccentric connectivity index of trees with perfect matchings

A graph possessing perfect matchings must have an even number of vertices. Therefore throughout this section we assume that n is even.

It is well known that if a tree T has a perfect matching, then this perfect matching M is unique: namely, a pendent vertex v has to be matched with its unique neighbor w, and then $M - \{vw\}$ forms the perfect matching of $T - v - w$.

Let $A_{n,\Delta}$ be a Δ-starlike tree $T(n-2\,\Delta, 2, 2, \dots, 2, 1)$ consisting of a central vertex v, a pendent vertex, a pendent path of length $n-2\,\Delta$, and $\Delta - 2$ pendant paths of length 2, all attached to v.

Theorem 4.1 *The tree $A_{n,\Delta}$ has maximum eccentric connectivity index among trees with perfect matching and maximum vertex degree Δ.*

Proof: Let T be an arbitrary tree with perfect matching and let v be a vertex of degree Δ, with neighbors $v_1, v_2, \dots, v_\Delta$. Let $T_1, T_2, \dots, T_\Delta$ be the maximal subtrees rooted at $v_1, v_2, \dots, v_\Delta$, respectively. Then at most one of the numbers $|T_1|, |T_2|, \dots, |T_\Delta|$ can be odd (if T_i and T_j have odd number of vertices, then their roots v_i and v_j will be unmatched). Since the number of vertices of T is even, there exists exactly one among $T_1, T_2, \dots, T_\Delta$ with odd number of vertices.

Using Theorem 2.1, we may transform each T_i into a path attached to v – while simultaneously decreasing ξ^c and keeping the existence of a perfect matching. Assume that T_Δ has odd number of vertices, while the remaining trees have even number of vertices. We apply a transformation similar to the one in Theorem 2.1, but instead of moving one vertex, we move two vertices in order to keep the existence of a perfect matching. Thus, if $p \geq q \geq 2$ then

$$\xi^c(G(p,q)) < \xi^c(G(p+2, q-2)) \ .$$

Using this transformation we may reduce T_Δ to one vertex, the trees $T_2, \dots, T_{\Delta-1}$ to two vertices, leaving T_1 with $n-2\Delta$ vertices, and thus obtaining $A_{n,\Delta}$. Since all times we strictly decreased ξ^c, we conclude that $A_{n,\Delta}$ has minimum eccentric connectivity index among the trees with perfect matching and maximum vertex degree Δ. □

The path $P_n \cong A_{n,2}$ has maximum, while $A_{n,n/2}$ has minimum eccentric connectivity index among trees with perfect matchings.

5 The minimum eccentric connectivity index of trees with fixed number of pendent vertices

In [22] the authors determinate the n-vertex trees with p pendent vertices, $2 \leq p \leq n-1$, with the maximum eccentric connectivity index, and, consecutively, the extremal trees with the maximum, second-maximum and third-maximum eccentric connectivity index for $n \geq 6$. For the completeness, here we determine the n-vertex trees with $2 \leq p \leq n-1$ pendent vertices that have minimum eccentric connectivity index.

Definition 5.1 *Let v be a vertex of a tree T of degree $m+1$. Suppose that $P_1, P_2, \ldots, P_m$ are pendent paths incident with v, with lengths $1 \leq n_1 \leq n_2 \leq \ldots \leq n_m$. Let w be the neighbor of v distinct from the starting vertices of paths $v_1, v_2, \ldots, v_m$, respectively. We form a tree $T' = \delta(T, v)$ by removing the edges $vv_1, vv_2, \ldots, vv_{m-1}$ from T and adding $m-1$ new edges $wv_1, wv_2, \ldots, wv_{m-1}$ incident with w. We say that T' is a δ-transform of T and write $T' = \delta(T, v)$.*

Theorem 5.1 *Let $T' = \delta(T, v)$ be a δ-transform of a tree T of order n. Let v be a non-central vertex, that is most distant from the root among all branching vertices (with degree greater than 2). Then*

$$\xi^c(T) \geq \xi^c(T')$$

with equality if and only if $n_1 = n_2 = \cdots = n_{m-1} = 1$.

Proof: The degrees of vertices v and w have changed – namely, $deg(v) - deg'(v) = deg'(w) - deg(w) = m-1$. Since the vertex most distant from v does not belong to $P_1, P_2, \ldots, P_m$ and $n_m \geq n_i$ for $i = 1, 2, \ldots, m-1$, it follows that the eccentricities of all vertices different from $P_1, P_2, \ldots, P_{m-1}, P_m$ do not change after the δ transformation. The eccentricities of vertices from P_m also remain the same, while the eccentricities of vertices from $P_1, P_2, \ldots, P_{m-1}$ decrease by 1. Using the equality $\varepsilon(v) = \varepsilon(w) + 1$, it follows that

$$\begin{aligned} \xi^c(T) - \xi^c(T') &= (n_1 + n_2 + \cdots + n_{m-1} + 0) - (m-1) \cdot \varepsilon(v) + (m-1) \cdot \varepsilon(w) \\ &= n_1 + n_2 + \cdots + n_{m-1} - (m-1) \geq 0 \,. \end{aligned}$$

The equality holds if and only if $n_1 = n_2 = \cdots = n_{m-1} = 1$, since $n_i \geq 1$. □

The p-starlike tree $SB_{n,p} = T(n_1, n_2, \ldots, n_p)$ is *balanced* if all paths have almost equal lengths, i. e., $|n_i - n_j| \leq 1$ for every $1 \leq i \leq j \leq p$.

Theorem 5.2 *The balanced p-starlike tree $SB_{n,p}$ has minimum eccentric connectivity index among trees with p pendent vertices, $2 < p < n-1$.*

Proof: Let T be a rooted n-vertex tree with p pendent vertices. If T contains only one vertex of degree greater than two, we can apply Theorem 2.1 in order to arrive at the balanced starlike tree $SB_{n,p}$, without changing the number of pendent vertices. If T has several vertices of degree greater than 2, such that there are only pendent paths attached below them, then we take the one most distant from the center vertex of T. By repetitive application of the δ transformation and balancing pendant paths, the eccentric connectivity index decreases.

Assume that we arrived at a tree with two centers $C = \{v, w\}$ with only pendent paths attached at both centers. If all pendent paths have equal lengths, then $n = kp + 2$. Since we can reattach $p - 2$ pendent paths at any central vertex without changing $\xi^c(T)$, it follows that there are exactly $\lfloor p/2 \rfloor$ extremal trees with minimum eccentric connectivity index in this special case.

Now, let R be the path with length $r = r(T) - 1$ attached to v and let Q be the shortest path of length q attached to w. After applying the δ transformation at vertex v, the eccentric connectivity index remains the same. If we apply the transformation from Theorem 2.1 to two pendant paths of lengths $r + 1$ and q attached at w, we will strictly decrease the eccentric connectivity index. Finally, we conclude that $SB_{n,p}$ is the unique extremal tree that minimizes ξ^c among n-vertex trees with p pendent vertices for $n \not\equiv 2 \pmod p$. $\square$

6 Chemical trees with minimal eccentric connectivity index

Theorem 6.1 *Let T be a rooted tree, with a center vertex c as root. Let u be the vertex closest to the root vertex, such that $deg(u) < \Delta$. Let w be the pendent vertex most distant from the root, adjacent to vertex v, such that $\varepsilon(v) > \varepsilon(u)$. Construct a tree T' by deleting the edge vw and inserting the new edge uw. Then*

$$\xi^c(T) > \xi^c(T') \ .$$

Proof: In the transformation $T \to T'$ the degrees of vertices other than u and v remain the same, while $deg'(u) = deg(u) + 1$ and $deg'(v) = deg(v) - 1$. Since the tree is rooted at the center vertex, the radius of T is equal to $r(T) = d(c, w)$. Furthermore, there exists a vertex w' in a different subtree attached to the center vertex, such that $d(c, w') = r(T)$ or $d(c, w') = r(T) - 1$. From the condition $\varepsilon(v) > \varepsilon(u)$, it follows that $d(c, w') > d(c, u)$ and $w' \neq u$.

By rotating the edge vw to uw, the eccentricity of vertices other than w decrease if and only if w is the only vertex at distance $r(T)$ from the center vertex. Otherwise the eccentricities remain the same. In both cases,

$$\begin{aligned}
\xi^c(T) - \xi^c(T') &\geq deg(v)\,\varepsilon(v) + deg(w)\,\varepsilon(w) + deg(u)\,\varepsilon(u) \\
&- \left[deg'(v)\,\varepsilon'(v) + deg'(w)\,\varepsilon'(w) + deg'(u)\,\varepsilon'(u)\right] \\
&\geq \varepsilon(v) + (\varepsilon(v) - \varepsilon(u)) - \varepsilon(u) = 2(\varepsilon(v) - \varepsilon(u)) > 0 \ .
\end{aligned}$$

This completes the proof. $\square$

The Volkmann tree $VT(n,\Delta)$ is a tree on n vertices and maximum vertex degree Δ, defined as follows [3, 4]. Start with the root having Δ children. Every vertex different from the root, which is not in one of the last two levels, has exactly $\Delta - 1$ children. In the last level, while not all vertices need to exist, the vertices that do exist fill the level consecutively. Thus, at most one vertex on the level second to last has its degree different from Δ and 1. For more details on Volkmann trees see [3, 4, 6]. In [3, 4] it was shown that among trees with fixed n and Δ, the Volkmann tree has minimum Wiener index. Volkmann trees have also other extremal properties among trees with fixed n and Δ [6, 8, 15, 20].

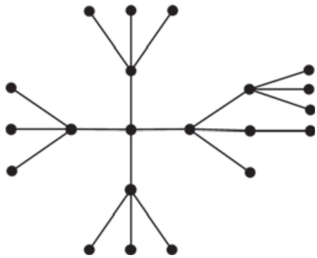

Figure 2: *The Volkmann tree* $VT(21,4)$.

Theorem 6.2 *Let T be an arbitrary tree on n vertices with maximum vertex degree Δ. Then*

$$\xi^c(T) \geq \xi^c(VT_{n,\Delta}).$$

Proof: Among n-vertex trees with maximum degree Δ, let T^* be the extremal tree with minimum eccentric connectivity index. Assume that u is a vertex closest to the root vertex c, such that $deg(u) < \Delta$ and let w be the pendent vertex most distant from the root, adjacent to vertex v. Also, let k be the greatest integer, such that

$$n \geq 1 + \Delta + \Delta(\Delta-1) + \Delta(\Delta-1)^2 + \cdots + \Delta(\Delta-1)^{k-1} \ .$$

First, we will show that the radius of T^* has to be less than or equal to $k+1$. Assume that $r(T^*) = d(c,w) > k+1$. Since the distance from the center vertex to u is less than or equal to k, it follows that

$$\varepsilon(v) \geq 2r(T^*) - 2 \geq k + r(T^*) \geq \varepsilon(u) \ .$$

If strict inequality holds, then we can apply Theorem 6.1 and decrease the eccentric connectivity index – which contradicts to the assumption that T^* is the tree with minimum ξ^c. Therefore, $\varepsilon(v) = \varepsilon(u)$

and after performing the transformation from Theorem 6.1, the eccentric connectivity index does not change. According to the definition of the number k, after finitely many transformations, the vertex w will be the only vertex at distance $r(T)$ from the center vertex and we will strictly decrease $\xi^c(T^*)$. Also, this means that for the case $n = 1 + \Delta + \Delta(\Delta-1) + \Delta(\Delta-1)^2 + \cdots + \Delta(\Delta-1)^{k-1}$, the Volkmann tree is the unique tree with minimum eccentric connectivity index.

Now, we can assume that the radius of T^* is equal $k+1$. If the distance $d(c,u)$ is less than $k-1$, it follows again that $\varepsilon(v) > \varepsilon(u)$, which is impossible. Therefore, the levels $1, 2, \ldots, k-1$ are full (level i contains exactly $\Delta(\Delta-1)^{i-1}$ vertices), while the k-th and $(k+1)$-th levels contain

$$L = n - \left[1 + \Delta + \Delta(\Delta-1) + \Delta(\Delta-1)^2 + \cdots + \Delta(\Delta-1)^{k-1}\right]$$

vertices.

Assume that T^* has only one center vertex – then $d(c,w) = k+1$ and $\varepsilon(v) = 2r(T^*) - 1$. If $d(c,u) = k-1$, we can apply the transformation from Theorem 6.1 and strictly decrease ξ^c. Thus, for $L > (\Delta-1)^k$, the k-th level is also full and the pendent vertices in the $(k+1)$-th level can be arbitrarily assigned. Using the same argument, for $L \leq (\Delta-1)^k$, the extremal trees are bicentral. By completing the k-th level, we do not change the eccentric connectivity index – since $\varepsilon(v) = \varepsilon(u)$. Finally, $\xi(T^*) = \xi(VT(n,\Delta))$ and the result follows. □

In Table 1 we give the minimum value of eccentric connectivity index among n vertex trees with maximum vertex degree Δ, together with the number of such extremal trees (of which one is the Volkman tree). Note that for $n \leq 2\Delta$ the number of extremal trees is 1, and for $\Delta > 2$ holds $\xi^c(VT(n,\Delta-1)) \geq \xi^c(VT(n,\Delta))$.

7 A linear algorithm for calculating the eccentric connectivity index of a tree

Let T be a rooted tree, with a center vertex as root. Let $c_1, c_2, \ldots, c_k$ be the neighbors of the center vertex c, and $T_1, T_2, \ldots, T_k$ be the corresponding rooted subtrees. Let r_i be the length of the longest path from c_i in the subtree T_i, $i = 1, 2, \ldots, k$.

Lemma 7.1 *The eccentricity of the vertex $v \in V(T_i)$ equals*

$$\varepsilon(v) = d(v,c) + 1 + \max_{i \neq k} r_k \ .$$

n	$\Delta=2$	$\Delta=3$	$\Delta=4$	$\Delta=5$	$\Delta=6$	$\Delta=7$	$\Delta=8$	$\Delta=9$	$\Delta=10$
11	150 ; 1	79 ; 3	62 ; 5	60 ; 6	49 ; 1	49 ; 1	49 ; 1	49 ; 1	30 ; 1
12	182 ; 1	88 ; 3	69 ; 4	67 ; 8	54 ; 1	54 ; 1	54 ; 1	54 ; 1	54 ; 1
13	216 ; 1	97 ; 1	76 ; 4	74 ; 9	72 ; 10	59 ; 1	59 ; 1	59 ; 1	59 ; 1
14	254 ; 1	106 ; 1	83 ; 3	81 ; 11	79 ; 12	64 ; 1	64 ; 1	64 ; 1	64 ; 1
15	294 ; 1	130 ; 7	90 ; 2	88 ; 11	86 ; 16	84 ; 14	69 ; 1	69 ; 1	69 ; 1
16	338 ; 1	141 ; 10	97 ; 1	95 ; 12	93 ; 19	91 ; 19	74 ; 1	74 ; 1	74 ; 1
17	384 ; 1	152 ; 7	104 ; 1	102 ; 11	100 ; 23	98 ; 24	96 ; 21	79 ; 1	79 ; 1
18	434 ; 1	163 ; 7	138 ; 24	109 ; 11	107 ; 25	105 ; 31	103 ; 27	84 ; 1	84 ; 1
19	486 ; 1	174 ; 4	147 ; 20	116 ; 9	114 ; 29	112 ; 37	110 ; 36	108 ; 29	89 ; 1
20	542 ; 1	185 ; 3	156 ; 18	123 ; 8	121 ; 30	119 ; 46	117 ; 45	115 ; 39	94 ; 1

n	$\Delta=11$	$\Delta=12$	$\Delta=13$	$\Delta=14$	$\Delta=15$	$\Delta=16$	$\Delta=17$	$\Delta=18$	$\Delta=19$
11									
12	33 ; 1								
13	59 ; 1	36 ; 1							
14	64 ; 1	64 ; 1	39 ; 1						
15	69 ; 1	69 ; 1	69 ; 1	42 ; 1					
16	74 ; 1	74 ; 1	74 ; 1	74 ; 1	45 ; 1				
17	79 ; 1	79 ; 1	79 ; 1	79 ; 1	79 ; 1	48 ; 1			
18	84 ; 1	84 ; 1	84 ; 1	84 ; 1	84 ; 1	84 ; 1	51 ; 1		
19	89 ; 1	89 ; 1	89 ; 1	89 ; 1	89 ; 1	89 ; 1	89 ; 1	54 ; 1	
20	94 ; 1	94 ; 1	94 ; 1	94 ; 1	94 ; 1	94 ; 1	94 ; 1	94 ; 1	57 ; 1

Table 1. The minimal value of the eccentricity connectivity index of trees with n vertices and maximum vertex degree Δ, and the number of such extremal trees.

Proof: We show that the longest path starting at vertex v has to traverse the center vertex c. This means that the eccentricity of v is equal to the sum of $d(v, c)$ and the longest path starting at c and not contained in T_i. Assume that the longest path P from v stays in the subtree T_i, and let w be the vertex from P at the smallest distance from the root c. Then $d(v, c) \geq d(v, w) + 1$. Since the root vertex is a center of T, we have $\max_{k \neq i} r_k + 1 \geq r_i$ and consequently

$$d(v, c) + \max_{k \neq i} r_k \geq d(v, w) + r_i \geq |P| \ .$$

This means that $d(v, c) + 1 + \max_{k \neq i} r_k$ is strictly greater than $|P|$, which is a contradiction. $\square$

We now present a simple linear algorithm for calculating the eccentric connectivity index of a tree T. First, find a center vertex of a tree – this can be done in time $O(n)$ (see [1] for details). For every vertex v, we have to find the length of the longest path from v in the subtree rooted at v. This can be done inductively using depth–first search, also in time $O(n)$. If $r[v]$ represents the length of the longest path in the subtree rooted at v, then

$$r[v] = 1 + \max_{(v,w)\in E(T),\ w\neq p[v]} r[w]$$

where $p[v]$ denotes the parent of vertex v in T. For all neighbors c_i of the center vertex c, we can calculate the maximum $\max_{i\neq j} r[c_j]$. Finally, for every vertex v we calculate the eccentricity $\varepsilon(v)$ in $O(1)$ using Lemma 7.1, and sum $deg(v)\cdot\varepsilon(v)$.

The time complexity of the algorithm is linear $O(n)$, and the memory used is $O(n)$, since we need three additional arrays of length n.

Acknowledgement. This work was supported by the research grants 144015G and 144007 of the Serbian Ministry of Science and Technological Development.

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