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On the eccentric connectivity index of a graph

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ABSTRACT

If G is a connected graph with vertex set V, then the eccentric connectivity index of G, $\xi^C(G)$, is defined as $\sum_{v\in V} \deg(v)\,\mathrm{ec}(v)$ where $\deg(v)$ is the degree of a vertex v and $\mathrm{ec}(v)$ is its eccentricity. We obtain an exact lower bound on $\xi^C(G)$ in terms of order, and show that this bound is sharp. An asymptotically sharp upper bound is also derived. In addition, for trees of given order, when the diameter is also prescribed, precise upper and lower bounds are provided.

1. Introduction

A critical step in pharmaceutical drug design continues to be the identification and optimization of compounds in a rapid and cost effective way. An important tool in this work is the prediction of physico-chemical, pharmacological and toxicological properties of a compound directly from its molecular structure. This analysis is known as the study of the quantitative structure–activity relationship (QSAR). In chemistry, a *molecular graph* represents the topology of a molecule, by considering how the atoms are connected. This can be modelled by a graph, where the points represent the atoms, and the edges symbolize the covalent bonds. Relevant properties of these graph models are then studied, giving rise to numerical graph invariants. The parameters derived from this graph-theoretic model of a chemical structure are being used not only in QSAR studies pertaining to molecular design and pharmaceutical drug design, but also in the environmental hazard assessment of chemicals.

Many such graph invariant 'topological indices' have been studied. The first, and most well-known parameter, the *Wiener index*, was introduced in the late 1940s in an attempt to analyze the chemical properties of paraffins (alkanes) [21]. This is a distance-based index, whose mathematical properties and chemical applications have been widely researched. Numerous other indices have been defined, and more recently, indices such as the *eccentric distance sum*, and the adjacency-cum-distance-based *eccentric connectivity index* have been considered [6,7,9,13,12,11,14,17,16,15,18,19]. These topological models have been shown to give a high degree of predictability of pharmaceutical properties, and may provide leads for the development of safe and potent anti-HIV compounds. Refinements of some of these indices have also been considered. For instance, the *augmented eccentric connectivity index* [1,2,8] and the *superaugmented eccentric connectivity index* [5] have been found to be useful indicators in chemical research.

We propose to investigate some mathematical properties of the eccentric connectivity index. The maximum value of the Wiener index, for a graph of given order and diameter, has not been established, but for other parameters, such as the degree distance [3,10], Gutman index and the edge-Wiener index [4,20], the maximum has been essentially established. In

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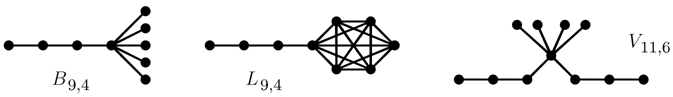

Fig. 1. Graphs $B_{9,4}$, $L_{9,4}$, $V_{11,6}$.

this paper we will consider the same problem, and establish bounds, both upper and lower, for the eccentric connectivity index.

2. Definitions and some examples

Consider a simple connected graph G, and let $V(G)$ and $E(G)$ denote its vertex and edge sets, respectively. $|V(G)| = n(G)$ is called the *order* of G. The *distance* between u and v in $V(G)$, $d_G(u, v)$, is the length of a shortest $u - v$ path in G. The *eccentricity*, $ec_G(u)$ of a vertex $u \in V(G)$ is the maximum distance between u and any other vertex in G. The *diameter* of G, d, is defined as the maximum value of the eccentricities of the vertices of G. Similarly, the *radius* of G is defined as the minimum value of the eccentricities of the vertices of G. A *central vertex* of G is any vertex whose eccentricity is equal to the radius of G. Finally, the degree of a vertex $w \in V(G)$, $\deg_G(w)$ is the number of edges incident to w. If no ambiguity is possible, the subscript G may be omitted.
We define the *eccentric connectivity* $\xi^C(G)$ of G as

$$\xi^C(G) = \sum_{v \in V(G)} \mathrm{ec}(v) \deg(v).$$

For special classes of graphs we have the following useful values for our parameter.

$$\xi^C(K_n) = n(n-1) \quad (\text{for } n \geq 2);$$
$$\xi^C(K_{a,b}) = 4\,a\,b \quad (\text{for } a, b \neq 1)$$

and the index reaches its maximum for $K_{a,b}$ when $a = b = n/2$.
For the star, cycle and path of order n,

$$\xi^C(S_n) = \xi^C(K_{1,n-1}) = 3(n-1) \quad (\text{for } n \geq 3);$$
$$\xi^C(C_n) = \begin{cases} n^2 & \text{for } n \text{ even} \\ n(n-1) & \text{for } n \text{ odd;} \end{cases}$$
$$\xi^C(P_n) = \begin{cases} \frac{1}{2}(3n^2 - 6n + 4) & \text{for } n \text{ even} \\ \frac{3}{2}(n-1)^2 & \text{for } n \text{ odd.} \end{cases}$$

Finally, we calculate the eccentric connectivity index for three other classes of graphs which will be important in our theorems. The *broom* graph $B_{n,d}$ consists of a path P_d, together with $(n-d)$ end vertices all adjacent to the same end vertex of P_d. The *lollipop* graph $L_{n,d}$ is obtained from a complete graph K_{n-d} and a path P_d, by joining one of the end vertices of P_d to all the vertices of K_{n-d}. The *volcano* graph $V_{n,d}$ is the graph obtained from a path P_{d+1} and a set S of $n-d-1$ vertices, by joining each vertex in S to a central vertex of P_{d+1}. See Fig. 1.
Straightforward calculations show that

$$\xi^C(B_{n,d}) = \begin{cases} 2dn - n - d^2/2 - d + 1 & \text{for } d \text{ even} \\ \frac{1}{2}(3 - 2d - d^2 - 2n + 4dn) & \text{for } d \text{ odd;} \end{cases}$$
$$\xi^C(L_{n,d}) = \begin{cases} \frac{1}{2}(2 - 2d + d^2 + 2d^3 - 2n + 2dn - 4d^2n + 2dn^2) & \text{for } d \text{ even} \\ \frac{1}{2}(3 - 2d + d^2 + 2d^3 - 2n + 2dn - 4d^2n + 2dn^2) & \text{for } d \text{ odd;} \end{cases}$$
$$\xi^C(V_{n,d}) = \begin{cases} nd + n + d^2/2 - 2d - 1 & \text{for } d \text{ even} \\ nd + 2n + d^2/2 - 3d - 3/2 & \text{for } d \text{ odd.} \end{cases}$$

3. Results

Theorem 1. *Let $G = (V, E)$ be a connected graph of order n, $n \geq 4$. Then*

$$\xi^C(G) \geq 3(n-1),$$

and the bound is tight.

Proof. Let $A = \{v \in V \mid \deg(v) = n-1\}$, $B = \{v \in V \mid n-2 \geq \deg(v) \geq 2\}$ and $C = \{v \in V \mid \deg(v) = 1\}$. Then letting $|A| = a,\ |B| = b$ and $|C| = c$, we obtain

$$a + b + c = n. \tag{1}$$

Since $\deg(v) \leq n-2$ for every vertex v in $B \cup C$, it is easy to see that, for $n \geq 4$,

$$\mathrm{ec}(v) \geq 2 \quad \text{for all } v \in B \cup C. \tag{2}$$

Case 1: $A \neq \emptyset$; i.e., $a \geq 1$. Then (1) and (2) in conjunction with $n > 3$, give

$$\begin{aligned}
\xi^C(G) &= \sum_{v \in A} \mathrm{ec}(v)\deg(v) + \sum_{v \in B \cup C} \mathrm{ec}(v)\deg(v) \\
&\geq \sum_{v \in A} 1 \cdot (n-1) + \sum_{v \in B \cup C} 2 \cdot 1 \\
&= a(n-1) + 2(b+c) \\
&= 2n + a(n-3) \\
&\geq 2n + n - 3,
\end{aligned}$$

as claimed.
Case 2: $A = \emptyset$; i.e., $a = 0$. It can be seen that $\mathrm{ec}(v) \geq 3$ for all $v \in C$. This, together with (1) and (2) yields

$$\begin{aligned}
\xi^C(G) &= \sum_{v \in B} \mathrm{ec}(v)\deg(v) + \sum_{v \in C} \mathrm{ec}(v)\deg(v) \\
&\geq \sum_{v \in B} 2 \cdot 2 + \sum_{v \in C} 3 \cdot 1 \\
&= 4b + 3c \\
&= 3n + b,
\end{aligned}$$

and the bound is established. The bound is attained by the star graph. □

Theorem 2. *Let G be a connected graph of order n and diameter d. Then*

$$\xi^C(G) \leq d(n-d)^2 + O(n^2),$$

and this bound is best possible.

Proof. For a vertex v of G, define $D(v) = \mathrm{ec}(v)\deg(u)$. Thus

$$\xi^C(G) = \sum_{v \in V(G)} D(v).$$

Let $P = u_0, u_1, \ldots, u_d$ be a diametral path, and let $M \subseteq V$ be the set of the remaining vertices which are not on P. Call $m = |M|$.

Claim 1. $\sum_{x \in V(P)} D(x) \leq O(n^2)$.

Write $d = 3q + r$ for $r \in \{0, 1, 2\}$, and partition the vertices of P as $V(P) = V_0 \cup V_1 \cup V_2$, where V_0, V_1 and V_2 are defined as follows: For the case when $r = 0$ we set

$$\begin{aligned}
V_0 &= \{u_0, u_3, u_6, \ldots, u_{3q}\} \\
V_1 &= \{u_1, u_4, u_7, \ldots, u_{3q-2}\} \\
V_2 &= \{u_2, u_5, u_8, \ \ldots, u_{3q-1}\}
\end{aligned}$$

and so for this case, $|V_1| = |V_2| = |V_0| - 1$. Similarly, for $r = 1$ or 2, all the vertices of P can be consecutively assigned to one of the three classes V_0, V_1, V_2.

Let $x, y \in V_i$, for some $i = 0, 1, 2$. Since the distance between x and y along P is at least 3, and P is a diametral path, we have that $N[x] \cap N[y] = \emptyset$, where $N[v]$ is the closed neighbourhood of v in G. Thus $\sum_{x \in V_i} \deg(x) \leq n - |V_i|$, for each $i = 0, 1, 2$. Now

$$\begin{aligned}
\sum_{x \in V(P)} D(x) &= \sum_{x \in V_0} D(x) + \sum_{x \in V_1} D(x) + \sum_{x \in V_2} D(x) \\
&\leq \sum_{x \in V_0} d\deg(x) + \sum_{x \in V_1} d\deg(x) + \sum_{x \in V_2} d\deg(x)
\end{aligned}$$

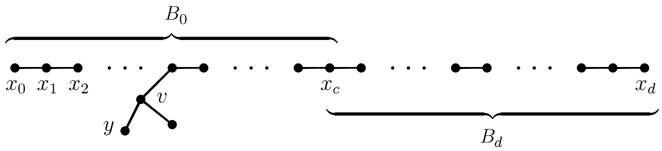

Fig. 2. Tree T in the proof of Theorem 3.

$$\begin{aligned} &= d\left(\sum_{x\in V_0}\deg(x)+\sum_{x\in V_1}\deg(x)+\sum_{x\in V_2}\deg(x)\right)\\ &\le d(n-|V_0|+n-|V_1|+n-|V_2|)\\ &= d(3n-d-1)\\ &= O(n^2). \end{aligned}$$

This argument holds for $r = 0$, 1 and 2, and thus the claim is proven.

Claim 2. *$D(v) \le d(n-d) + O(n)$ for all $v \in M$.*

Since P is a diametral path, $v \in M$ is adjacent to at most 3 vertices of P. Hence, $\deg(v) \le n-d+1$ and so

$$D(v) \le d(n-d+1) \le d(n-d) + O(n),$$

as required.

Finally, combining Claims 1 and 2 we obtain

$$\begin{aligned} \xi^c(G) = \sum_{v\in M} D(v) + \sum_{x\in P} D(x) &\le m\{d(n-d)+O(n)\} + O(n^2)\\ &= (n-d-1)d(n-d) + O(n^2)\\ &= d(n-d)^2 + O(n^2) \end{aligned}$$

which completes the proof.

This bound is sharp, since the lollipop graph attains this upper value. In fact, it can be verified that

$$\xi^C(L_{n,d}) = d(d-n)^2 + O(n^2).$$

□

A simple maximization of the bound in Theorem 2 results in a maximum eccentricity value at $d = n/3$, and hence we have

Corollary 1. *Let G be a connected graph of order n. Then*

$$\xi^C(G) \le \frac{4}{27}n^3 + O(n^2),$$

and the bound is sharp.

Again, the lollipop graph, $L_{n,n/3}$ shows that this bound is best possible.

Theorem 3. *Let T be a tree of order n, $n \ge 2$. Then*

$$\xi^C(T) \le \xi^C(P_n) = \begin{cases} \frac{1}{2}(3n^2-6n+4) & \text{for } n \text{ even}\\ \frac{3}{2}(n-1)^2 & \text{for } n \text{ odd}. \end{cases} \tag{3}$$

Proof (*By Reverse Induction on the Diameter d of T*)**.** Firstly, if $d = n-1$, then $T = P_n$ and the theorem is true. The same is true when $n = 2$ or 3. Call ε the number of end vertices of T: clearly $\varepsilon \ge 3$, if T is not a path.

So, assume that $n \ge 4$, $d \le n-2$ and that (3) holds if $d = k+1$, for $2 \le k \le n-2$.

Now, consider a tree T with diameter $d = k$.

Let $P : x_0, x_1, \dots, x_c, \dots, x_d$ be a diametral path in T, where x_c is a central vertex of T. Observe that for each vertex w in $V(T)$, $\mathrm{ec}(w) \in \{d(w, x_0), d(w, x_d)\}$.

Let B_0 and B_d be the branches at x_c containing, respectively, x_0 and x_d. Also, let y be an end vertex of T, where $y \notin \{x_0, x_d\}$. Say, without loss of generality, that y is not in B_d, and let $vy \in E(T)$. See Fig. 2.

Define $T' = (T - \{v\,y\}) \cup \{y\,x_0\}$. Then $d(T') = k + 1$ and $|V(T')| = n$, so by the induction hypothesis

$$\xi^C(T') \le \xi^C(P_n). \tag{4}$$

For $z \in V(T) - \{y, v, x_0\}$, we have $\mathrm{ec}_{T'}(z) \ge \mathrm{ec}_T(z)$ (and certainly, $\mathrm{ec}_{T'}(z) > \mathrm{ec}_T(z)$ if z is in B_d.) Furthermore, $\deg_{T'}(v) = \deg_T(v) - 1$, $\deg_{T'}(x_0) = \deg_T(x_0) + 1$, and $\mathrm{ec}_{T'}(y) = d + 1 \ge \mathrm{ec}_T(y) + 1$. Thus,

$$\begin{aligned}\xi^C(T') - \xi^C(T) &> \mathrm{ec}_T(v)(\deg_T(v) - 1) + (\mathrm{ec}_T(x_0)) \cdot 2 + (\mathrm{ec}_T(y) + 1) \cdot 1 - \{\mathrm{ec}_T(v) \deg_T(v) + d \cdot 1 + \mathrm{ec}_T(y) \cdot 1\}\\ &= d - \mathrm{ec}_T(v) + 1\\ &\ge 1.\end{aligned}$$

Combining this inequality with (4), we conclude that $\xi^C(T) < \xi^C(T') \le \xi^C(P_n)$. and the proof is complete. □

Theorem 4. *If T is a tree of order n and diameter d, then $\xi^C(T) \le \xi^C(B_{n,d})$.*

Proof. Let $P : x_0, x_1, \ldots, x_d$ be a diametral path in T.

If $T = B_{n,d}$, then there is nothing to be proved; so assume that there exists an end vertex v of T, $v \neq x_0$, such that v is adjacent to a vertex u, where $u \neq x_{d-1}$. (It is possible that u lies on P.) Denote by $\{v_1, v_2, \ldots, v_k\}$ the set of end vertices which are adjacent to u; and $v_i \neq x_0$ for $i = 1, 2, \ldots, k$. Let $\deg(u) = r + k$, for some $r \ge 1$.

Form another tree, T', by replacing the k edges $u\,v_i$ with $x_{d-1}\,v_i$ for $i = 1, 2, \ldots, k$. Note that T' has the same order and diameter as T.

We show that T' has a larger eccentric connectivity index than T.

$$\begin{aligned}\xi^C(T) &= \sum_{i=1}^{k} \mathrm{ec}_T(v_i) \deg_T(v_i) + \mathrm{ec}_T(u) \deg_T(u) + (d-1) \deg_T(x_{d-1}) + N\\ &\le k \cdot (d)(1) + \mathrm{ec}_T(u)(r+k) + (d-1)\deg_T(x_{d-1}) + N,\end{aligned}$$

where $N = \sum_{x \in V(T) - \{v_1, v_2, \ldots, v_k, u, x_{d-1}\}} \mathrm{ec}_T(x) \deg_T(x)$.

In comparison,

$$\xi^C(T') = k \cdot (d)(1) + \mathrm{ec}_T(u)\,r + (d-1)(k + \deg_T(x_{d-1})) + N.$$

So, since $\mathrm{ec}(u) \le d - 1$,

$$\xi^C(T') - \xi^C(T) \ge -k\,\mathrm{ec}_T(u) + k(d-1) \ge 0.$$

Continue this procedure, forming new trees, until all the end vertices in $V(T) - \{x_0\}$ are adjacent to x_{d-1}. Thus, a broom $B_{n,d}$ is obtained, of order n and diameter d, with the property that $\xi^C(B_{n,d}) \ge \xi^C(T)$. □

Theorem 5. *If T is a tree of order $n \ge 3$ and diameter d, then*

$$\xi^C(T) \ge \xi^C(V_{n,d}). \tag{5}$$

Proof. The statement (5) holds if $n = 3$ or 4, and if $d = n - 1$. Let us assume that there exists a tree T with $\xi^C(T) < \xi^C(V_{n,d})$, where d is the diameter of T and, of such counterexamples to (5), choose T to have the smallest possible order, n.

Let $P : x_0, x_1, \ldots, x_d$ be a diametral path in T.

Suppose there exists an end vertex x in $V(T) - V(P)$ adjacent to a vertex y, and let $T' = T - x$. Then, since $n(T') < n(T)$ we have

$$\xi^C(T') \ge \xi^C(V_{n-1,d}) \quad \text{while } \xi^C(T) < \xi^C(V_{n,d}).$$

Hence $\xi^C(T) - \xi^C(T') < \xi^C(V_{n,d}) - \xi^C(V_{n-1,d}) \le \begin{cases} d+1 & \text{for } d \text{ even} \\ d+2 & \text{for } d \text{ odd.} \end{cases}$

$$\begin{aligned}\text{However,}\quad \xi^C(T) - \xi^C(T') &\ge \mathrm{ec}(x) \cdot 1 + \mathrm{ec}(y) \cdot 1\\ &\ge (\lceil d/2 \rceil + 1) + \lceil d/2 \rceil\\ &\ge \begin{cases} d+1 & \text{for } d \text{ even} \\ d+2 & \text{for } d \text{ odd.} \end{cases}\end{aligned}$$

This is a contradiction, and the proof is complete. □

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