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# A lower bound on the eccentric connectivity index of a graph

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ABSTRACT

In pharmaceutical drug design, an important tool is the prediction of physicochemical, pharmacological and toxicological properties of compounds directly from their structure. In this regard, the Wiener index, first defined in 1947, has been widely researched, both for its chemical applications and mathematical properties. Many other indices have since been considered, and in 1997, Sharma, Goswami and Madan introduced the *eccentric connectivity index*, which has been identified to give a high degree of predictability. 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 vertex $v$ and $\mathrm{ec}(v)$ is its eccentricity. Several authors have determined extremal graphs, for various classes of graphs, for this index. We show that a known tight lower bound on the eccentric connectivity index for a tree $T$, in terms of order and diameter, is also valid for a general graph $G$, of given order and diameter.



## 1. Introduction

Topological indices, such as the eccentric connectivity index, are graph-theoretical invariants designed to find relationships between the structure of chemical molecules and their physical properties. These indices have been used for isomer discrimination, chemical documentation, drug design, quantitative structure versus activity (or property) relationships (QSAR/QSPR's), combinatorial library design, and toxicology hazard assessments [4,5,7,11]. In pharmaceutical research, QSAR information is used to select the most promising compounds for a desired property, and hence decreases the number of compounds which need to be synthesized during the process of designing new drugs [3,9,12].

Many topological indices have been defined and used. The first, the Wiener index, was introduced in 1947. The Hosoya index, Randić's molecular connectivity index, Zagreb group parameters and Balaban's index were introduced in the 1970's and 1980's [8]. Dozens of other topological descriptors can be found in the literature. In 1997, the eccentric connectivity index was put forward by Sharma et al. [16].

Research continues on the eccentric connectivity index [7,10] with current focus on nanotubes [1,2,15]. In this paper, we investigate mathematical properties of the eccentric connectivity index. More specifically, we will consider extremal values of this molecular descriptor. The investigation of extremal values is closely linked to isomer enumeration [13]. Suppose an integral index $X$ is shown to have minimum and maximum values of $X_m$ and $X_M$ respectively, and that a particular class of chemical compounds under consideration has $N$ isomers. If $N > (X_M - X_m)$, then two or more isomers will have the same value of the chosen index $X$. This type of 'degeneracy' is a serious problem encountered with topological indices. The eccentric connectivity index has been found to have quite low degeneracy [6].

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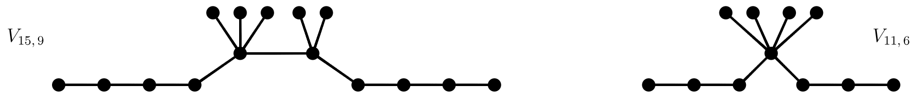


**Fig. 1.** Volcano graphs $V_{15,\,9}$, and $V_{11,\,6}$.

## 2. Definitions and preliminaries

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*, $\mathrm{ec}_G(u)$, 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 $G$. The *centre* of a graph is the subgraph induced by its central vertices. Denote by $C(G)$ the set of central vertices of $G$. Also, the degree of a vertex $w \in V(G)$, $\deg_G(w)$, is the number of edges incident to $w$. A vertex of degree 1 is called a *pendant* vertex. The *neighbourhood* of a vertex $v \in V(G)$, $N_G(v)$, consists of all vertices which are adjacent to $v$. Similarly, for $H \subseteq G$, the neighbourhood of $H$, $N(H)$, is composed of the neighbours of all the vertices in $H$. A vertex is a *cut-vertex* if its removal disconnects the graph. If no ambiguity is possible, the subscript $G$ may be omitted in these notations.

The *eccentric connectivity index* $\xi^C(G)$ of $G$ is defined as

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

Formulae for the eccentric connectivity index of the complete graph $K_n$, complete bipartite graph $K_{p,q}$, cycle graph $C_n$, star graph $S_n$ and the path $P_n$ have been calculated independently by several authors [6,14,18].

The *volcano* graph $V_{n,\,d}$, first defined in [14], is a 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. Note that for a fixed value of $n$, when $d$ is even, the volcano graph $V_{n,d}$ is unique; whereas when $d$ is odd, there may be several non-isomorphic volcano graphs $V_{n,d}$. The eccentric connectivity index for the volcano graph $V_{n,\,d}$ is

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

A number of authors have recently considered the extremal values for the eccentric connectivity index. It was proved independently by Morgan et al. [14], as well as Zhou and Du [18], that the minimum eccentric connectivity index for a graph of order $n$ is attained by the star graph. An asymptotic maximum has also been identified [6,14], and the exact formula for the eccentric connectivity index of this extremal graph has been calculated [14]. Not surprisingly, the maximum index value for trees of order $n$ is attained by the path graph [6,14,18]. For trees of order $n$ and diameter $d$, a sharp upper bound has been found [14]. The lower bound is attained by the volcano graph. Thus, if $T$ is a tree of order $n \geq 3$ and diameter $d$, then

$$\xi^C(T) \geq \xi^C(V_{n,\,d}). \tag{1}$$

This inequality was derived, using different approaches, by Morgan et al. [14], by Zhou and Du [18]; and Yu et al. [17] indirectly deduced the same result.

In this paper, we generalize inequality (1), by proving that the volcano graph achieves the lowest value for the eccentric connectivity index over all general graphs (rather than only trees), of fixed order $n$ and diameter $d$.

This simple generalization has been quite challenging to prove. The difficulty in achieving the sharp bound lies with some 'problem vertices'.

Observe that since the eccentricity of any vertex is bounded below by the radius of the graph, we have that

$$\text{for all vertices } w \in V(G), \quad \mathrm{ec}(w) \geq \lceil d/2 \rceil. \tag{2}$$

The problem vertices have degree two, and precisely meet this eccentricity lower bound.

*Notation*

Given a connected graph $G$ with diameter $d$, we denote by $t(G)$ the number of vertices in $G$ of degree 2 and eccentricity precisely $\lceil d/2 \rceil$, i.e.,

$$t(G) := |\{x \in V(G) \mid \deg(x) = 2 \text{ and } \mathrm{ec}(x) = \lceil d/2 \rceil\}|.$$

## 3. Results

Consider a connected graph $G$ of order $n$ and diameter $d$. If $d = 2$, note that from the previous section, $\xi^C(G) \geq \xi^C(S_n) = \xi^C(V_{n,\,2})$.

Hence from now onwards in this paper, we only consider $d \geq 3$.

**Theorem 1.** *Let $G = (V, E)$ be a connected graph of order $n$, and diameter $d \geq 3$. Then*

$$\xi^C(G) \geq \xi^C(V_{n,d}).$$

**Proof.** *Part A*

We first prove that the theorem holds when $G$ contains at least one problem vertex. So, assume that $t(G) \geq 1$. We must show that $\xi^C(G) \geq \xi^C(V_{n,d})$.

Suppose, to the contrary, that there exists a counterexample $G$, for which $t(G) \geq 1$ and

$$\xi^C(G) < \xi^C(V_{n,d}). \tag{3}$$

Of all such counterexamples, choose $G$ to have the smallest possible order, $n$. Hence, any graph $G'$ with diameter $d'$, at least one problem vertex, and $n' < n$ vertices, will satisfy

$$\xi^C(G') \geq \xi^C(V_{n',d'}). \tag{4}$$

Let $P : v_0, v_1, \ldots, v_d$ be a diametral path in $G$, and define $S = V - V(P)$.

We will need two general properties of the distance from a vertex $w \in G$ to $v_0$ or $v_d$, for any arbitrary graph $G$.

$$\text{For all vertices } w \in V(G), \quad d(w, v_0) \geq \lceil d/2 \rceil \quad \text{or} \quad d(w, v_d) \geq \lceil d/2 \rceil. \tag{5}$$

To see that (5) holds, suppose, by contradiction, that both $d(w, v_0) < \lceil d/2 \rceil$ and $d(w, v_d) < \lceil d/2 \rceil$. By the triangle inequality, $d = d(v_0, v_d) \leq d(v_0, w) + d(w, v_d)$ which implies

$$d \leq (\lceil d/2 \rceil - 1) + (\lceil d/2 \rceil - 1) = 2\lceil d/2 \rceil - 2 = \begin{cases} d-2 & \text{for } d \text{ even} \\ d-1 & \text{for } d \text{ odd}, \end{cases}$$

which is impossible, and (5) is proven.

It follows from the definition of eccentricity, and (5), that

$$\text{for } w \in V(G), \quad \text{if } \mathrm{ec}(w) = \lceil d/2 \rceil, \quad \text{then } d(w, v_0) = \lceil d/2 \rceil \quad \text{or} \quad d(w, v_d) = \lceil d/2 \rceil. \tag{6}$$

We will apply these two general properties of graphs to our counterexample graph $G$.

**Claim A1.** *There are no pendant vertices in $S$.*

**Proof of Claim A1.** Suppose to the contrary, that $S$ contains a pendant vertex $x$, and let $y$ be the neighbour of $x$. Form $G'$ by removing the vertex $x$, viz. set $G' = G - x$.

**Fact 1.** (i) The diameter of $G'$ is $d$, since $x$ is not on the diametral path $P$.
(ii) $n(G') = n - 1 < n(G)$.
(iii) $t(G') \geq 1$.

To establish (iii), we show that $G'$ indeed has a problem vertex. Since $t(G) \geq 1$, let $z$ be a problem vertex of $G$, i.e., $\deg_G(z) = 2$ and $\mathrm{ec}_G(z) = \lceil d/2 \rceil$. We first show that $z \neq y$. If $z$ is equal to $y$, then $\deg_G(y) = 2$. Let $w$ be the other neighbour of $y$. Note that any path from $\{v_0, v_d\}$ to $y$ must pass through $w$. We can assume, without loss of generality, that $d_G(w, v_d) \geq d_G(w, v_0)$. Then, by (5),

$$\mathrm{ec}_G(y) \geq d_G(y, v_d) = d_G(y, w) + d_G(w, v_d) \geq 1 + \lceil d/2 \rceil,$$

and this contradicts the fact that $\mathrm{ec}_G(y) = \mathrm{ec}_G(z) = \lceil d/2 \rceil$. Thus, $z \neq y$, and this implies that $\deg_{G'}(z) = 2$.

Since $\mathrm{ec}_G(z) = \lceil d/2 \rceil$, (6) implies that in $G$, $z$ is at distance $\lceil d/2 \rceil$ from one of $v_0$ or $v_d$, say, $v_d$. Then, since $x$ is not on any such shortest path between $z$ and $v_d$, $\lceil d/2 \rceil = d_G(z, v_d) = d_{G'}(z, v_d)$. So, $\mathrm{ec}_{G'}(z) \geq \lceil d/2 \rceil$. But the removal of a pendant vertex cannot increase the eccentricity of any other vertex in the graph ($\mathrm{ec}_{G'}(z) \leq \mathrm{ec}_G(z)$), so we conclude that $\mathrm{ec}_{G'}(z) = \lceil d/2 \rceil$, and hence $z$ is a problem vertex of $G'$. This completes the proof of Fact 1.

From Fact 1, $G'$ is not a counterexample, and thus by (4)

$$\xi^C(G') \geq \xi^C(V_{n-1,d}). \tag{7}$$

Note that for all $u \in V(G') - \{y\}$, $\deg_G(u) = \deg_{G'}(u)$, and $\mathrm{ec}_G(u) \geq \mathrm{ec}_{G'}(u)$. Also, $\mathrm{ec}_G(y) = \mathrm{ec}_{G'}(y)$. These observations, as well as (2), imply

$$\begin{aligned}
\xi^C(G) - \xi^C(G') &\geq \deg_G(x)\,\mathrm{ec}_G(x) + \deg_G(y)\,\mathrm{ec}_G(y) - \deg_{G'}(y)\,\mathrm{ec}_{G'}(y) \\
&= 1 \cdot \mathrm{ec}_G(x) + \deg_G(y)\,\mathrm{ec}_G(y) - (\deg_G(y) - 1)\,\mathrm{ec}_{G'}(y) \\
&= \mathrm{ec}_G(x) + 1 \cdot \mathrm{ec}_G(y) \\
&\geq (\lceil d/2 \rceil + 1) + \lceil d/2 \rceil \\
&= 2(\lceil d/2 \rceil) + 1.
\end{aligned}$$

Thus

$$\xi^C(G') + 2(\lceil d/2 \rceil) + 1 \le \xi^C(G).$$

Combining this with (7) yields

$$\xi^C(V_{n-1,\,d}) + 2(\lceil d/2 \rceil) + 1 \le \xi^C(G),$$

and since $G$ is a counterexample, (3) gives

$$\xi^C(V_{n-1,\,d}) + 2(\lceil d/2 \rceil) + 1 \le \xi^C(G) < \xi^C(V_{n,\,d}). \tag{8}$$

But, straightforward calculations yield

$$\begin{aligned}
\xi^C(V_{n-1,\,d}) + 2(\lceil d/2 \rceil) + 1 &= \begin{cases} (n-1)(d+1) + d^2/2 - 2d - 1 + (d+1) & \text{for } d \text{ even} \\ (n-1)(d+2) + d^2/2 - 3d - 3/2 + (d+2) & \text{for } d \text{ odd} \end{cases} \\
&= \begin{cases} n(d+1) + d^2/2 - 2d - 1 & \text{for } d \text{ even} \\ n(d+2) + d^2/2 - 3d - 3/2 & \text{for } d \text{ odd} \end{cases} \\
&= \xi^C(V_{n,\,d}).
\end{aligned}$$

So (8) reduces to $\xi^C(V_{n,\,d}) < \xi^C(V_{n,\,d})$, a contradiction. Therefore, Claim A1 is proven. □

**Fact 2.** Every vertex in $G$ has degree at least 2, except possibly for $v_0$ and $v_d$.

To see that Fact 2 holds, recall that $V = S \cup \{v_1, v_2, \dots, v_{d-1}\} \cup \{v_0,\ v_d\}$. Then, observe that by Claim A1, every vertex in $S$ has degree at least 2. Also, for every $v_i,\ i = 1, \dots, (d-1)$, on $P$, we have $\deg(v_i) \ge 2$, and hence, Fact 2 is established.

We now look at two cases separately, depending on the parity of $d$. In each case, we will partition the vertex set of the counterexample graph $G$ into several sets, in order to calculate a lower bound on the eccentric connectivity index of $G$ in terms of the index value of the volcano graph $V_{n,\,d}$, in order to arrive at a contradiction.

*Case* 1. $d$ is even.

Here $\lceil d/2 \rceil = d/2$. Let $Q$ be the set of problem vertices, i.e., $Q := \{x \in V(G) \mid \deg(x) = 2,\ \mathrm{ec}(x) = d/2\}$.

**Claim 2.** *Every vertex $u \in Q$ is adjacent to some vertex $u'$ satisfying*

$$\mathrm{ec}(u') \ge (d/2) + 1.$$

**Proof of Claim 2.** Consider a problem vertex $u \in Q$. Since $\mathrm{ec}(u) = \lceil d/2 \rceil$, (6) implies that $u$ is at a distance $d/2$ from one of $v_0$ or $v_d$, say, $v_d$. Consider a shortest path connecting $u$ and $v_d$ : $u, u_1, u_2, \dots, v_d$. Since $d(u, v_d) = d/2$, and $u, u_1, u_2, \dots, v_d$ is a shortest path, then $d(u_1, v_d) = (d/2) - 1$. We show that $d(u_1, v_0) \ge (d/2) + 1$. If not, then by the triangle inequality,

$$d = d(v_0, v_d) \le d(v_0, u_1) + d(u_1, v_d) \le (d/2) + ((d/2) - 1) = d - 1$$

which is impossible. Thus, $d(u_1, v_0) \ge (d/2) + 1$, and hence $\mathrm{ec}(u_1) \ge (d/2) + 1$. Setting $u' = u_1$, completes the proof of Claim 2. □

For every $u \in Q$, choose a vertex $u'$ as found in Claim 2, and denote it by $f(u)$.

Let $Q' := \{f(u) \mid u \in Q\}$, and set $|Q| = q$ and $|Q'| = q'$. Since the mapping $f(u) = u'$ is not necessarily injective, we have that $q' \le q$.

Observe that Claim 2 gives $\mathrm{ec}(f(u)) \ge (d/2) + 1$, and this implies that $Q'$ cannot contain any problem vertices. Therefore, $Q \cap Q' = \emptyset$.

**Fact 3.** $\deg(u') \ge 2$ for all $u' \in Q'$.

To prove this fact, it suffices, by Fact 2, to show that if $u' \in Q'$, then $u' \notin \{v_0, v_d\}$. Suppose, to the contrary, that $u' \in \{v_0, v_d\}$. Then $\mathrm{ec}(u') = d$. Also, since $u' \in Q'$, $u'$ is a neighbour of some problem vertex $u \in Q$. Thus $|\mathrm{ec}(u') - \mathrm{ec}(u)| \le 1$, i.e., $|\,d - d/2| \le 1$, which contradicts the fact that $d \ge 3$. Hence, Fact 3 is proven.

We now find a lower bound for $\sum_{w \in Q'} \mathrm{ec}(w)\ \deg(w)$.

By Fact 3, $\sum_{w \in Q'} \deg(w) \ge 2\,q'$. On the other hand, since every vertex in $Q$ is adjacent to some vertex in $Q'$, we have $\sum_{w \in Q'} \deg(w) \ge q$. Summing these two inequalities gives $2 \sum_{w \in Q'} \deg(w) \ge 2\,q' + q$. Therefore,

$$\sum_{w \in Q'} \deg(w) \ge q' + q/2. \tag{9}$$

For $w \in Q'$, by Claim 2, we have that $\mathrm{ec}(w) \geq (d/2) + 1$. This, in conjunction with (9), yields

$$\begin{aligned}\sum_{w\in Q'} \mathrm{ec}(w)\ \deg(w) &\geq \sum_{w\in Q'} ((d/2)+1)\ \deg(w)\\ &= ((d/2)+1) \sum_{w\in Q'} \deg(w)\\ &\geq ((d/2)+1)\,(q'+q/2).\end{aligned}$$

Hence, from the definition of $Q$, and the above inequality, we have

$$\begin{aligned}\sum_{v\in(Q\cup Q')} \mathrm{ec}(v)\ \deg(v) &= \sum_{v\in Q} \mathrm{ec}(v)\ \deg(v) + \sum_{w\in Q'} \mathrm{ec}(w)\ \deg(w)\\ &\geq 2\,q\,(d/2) + ((d/2)+1)\,(q'+q/2)\\ &= q\cdot((5d+2)/4) + q'\cdot((d/2)+1). \end{aligned} \tag{10}$$

Next, set $P' := \{v_0, \ldots, v_{(d/2)-2},\ v_{(d/2)+2}, \ldots, v_d\}$. (If $d = 4$, then $P' := \{v_0, v_4\}$.)
It can be seen that $Q,\ Q'$ and $P'$ are all pairwise disjoint. Note that $|P'| = d - 2$.
A bound for the eccentric connectivity index of $P'$ can be found by direct calculation. If $d \geq 6$ we have:

$$\begin{aligned}\sum_{v\in P'} \mathrm{ec}(v)\ \deg(v) &= \mathrm{ec}(v_0)\ \deg(v_0) + \mathrm{ec}(v_d)\ \deg(v_d) + \sum_{i=1}^{(d/2)-2} \mathrm{ec}(v_i)\ \deg(v_i) + \sum_{i=(d/2)+2}^{d-1} \mathrm{ec}(v_i)\ \deg(v_i)\\ &\geq d\cdot 1 + d\cdot 1 + 2\sum_{i=1}^{(d/2)-2} (d-i)\cdot 2\\ &= 2d + 4\cdot \sum_{i=1}^{(d/2)-2} (d-i)\\ &= 3\,d^2/2 - 3d - 4.\end{aligned} \tag{11}$$

(And if $d = 4$, (11) still holds.)
Define $S' = V - (P' \cup Q \cup Q')$.
Since $v_0,\ v_d \in P'$, then $v_0,\ v_d \notin S'$, and it follows from Fact 2 that $S'$ has no pendant vertices. This allows us to partition $S'$ as follows:
let $A = \{x \in S' \mid \deg(x) = 2\}$, $B = \{x \in S' \mid \deg(x) \geq 3\}$. Setting $|A| = a$, and $|B| = b$, we obtain

$$a + b + (d-2) + q + q' = n. \tag{12}$$

Combining (2) with the fact that there are no problem vertices in $S'$, we have that for all vertices $x$ in $A$, $\mathrm{ec}(x) \geq (d/2) + 1$. Applying this inequality, (2), (10) and (11), we calculate

$$\begin{aligned}\xi^C(G) &= \sum_{x\in A} \mathrm{ec}(x)\ \deg(x) + \sum_{u\in B} \mathrm{ec}(u)\ \deg(u)\\ &\quad + \sum_{v\in P'} \mathrm{ec}(v)\ \deg(v) + \sum_{v\in Q} \mathrm{ec}(v)\ \deg(v) + \sum_{w\in Q'} \mathrm{ec}(w)\ \deg(w)\\ &\geq 2a\,(d/2+1) + 3b\,(d/2) + (3\,d^2/2 - 3d - 4) + q\cdot((5d+2)/4) + q'\cdot((d/2)+1)\\ &= a\,(d+2) + b\,(3d/2) + (3\,d^2/2 - 3d - 4) + q\,((5d+2)/4) + q'\left(\frac{1}{2}d + 1\right).\end{aligned} \tag{13}$$

We will minimize (13) by optimizing the coefficients $a,\ b,\ q$ and $q'$ in two stages. First, recall that $q' \leq q$. Fixing $a$ and $b$, the sum of the last two terms in (13) is as small as possible when $q'$ is as large as possible, i.e., when $q' = q$. This gives

$$\xi^C(G) \geq a(d+2) + b(3d/2) + (3/2)\,d^2 - 3d - 4 + q\cdot((7d+6)/4), \tag{14}$$

and now (12) has been reduced to $a + b + 2q = n - d + 2$.
Second, if $d \geq 4$, (14) is minimized for $b = 0,\ q = 0$, and $a = n - d + 2$. Thus,

$$\begin{aligned}\xi^C(G) &\geq (n-d+2)(d+2) + (3/2)\,d^2 - 3d - 4\\ &= n(d+1) + n - d^2 - 2d + 2d + 4 + (3/2)\,d^2 - 3d - 4\\ &= n(d+1) + d^2/2 - 2d - 1 + n - d + 1\\ &= \xi^C(V_{n,d}) + n - d + 1.\end{aligned}$$

Since $n \geq d+1 > d-1$, we have $\xi^C(G) \geq \xi^C(V_{n,d}) + n - d + 1 > \xi^C(V_{n,d})$, which contradicts (3). It follows that for $d$ even, $\xi^C(G) \geq \xi^C(V_{n,d})$.

Continuing in Part A, we now turn to the case with $d$ odd.

*Case* 2. $d$ is odd.

Here $\lceil d/2 \rceil = (d+1)/2$. In this case, a class of problem vertices with both neighbours in the centre of the graph, will require special attention. So, it will now be necessary to partition the vertex set of the counterexample graph $G$ into even more sets than were needed in the $d$ even case.

Let $R = \{x \in V \mid \deg(x) = 2,\ \mathrm{ec}(x) = \lceil d/2 \rceil\}$. So $R$ is the set of problem vertices of $G$, and clearly, $|R| = t \geq 1$.

Partition $R$ as follows: $R = Q \cup H$, where

$$Q := \{x \in R \mid x \text{ is adjacent to a vertex outside } C(G)\} \quad \text{and}$$
$$H := \{x \in R \mid \text{both neighbours of } x \text{ are in } C(G)\}.$$

Since they partition $R$, we have that

$$Q \cap H = \emptyset. \tag{15}$$

**Claim 2′.** *Every vertex $u \in Q$ is adjacent to some vertex $u'$ satisfying*

$$\mathrm{ec}(u') \geq ((d+1)/2) + 1.$$

**Proof of Claim 2′.** Consider $u \in Q$. By the definition of $Q$, the problem vertex $u$ is adjacent to a vertex, $u'$, which is not a central vertex. So, $\mathrm{ec}(u') \geq (d+1)/2 + 1$, and Claim 2′ is proven. □

For every $u \in Q$, choose a vertex $u'$ as found in Claim 2′, and denote it by $f(u)$.

Let $Q' := \{f(u) \mid u \in Q\}$, and set $|Q| = q$ and $|Q'| = q'$. Since the mapping $f(u) = u'$ is not necessarily injective, we have that $q' \leq q$. Also, Claim 2′ gives $\mathrm{ec}(f(u)) \geq ((d+1)/2) + 1$, while all vertices in $Q$ have eccentricity $(d+1)/2$, so

$$Q \cap Q' = \emptyset. \tag{16}$$

**Claim 3.**

$$\sum_{w \in Q'} \mathrm{ec}(w)\ \deg(w) \geq q((d+3)/4) + q'((d+3)/2) - 3. \tag{17}$$

**Proof of Claim 3.** Since every vertex in $Q$ is adjacent to some vertex in $Q'$, we have

$$\sum_{w \in Q'} \deg(w) \geq |Q| = q. \tag{18}$$

Then, Claim 2′ and (18) give

$$\sum_{w \in Q'} \mathrm{ec}(w)\ \deg(w) \geq (((d+1)/2) + 1)\ q. \tag{19}$$

Observe that by Fact 2, $Q'$ can contain at most 2 pendant vertices, possibly $v_0$ or $v_d$. We look at three cases, separately.

(i) If $Q'$ contains no pendant vertices, then $\sum_{w \in Q'} \deg(w) \geq \sum_{w \in Q'} 2 = 2q'$. Summing this inequality with (18) gives $2\sum_{w \in Q'} \deg(w) \geq q + 2q'$, and therefore

$\sum_{w \in Q'} \deg(w) \geq q/2 + q'$. From this result, and Claim 2′, it follows that

$$\begin{aligned}
\sum_{w \in Q'} \mathrm{ec}(w)\ \deg(w) &\geq \sum_{w \in Q'} (((d+1)/2) + 1)\ \deg(w) \\
&\geq (((d+1)/2) + 1)\ (q/2 + q') \\
&= q((d+3)/4) + q'((d+3)/2) \\
&> q((d+3)/4) + q'((d+3)/2) - 3
\end{aligned}$$

and (17) holds for case (i).

(ii) If $Q'$ contains exactly one pendant vertex, say, without loss of generality, $v_0$, then, by Claim 2′,

$$\begin{aligned}
\sum_{w \in Q'} \mathrm{ec}(w)\ \deg(w) &= \mathrm{ec}(v_0)\ \deg(v_0) + \sum_{w \in Q' - \{v_0\}} \mathrm{ec}(w)\ \deg(w) \\
&\geq d \cdot 1 + 2 \cdot (q' - 1)(((d+1)/2) + 1).
\end{aligned}$$

Summing this with (19) gives

$$2\sum_{w\in Q'} \mathrm{ec}(w)\ \deg(w) \ge d + 2\cdot(q'-1)((d+1)/2+1) + q\,(((d+1)/2)+1)$$
$$= q'\,(d+3) + q\,((d+3)/2) - 3$$

and this simplifies to

$$\sum_{w\in Q'} \mathrm{ec}(w)\ \deg(w) \ge q\,((d+3)/4) + q'\,((d+3)/2) - 3/2$$
$$> q((d+3)/4) + q'((d+3)/2) - 3$$

and (17) holds for case (ii).

The final case is

(iii) if both $v_0$ and $v_d$ are in $Q'$, and they both have degree 1. Proceeding as in case (ii), we have that

$$\sum_{w\in Q'} \mathrm{ec}(w)\ \deg(w) \ge 2\,d + 2\cdot(q'-2)(((d+1)/2)+1).$$

Summing this with (19) gives

$$2\sum_{w\in Q'} \mathrm{ec}(w)\ \deg(w) \ge 2\,d + 2\cdot(q'-2)((d+1)/2+1) + q((d+3)/2)$$

and this simplifies to

$$\sum_{w\in Q'} \mathrm{ec}(w)\ \deg(w) \ge q\,((d+3)/4) + q'\,((d+3)/2) - 3,$$

which completes case (iii), and hence, Claim 3 is proven. □

Thus, from the fact that $Q \subseteq R$, and Claim 3,

$$\sum_{v\in(Q\cup Q')} \mathrm{ec}(v)\ \deg(v) = \sum_{v\in Q} \mathrm{ec}(v)\ \deg(v) + \sum_{v\in Q'} \mathrm{ec}(v)\ \deg(v)$$
$$\ge 2q((d+1)/2) + q((d+3)/4) + q'((d+3)/2) - 3$$
$$= q((5d+7)/4) + q'((d+3)/2) - 3. \tag{20}$$

Next we consider the extra vertex set $H$ and define its neighbourhood, $H' := N(H)$. Note that by the definition of $H$, $N(H) \subseteq C(G)$. Set $|H| = h$ and $|H'| = h'$. Since each vertex in $H$ has degree 2, and $H'$ is the neighbourhood of $H$, we have that $h' \le 2h$. Also note that by Claim 2′, $\mathrm{ec}(u') \ge ((d+1)/2) + 1$, for each $u' \in Q'$; whereas all the vertices in $H$, and in $H'$ are central vertices. This implies that

$$Q' \cap (H \cup H') = \emptyset. \tag{21}$$

In order to find a bound on the degrees of the vertices in $H'$, we need the following two claims.

**Claim 4.** *Let $x \in H$. Then its two neighbours each have degree at least* 3.

**Proof of Claim 4.** Let $w$ and $y$ be the two neighbours of $x$. So, by the definition of $H$, they are both central vertices, i.e., $\mathrm{ec}(w) = (d+1)/2 = \mathrm{ec}(y)$. This immediately implies

$$d(w, v_0),\ d(w, v_d) \le (d+1)/2. \tag{22}$$

Also, by (6) we have that $y$ lies at a distance $(d+1)/2$ from $v_0$ or $v_d$. Assume, without loss of generality, that

$$d(y, v_d) = (d+1)/2. \tag{23}$$

First, we show that $d(w, v_0) \ge (d-1)/2$. If not, then by (22) and the triangle inequality

$$d = d(v_0, v_d) \le d(v_0, w) + d(w, v_d) \le ((d-1)/2 - 1) + ((d+1)/2) = d - 1,$$

which is impossible. So,

$$d(w, v_0) \ge (d-1)/2. \tag{24}$$

Similarly,

$$d(w, v_d) \ge (d-1)/2. \tag{25}$$

Now, continuing the proof of Claim 4, assume by contradiction, that $\deg(y) \le 2$.

Since $y \in C(G)$, $y \neq v_0,\ v_d$, and hence, by Fact 2, $\deg(y) \neq 1$.

It follows that $\deg(y) = 2$. Then label as $z$, the second neighbour of $y$.

If $z = w$, then $w$ is a cut-vertex, since its removal would disconnect the edge $xy$ from the rest of the graph. Thus, every path from $\{v_0,\ v_d\}$ to $y$ must go through $w$. But then (5) implies that $\mathrm{ec}(y) \geq 1+\max\{d(w, v_0),\ d(w, v_d)\} \geq 1+(d+1)/2$, which contradicts the fact that $\mathrm{ec}(y) = (d+1)/2$. So, $z \neq w$.

Next, by (24) and (25), any shortest path from $\{v_0,\ v_d\}$ to $y$ which goes through $w$ and $x$, has length at least $(d-1)/2 + d(w,\ x)+d(x,\ y) = (d+1)/2+1$. Hence, since $\mathrm{ec}(y) = (d+1)/2$, we have that any shortest path from $\{v_0,\ v_d\}$ to $y$ cannot pass through $w$ and $x$. Note again that since $y \in C(G)$, $y \neq v_0,\ v_d$. Hence, any shortest path from $y$ to $\{v_0,\ v_d\}$ must pass through $z$. Thus, from (23), and since any shortest $y$–$v_d$ path must pass through $z$, we have that $d(z, v_d) = (d+1)/2 - 1$. However, this then gives that $d(z, v_0) \geq (d+1)/2$, since otherwise, by the triangle inequality

$$d = d(v_0, v_d) \leq d(v_0, z) + d(z, v_d) \leq ((d+1)/2 - 1) + (((d+1)/2) - 1) = d - 1$$

which is impossible. So, $d(z, v_0) \geq (d+1)/2$, which in turn implies that a shortest $y$–$v_0$ path which passes through $z$ must have length at least $((d+1)/2)+1$, contrary to the fact that $\mathrm{ec}(y) = (d+1)/2$. Therefore, a shortest $v_0$–$y$ path cannot pass through $z$, a contradiction. So, $\deg(y) \neq 2$.

Thus, $\deg(y) \not\leq 2$, i.e., $\deg(y) \geq 3$. By an equivalent argument, $\deg(w) \geq 3$, which completes the proof of Claim 4. □

From Claim 4 we have that all the vertices of $H'$ have degree at least 3; whereas all the vertices in $H$ and $Q$ have degree 2, since they are problem vertices. Thus,

$$H' \cap (Q \cup H) = \emptyset. \tag{26}$$

Summarizing, thus far, by (15), (16), (21) and (26) we have shown that $Q,\ Q',\ H$ and $H'$ are all pairwise disjoint.

**Claim 5.** $\sum_{x\in H'} \deg(x) \geq h + (3/2)h'$.

**Proof of Claim 5.** On the one hand, since by Claim 4, $\deg(x) \geq 3$, for all $x \in H'$, we have that $\sum_{x\in H'} \deg(x) \geq 3h'$. On the other hand, since every vertex in $H$ has two neighbours in $H'$, we have $\sum_{x\in H'} \deg(x) \geq 2h$. Summing these two inequalities, we get $2\sum_{x\in H'} \deg(x) \geq 2h + 3h'$, and upon division by 2, Claim 5 is proven. □

Claim 5, and the definitions of $H$ and $H'$, give a lower bound for the eccentric connectivity index over $H \cup H'$ as follows:

$$\begin{aligned}\sum_{x\in(H\cup H')} \mathrm{ec}(x)\ \deg(x) &= \sum_{x\in H} \mathrm{ec}(x)\ \deg(x) + \sum_{x\in H'} \mathrm{ec}(x)\ \deg(x)\\ &= h((d+1)/2)\cdot 2 + ((d+1)/2)\sum_{x\in H'} \deg(x)\\ &\geq h(d+1) + ((d+1)/2)(h+(3/2)h')\\ &= h(3(d+1)/2) + h'(3(d+1)/4).\end{aligned} \tag{27}$$

Next, set $P' := \{v_0, \ldots, v_{(d-5)/2},\ v_{(d+5)/2}, \ldots, v_d\}$. (If $d = 3$, then $P' := \emptyset$; whereas if $d = 5$, then $P' := \{v_0,\ v_5\}$.) It can be seen that $P' \cap (Q \cup Q' \cup H \cup H') = \emptyset$. Note that $|P'| = d - 3$.

A bound for the eccentric connectivity index of $P'$ can be found by direct calculation. If $d \geq 7$, we have:

$$\begin{aligned}\sum_{v\in P'} \mathrm{ec}(v)\ \deg(v) &= \mathrm{ec}(v_0)\ \deg(v_0) + \mathrm{ec}(v_d)\ \deg(v_d) + \sum_{i=1}^{(d-5)/2} \mathrm{ec}(v_i)\ \deg(v_i) + \sum_{i=(d+5)/2}^{d-1} \mathrm{ec}(v_i)\ \deg(v_i)\\ &\geq d\cdot 1 + d\cdot 1 + 2\sum_{i=1}^{(d-5)/2} (d-i)\cdot 2\\ &= 2d + 4\cdot \sum_{i=1}^{(d-5)/2} (d-i)\\ &= 3d^2/2 - 4d - 15/2.\end{aligned} \tag{28}$$

(And (28) also holds for $d = 5$.)

For $d = 3$, we have

$$\sum_{v\in P'} \mathrm{ec}(v)\ \deg(v) = 0. \tag{29}$$

Define $S' = V - (Q \cup Q' \cup H \cup H' \cup P')$.

For now, assume that $d \geq 5$. (We will consider the case for $d = 3$, below.) Since $v_0,\ v_d \in P'$, then $v_0,\ v_d \notin S'$. It follows from Fact 2, that $S'$ has no pendant vertices, and this allows us to partition $S'$ as follows:

let $A = \{x \in S' \mid \deg(x) = 2\}$, $B = \{x \in S' \mid \deg(x) \geq 3\}$. Setting $|A| = a$, and $|B| = b$, we obtain

$$a + b + q + q' + h + h' + (d - 3) = n. \tag{30}$$

Combining (2) with the fact that there are no problem vertices in $S'$, we have that for all vertices $x$ in $A$, $\mathrm{ec}(x) \geq ((d+1)/2)+1$.

Applying this inequality, and (2), an upper bound for the index over the vertices of $S'$ is

$$\begin{aligned}\sum_{x\in A} \mathrm{ec}(x)\ \deg(x) + \sum_{u\in B} \mathrm{ec}(u)\ \deg(u) &\geq 2a((d+1)/2+1) + 3b((d+1)/2)\\ &= a(d+3) + b(3(d+1)/2).\end{aligned}$$

Combining this inequality, (20), (27) and (28) we have

$$\begin{aligned}\xi^C(G) &= \sum_{x\in A} \mathrm{ec}(x)\ \deg(x) + \sum_{u\in B} \mathrm{ec}(u)\ \deg(u) + \sum_{v\in Q} \mathrm{ec}(v)\ \deg(v) + \sum_{w\in Q'} \mathrm{ec}(w)\ \deg(w) + \sum_{v\in H} \mathrm{ec}(v)\ \deg(v)\\ &\quad + \sum_{v\in H'} \mathrm{ec}(v)\ \deg(v) + \sum_{v\in P'} \mathrm{ec}(v)\ \deg(v)\\ &\geq a(d+3) + b(3(d+1)/2) + q((5d+7)/4) + q'((d+3)/2) - 3\\ &\quad + h(3(d+1)/2) + h'(3(d+1)/4) + 3d^2/2 - 4d - 15/2.\end{aligned} \tag{31}$$

We will minimize (31) by optimizing the coefficients $a$, $b$, $q$, $q'$, $h$, and $h'$ in three stages. First, recall that $q' \leq q$. Fixing $a$, $b$, $h$ and $h'$, (31) is as small as possible when $q'$ is as large as possible, i.e., when $q' = q$. This gives

$$\begin{aligned}\xi^C(G) &\geq a(d+3) + b(3(d+1)/2) + q\,((7d+13)/4) - 3\\ &\quad + h(3(d+1)/2) + h'(3(d+1)/4) + 3d^2/2 - 4d - 15/2\end{aligned} \tag{32}$$

and now (30) has been reduced to

$$a + b + 2q + h + h' = n - d + 3. \tag{33}$$

Second, recall that $h' \leq 2h$. Fixing $a$, $b$ and $q$, (32) is as small as possible when $h'$ is as large as possible, i.e., when $h' = 2h$. This gives

$$\begin{aligned}\xi^C(G) &\geq a(d+3) + b(3(d+1)/2) + q((7d+13)/4) - 3\\ &\quad + h\,(3(d+1)) + 3d^2/2 - 4d - 15/2\end{aligned} \tag{34}$$

and now (33) has been reduced to $a + b + 2q + 3h = n - d + 3$.

Third, if $d \geq 3$, (34) is minimized for $b = q = h = 0$ and $a = n - d + 3$, to give

$$\begin{aligned}\xi^C(G) &\geq (n-d+3)(d+3) - 3 + (3/2)\,d^2 - 4d - 15/2\\ &= n(d+2) + d^2/2 - 3d - 3/2 + n - d\\ &= \xi^C(V_{n,d}) + n - d.\end{aligned}$$

Since $n \geq d+1 \geq d$, we have $\xi^C(G) \geq \xi^C(V_{n,d}) + n - d \geq \xi^C(V_{n,d})$, which contradicts (3), and Case 2, for $d \geq 5$ odd, is complete.

Now, assume that $d = 3$. Here we partition $S'$ as $S' = F \cup A \cup B$, where $F = \{v_0, v_3\}$, and where $A$ and $B$ are defined as previously, i.e., $A = \{x \in S' \mid \deg(x) = 2\}$, $B = \{x \in S' \mid \deg(x) \geq 3\}$. Setting $|A| = a$, and $|B| = b$, we obtain

$$2 + a + b + q + q' + h + h' + 0 = n. \tag{35}$$

Notice that $\sum_{x\in F} \mathrm{ec}(x)\ \deg(x) \geq d + d$.

Using this, (29), and as in (31), we get

$$\begin{aligned}\xi^C(G) &\geq a(d+3) + b(3(d+1)/2) + q((5d+7)/4) + q'((d+3)/2) - 3\\ &\quad + h(3(d+1)/2) + h'(3(d+1)/4) + 0 + 2d.\end{aligned} \tag{36}$$

Minimizing as above, after the second stage, (35) reduces to

$$a + b + 2q + 3h = n - 2.$$

Then, for the third stage, we set $b = q = h = 0$ and $a = n - 2$. Thus, (36) becomes

$$\begin{aligned}\xi^C(G) &\geq (n-2)(d+3) - 3 + 2d\\ &= 6n - 9\\ &= \xi^C(V_{n,3}) + n - d,\end{aligned}$$

and as above, we get a contradiction to (3). Thus, Case 2, for $d = 3$, is complete.

This concludes the proof for Part A, and we have shown that for $t(G) \geq 1$, $\xi^C(G) \geq \xi^C(V_{n,d})$.

*Part B*

The remaining part of the proof of the theorem is for $t(G) = 0$ (no problem vertices). The proof will parallel the proof given in Part A, but with the even and odd cases considered simultaneously. Again we must show that $\xi^C(G) \geq \xi^C(V_{n,d})$.

Suppose, to the contrary, that there exists a counterexample $G$, for which $t(G) = 0$, and

$$\xi^C(G) < \xi^C(V_{n,d}). \tag{37}$$

Of all such counterexamples, choose $G$ to have the smallest possible order, $n$. Hence, any graph $G'$ with diameter $d'$, no problem vertices, and $n' < n$ vertices, will satisfy

$$\xi^C(G') \geq \xi^C(V_{n',d'}). \tag{38}$$

Let $P : v_0, v_1, \ldots, v_d$ be a diametral path in $G$, and define $S = V - V(P)$.

**Claim B1.** *There are no pendant vertices in $S$.*

**Proof of Claim B1.** Suppose to the contrary, that $S$ contains a pendant vertex $x$, and let $y$ be the neighbour of $x$. Set $G' = G - x$.

**Fact 4.** (i) The diameter of $G'$ is $d$, since $x$ is not on the diametral path $P$.
(ii) $n(G') = n - 1 < n(G)$.

We now show that

$$\xi^C(G') \geq \xi^C(V_{n-1,d}). \tag{39}$$

If on the one hand $t(G') = 0$, then along with Fact 4, we conclude that $G'$ is not a counterexample, (38) applies, and (39) follows. If on the other hand $t(G') \geq 1$, then $G'$ satisfies the conditions of Part A, and (39) follows immediately.

Continuing from this point onwards, the proof of Claim B1 is identical to that of Claim A1. We arrive at a contradiction, and thus Claim B1 is proven. $\square$

Claim B1 allows us to partition $S$ as follows:
let $A = \{x \in S \mid \deg(x) = 2\}$, $B = \{x \in S \mid \deg(x) \geq 3\}$. Setting $|A| = a$, and $|B| = b$, we obtain

$$a + b + d + 1 = n. \tag{40}$$

Analogous to (11), a simple calculation gives

$$\sum_{v \in V(P)} \mathrm{ec}(v)\ \deg(v) \geq \begin{cases} \dfrac{3}{2}d^2 & \text{for } d \text{ even} \\ \dfrac{3}{2}d^2 + 1/2 & \text{for } d \text{ odd.} \end{cases} \tag{41}$$

Combining (2) with $t(G) = 0$, we have that for all vertices $x$ in $A$, $\mathrm{ec}(x) \geq \lceil d/2 \rceil + 1$. This inequality, in conjunction with (2) and (41), gives us

$$\begin{aligned} \xi^C(G) &= \sum_{v \in V(P)} \mathrm{ec}(v)\ \deg(v) + \sum_{x \in A} \mathrm{ec}(x)\ \deg(x) + \sum_{u \in B} \mathrm{ec}(u)\ \deg(u) \\ &\geq \sum_{v \in V(P)} \mathrm{ec}(v)\ \deg(v) + 2\,a(\lceil d/2 \rceil + 1) + 3\,b(\lceil d/2 \rceil) \\ &\geq \begin{cases} \dfrac{3}{2}\,d^2 + a\,(d+2) + b\,(3d/2) & \text{for } d \text{ even} \\ \dfrac{3}{2}\,d^2 + 1/2 + a\,(d+3) + b\,(3\,(d+1)/2) & \text{for } d \text{ odd.} \end{cases} \end{aligned} \tag{42}$$

We will minimize (42) by optimizing the coefficients $a$ and $b$. If $d \geq 3$, the right hand side of the inequality is minimized when $a$ is as large as possible, so, by (40), set $a = n - d - 1$, and $b = 0$. Thus,

$$\begin{aligned} \xi^C(G) &\geq \begin{cases} (n-d-1)(d+2) + \dfrac{3}{2}\,d^2 & \text{for } d \text{ even} \\ (n-d-1)(d+3) + \dfrac{3}{2}\,d^2 + 1/2 & \text{for } d \text{ odd} \end{cases} \\ &= \begin{cases} n(d+1) + n + \dfrac{3}{2}\,d^2 - d^2 - 2d - d - 2 & \text{for } d \text{ even} \\ n(d+2) + \dfrac{3}{2}\,d^2 + n - d^2 - 3d - d - 3 + 1/2 & \text{for } d \text{ odd} \end{cases} \end{aligned}$$

$$= \begin{cases} n(d+1) + \dfrac{1}{2}d^2 - 2d - 1 + n - d - 1 & \text{for } d \text{ even} \\ n(d+2) + \dfrac{1}{2}d^2 - 3d - 3/2 + n - d - 1 & \text{for } d \text{ odd} \end{cases}$$
$$= \xi^C(V_{n,d}) + n - d - 1.$$

Finally, since $n \geq d+1$, we have $\xi^C(G) \geq \xi^C(V_{n,d}) + n - d - 1 \geq \xi^C(V_{n,d})$, which contradicts (37). This contradiction completes the proof of Part B, and hence completes the proof of the theorem. □

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