Maximum Eccentric Connectivity Index
for Graphs with Given Diameter

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Abstract
The eccentricity of a vertex $v$ in a graph $G$ is the maximum distance between $v$ and any other vertex of $G$. The diameter of a graph $G$ is the maximum eccentricity of a vertex in $G$. The eccentric connectivity index of a connected graph is the sum over all vertices of the product between eccentricity and degree. Given two integers $n$ and $D$ with $D \leq n - 1$, we characterize those graphs which have the largest eccentric connectivity index among all connected graphs of order $n$ and diameter $D$. As a corollary, we also characterize those graphs which have the largest eccentric connectivity index among all connected graphs of a given order $n$.

1 Introduction

Let $G = (V, E)$ be a simple connected undirected graph. The distance $d(u, v)$ between two vertices $u$ and $v$ in $G$ is the number of edges of a shortest path in $G$ connecting $u$ and $v$. The eccentricity $\epsilon(v)$ of a vertex $v$ is the maximum distance between $v$ and any other vertex, that is $\max\{d(v, w) \mid w \in V\}$. The diameter of $G$ is the maximum eccentricity among all vertices of $G$. The eccentric connectivity index $\xi^e(G)$ of $G$ is defined by

$$\xi^e(G) = \sum_{v \in V} \deg(v)\epsilon(v).$$

This index was introduced by Sharma et al. in [3]. Alternatively, $\xi^e$ can be computed by summing the eccentricities of the extremities of each edge:

$$\xi^e(G) = \sum_{vw \in E} \epsilon(v) + \epsilon(w).$$

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We define the weight of a vertex by $W(v) = \deg(v)\epsilon(v)$, and we thus have $\xi^c(G) = \sum_{v \in V} W(v)$. Morgan et al. [2] give the following asymptotic upper bound on $\xi^c(G)$ for a graph $G$ of order $n$ and with a given diameter $D$.

**Theorem 1** (Morgan, Mukwembi and Swart, 2011 [2]). Let $G$ be a connected graph of order $n$ and diameter $D$. Then, 
\[ \xi^c(G) \leq D(n - D)^2 + O(n^2). \]

In what follows, we write $G \simeq H$ if $G$ and $H$ are two isomorphic graphs, and we let $K_n$ and $P_n$ be the complete graph and the path of order $n$, respectively. We refer to Diestel [1] for basic notions of graph theory that are not defined here. A lollipop $L_{n,D}$ is a graph obtained from a path $P_D$ by joining an end vertex of this path to $K_{n-D}$. Morgan et al. [2] state that the above asymptotic bound is best possible by showing that $\xi^c(L_{n,D}) = D(n - D)^2 + O(n^2)$.

The aim of this paper is to give a precise upper bound on $\xi^c(G)$ in terms of $n$ and $D$, and to completely characterize those graphs that attain the bound. As a result, we will observe that there are graphs $G$ of order $n$ and diameter $D$ such that $\xi^c(G)$ is strictly larger than $\xi^c(L_{n,D})$.

Morgan et al. [2] also give an asymptotic upper bound on $\xi^c(G)$ for graphs $G$ of order $n$ (but without a fixed diameter), and show that this bound is sharp by observing that it is attained by $L_{n,\frac{n}{2}}$.

**Theorem 2** (Morgan, Mukwembi and Swart, 2011 [2]). Let $G$ be a connected graph of order $n$. Then, 
\[ \xi^c(G) \leq \frac{4}{27}n^3 + O(n^2). \]

We give a precise upper bound on $\xi^c(G)$ for graphs $G$ of order $n$, and characterize those graphs that reach the bound. As a corollary, we show that for every lollipop, there is another graph $G$ of same order, but with a strictly larger eccentric connectivity index.

## 2 Results for a fixed order and a fixed diameter

The only graph with diameter 1 is the clique, and clearly, $\xi^c(K_n) = n(n-1)$. Also, the only connected graph with 3 vertices and diameter 2 is $P_3$, and $\xi^c(P_3) = \xi^c(K_3) = 6$. The next theorem characterizes the graphs with maximum eccentric connectivity index among those with $n \geq 4$ vertices and diameter 2. Let $M_n$ be the graph obtained from $K_n$ by removing a maximum matching (i.e., $\lfloor \frac{n}{2} \rfloor$ disjoint edges) and, if $n$ is odd, an additional edge adjacent to the unique vertex that still has degree $n-1$. In other words, all vertices in $M_n$ have degree $n-2$, except possibly one that has degree $n-3$. For illustration, $M_6$ and $M_7$ are drawn in Figure [1].

**Theorem 3.** Let $G$ be a connected graph of order $n \geq 4$ and diameter 2. Then, 
\[ \xi^c(G) \leq 2n^2 - 4n - 2(n \text{ mod } 2) \]

with equality if and only if $G \simeq M_n$ or $n = 5$ and $G \simeq H_1$ (see Figure [7]).

**Proof.** Let $G$ be a graph of order $n$ and diameter 2, and let $x$ be the number of vertices of degree $n-1$ in $G$. Clearly, $W(v) = n-1$ for all vertices $v$ of degree $n-1$, while $W(v) \leq 2(n-2)$ for 2.
for all other vertices \( v \). Note that if \( n - x \) is odd, then at least one vertex in \( G \) has degree at most \( n - 3 \). Hence,

\[
\xi^c(G) \leq x(n - 1) + 2(n - x)(n - 2) - 2((n - x) \mod 2)
\]

\[
= 2n^2 - 4n + x(3 - n) - 2((n - x) \mod 2).
\]

For \( n = 4 \) or \( n \geq 6 \), this value is maximized with \( x = 0 \). For \( n = 5 \), both \( x = 1 \) (i.e., \( G \simeq H_1 \)) and \( x = 0 \) (i.e., \( G \simeq M_5 \)) give the maximum value \( 28 = 2n^2 - 4n + (3 - n) - 2((n - 1) \mod 2) = 2n^2 - 4n - 2(n \mod 2) \).

Before giving a similar result for graphs with diameter \( D \geq 3 \), we prove the following useful property.

**Lemma 4.** Let \( G \) be a connected graph of order \( n \geq 4 \) and diameter \( D \geq 3 \). Let \( P \) be a shortest path in \( G \) between two vertices at distance \( D \), and assume there is a vertex \( u \) on \( P \) such that \( \epsilon(u) \) is strictly larger than the longest distance \( L \) from \( u \) to an extremity of \( P \). Finally, let \( v \) be a vertex in \( G \) such that \( d(v, u) = \epsilon(u) \) and let \( v = v_1 - v_2 - \ldots - v_{\epsilon(u)+1} = u \) be a path of length \( \epsilon(u) \) linking \( v \) to \( u \) in \( G \). Then

- vertices \( w_1, \ldots, w_{\epsilon(u)-L} \) do not belong to \( P \);
- vertex \( w_{\epsilon(u)-L} \) has either no neighbor on \( P \), or its unique neighbor on \( P \) is an extremity at distance \( L \) from \( u \);
- if \( \epsilon(u) - L > 1 \) then vertices \( w_1, \ldots, w_{\epsilon(u)-L-1} \) have no neighbor on \( P \).

**Proof.** No vertex \( w_i \) with \( 1 \leq i \leq \epsilon(u) - L \) is on \( P \), since this would imply \( d(u, w_i) \leq L \), and hence \( d(u, v) = d(u, w_1) \leq L+i-1 \leq \epsilon(u)-1 \). Similarly, no vertex \( w_i \) with \( 1 \leq i \leq \epsilon(u) - L - 1 \) has a neighbor on \( P \), since this would imply \( d(u, w_i) \leq L + 1 \), and hence \( d(u, v) = d(u, w_1) \leq L + 1 + i - 1 \leq \epsilon(u) - 1 \). If vertex \( w_{\epsilon(u)-L} \) has at least one neighbor on \( P \), then this neighbor is necessarily an extremity of \( P \) at distance \( L \) from \( u \), else we would have \( d(u, w_{\epsilon(u)-L}) \leq L \), which would imply \( d(u, v) = d(u, w_1) \leq L + (\epsilon(u) - L - 1) = \epsilon(u) - 1 \). We conclude the proof by observing that if both extremities of \( P \) are at distance \( L \) from \( u \), then \( w_{\epsilon(u)-L} \) is adjacent to at most one of them since \( D \geq 3 \). \( \square \)
Let \( n, D \) and \( k \) be integers such that \( n \geq 4, 3 \leq D \leq n-1 \) and \( 0 \leq k \leq n-D-1 \), and let \( E_{n,D,k} \) be the graph (of order \( n \) and diameter \( D \)) constructed from a path \( u_0 - u_1 - \ldots - u_D \) by joining each vertex of a clique \( K_{n-D-1} \) to \( u_0 \) and \( u_1 \), and \( k \) vertices of the clique to \( u_2 \). (see Figure \([\star]\)). Observe that \( E_{n,D,0} \) is the lollipop \( L_{n,D} \) and that \( E_{n,D,n-D-1} \) can be viewed as a lollipop with a missing edge between \( u_0 \) and \( u_2 \). Also, if \( D = n - 1 \), then \( k = 0 \) and \( E_{n,n-1,0} \simeq P_n \).

**Lemma 5.** Let \( n, D \) and \( k \) be integers such that \( n \geq 4, 3 \leq D \leq n-1 \) and \( 0 \leq k \leq n-D-1 \), then

\[
\xi_c(E_{n,D,k}) = 2 \sum_{i=0}^{D-1} \max\{i, D-i\} + (n - D - 1)(2D - 1 + D(n - D)) + k(2D - n - 1 + \max\{2, D - 2\}).
\]

**Proof.** The sum of the weights of the vertices outside \( P \) is

\[
\sum_{v \in V \setminus V(P)} W(v) = k(n - D + 1)(D - 1) + (n - D - 1 - k)(n - D)D,
\]

\[
= k(2D - n - 1) + (n - D - 1)(n - D)D.
\]

We now consider the weights of the vertices in \( P \). The weight of \( u_0 \) is \( D(n - D) \), the weight of \( u_1 \) is \((D - 1)(n - D + 1)\), and the weight of \( u_2 \) is \((k + 2) \max\{2, D - 2\}\). The weight of \( u_i \) for \( i = 3, \ldots, D - 1 \) is \( 2 \max\{i, D - i\} \), and the weight of \( u_D \) is \( D \). Hence, the total weight of the vertices on \( P \) is

\[
(n - D)D + (n - D + 1)(D - 1) + (k + 2) \max\{2, D - 2\} + 2 \sum_{i=3}^{D-1} \max\{i, D-i\} + D
\]

\[
= \left( (n - D - 1)D + D \right) + \left( (n - D - 1)(D - 1) + 2(D - 1) \right)
\]

\[
+ \left( k \max\{2, D - 2\} + 2 \max\{2, D - 2\} \right) + 2 \sum_{i=3}^{D-1} \max\{i, D-i\} + D
\]

\[
= 2 \sum_{i=0}^{D-1} \max\{i, D-i\} + (n - D - 1)(2D - 1) + k \max\{2, D - 2\}
\]

By summing up all weight in \( G \), we obtain the desired result. \( \Box \)

In what follows, we denote \( f(n, D) = \max_{k=0}^{n-D-1} \xi_c(E_{n,D,k}) \). It follows from the above lemma that

\[
f(n, D) = \begin{cases} 
14 + \left( n - 4 \right) \left( 3n - 4 + \max\{0, 2D - n + 1\} \right) & \text{if } D = 3; \\
2 \sum_{i=0}^{D-1} \max\{i, D-i\} + \left( n - D - 1 \right) \left( 2D - 1 + D(n - D) + \max\{0, 3D - n - 3\} \right) & \text{if } D \geq 4.
\end{cases}
\]

Lemma \([\star]\) allows to know for which values of \( k \) we have \( \xi_c(E_{n,D,k}) = f(n, D) \).
Corollary 6. Let \( n \) and \( k \) be integers such that \( n \geq 4 \), and \( 0 \leq k \leq n - 4 \).

- If \( n < 7 \), then \( \xi^c(E_{n,3,k}) \leq f(n,3) = 2n^2 - 5n + 2 \), with equality if and only if \( k = n - 4 \).
- If \( n > 7 \), then \( \xi^c(E_{n,3,k}) \leq f(n,3) = 3n^2 - 16n + 30 \) with equality if and only if \( k = 0 \).
- If \( n = 7 \), then all \( \xi^c(E_{n,3,k}) \) are equal to 65 for \( k = 0, \ldots, n - 4 \).

Corollary 7. Let \( n, D \) and \( k \) be integers such that \( n \geq 5, 4 \leq D \leq n - 1 \) and \( 0 \leq k \leq n - D - 1 \).

- If \( n < 3(D - 1) \), then \( \xi^c(E_{n,D,k}) = f(n,D) \) if and only if \( k = n - D - 1 \).
- If \( n > 3(D - 1) \), then \( \xi^c(E_{n,D,k}) = f(n,D) \) if and only if \( k = 0 \).
- If \( n = 3(D - 1) \), then \( \xi^c(E_{n,D,k}) = f(n,D) \) if and only if \( k \in \{0, \ldots, n - D - 1\} \).

The graph \( H_2 \) of Figure 1 has 6 vertices, diameter 3, and is not isomorphic to \( E_{6,3,k} \), while \( \xi^c(H_2) = f(6,3) = 44 \). Similarly, the graph \( H_3 \) of Figure 1 has 7 vertices, diameter 3, and is not isomorphic to \( E_{7,3,k} \), while \( \xi^c(H_3) = f(7,3) = 65 \). In what follows, we prove that all graphs \( G \) of order \( n \) and diameter \( D \geq 3 \) have \( \xi^c(G) \leq f(n,D) \). Moreover, we show that if \( G \) is not isomorphic to a \( E_{n,D,k} \), then equality can only occur if \( G \cong H_2 \) or \( G \cong H_3 \). So, for every \( n \geq 4 \) and \( 3 \leq D \leq n - 1 \), let us consider the following graph class \( \mathcal{C}_n^D \):

\[
\mathcal{C}_n^D = \begin{cases} 
\{E_{n,3,n-4}\} & \text{if } n = 4,5 \text{ and } D = 3; \\
\{E_{n,3,2}, H_2\} & \text{if } n = 6 \text{ and } D = 3; \\
\{E_{n,3,0}, \ldots, E_{n,3,3}, H_3\} & \text{if } n = 7 \text{ and } D = 3; \\
\{E_{n,3,0}\} & \text{if } n > 7 \text{ and } D = 3; \\
\{E_{n,D,n-D-1}\} & \text{if } n < 3(D - 1) \text{ and } D \geq 4; \\
\{E_{n,D,0}, \ldots, E_{n,D,n-D-1}\} & \text{if } n = 3(D - 1) \text{ and } D \geq 4; \\
\{E_{n,D,0}\} & \text{if } n > 3(D - 1) \text{ and } D \geq 4.
\end{cases}
\]

Note that while Morgan et al. [2] state that the lollipops reach the asymptotic upper bound of the eccentric connectivity index, we will prove that they reach the more precise upper bound only if \( D = n - 1, D = 3 \) and \( n \geq 7 \), or \( D \geq 4 \) and \( n \geq 3(D - 1) \).

Theorem 8. Let \( G \) be a connected graph of order \( n \geq 4 \) and diameter \( 3 \leq D \leq n - 1 \). Then \( \xi^c(G) \leq f(n,D) \), with equality if and only if \( G \) belongs to \( \mathcal{C}_n^D \).

Proof. We have already observed that all graphs \( G \) in \( \mathcal{C}_n^D \) have \( \xi^c(G) = f(n,D) \). So let \( G \) be a graph of order \( n \), diameter \( D \) such that \( \xi^c(G) \geq f(n,D) \). It remains to prove that \( G \) belongs to \( \mathcal{C}_n^D \).

Let \( P = u_0 - u_1 - \cdots - u_D \) be a shortest path in \( G \) that connects two vertices \( u_0 \) and \( u_D \) at distance \( D \) from each other. In what follows, we use the following notations for all \( i = 0, \ldots, D \):

- \( \alpha_i \) is the number of vertices outside \( P \) and adjacent to \( u_i \);
- \( \delta_i = \max\{i, D - i\} \);
- \( r_i = \epsilon(u_i) - \delta_i \).

Also, let \( r^* = \max_{i=1}^{D-1} r_i \). Note that \( r^* \geq 2 \) and \( r_i \leq \left\lfloor \frac{D}{2} \right\rfloor \) for all \( i \), and \( r_0 = r_D = 0 \) since \( \epsilon(u_0) = \epsilon(u_D) = \delta_0 = \delta_D = D \). Since \( P \) is a shortest path linking \( u_0 \) to \( u_D \), no vertex outside \( P \) can have more than three neighbors in \( P \). We consider the following partition of the vertices outside \( P \) in 4 disjoint sets \( V_0, V_1, V_2^{D-1}, V_3^D \), and denote by \( n_0, n_1, n_2^{D-1}, n_3^D \) their respective size:
• $V_0$ is the set of vertices outside $P$ with no neighbor on $P$;
• $V_{1,2}$ is the set of vertices outside $P$ with one or two neighbors in $P$;
• $V_{3}^{D-1}$ is the set of vertices $v$ outside $P$ with three neighbors in $P$ and $\epsilon(v) \leq D - 1$;
• $V_{3}^{D}$ is the set of vertices $v$ outside $P$ with three neighbors in $P$ and $\epsilon(v) = D$.

Clearly, all vertices $v$ outside $P$ can have $\epsilon(v) = D$ except those in $V_{3}^{D-1}$. The maximum degree of a vertex in $V_0$ is $n - D - 2$, while it is $n - D$ for those in $V_{1,2}$ and $n + D + 1$ for those in $V_{3}^{D-1} \cup V_{3}^{D}$. For a vertex $v \in V_{1,2} \cup V_{3}^{D-1} \cup V_{3}^{D}$, let

$$\rho(v) = \max\{r_i \mid u_i \text{ is adjacent to } v\}$$

$$\rho^* = \max_{v \in V_{1,2} \cup V_{3}^{D-1} \cup V_{3}^{D}} \rho(v)$$

Hence, $r^* \geq \rho^*$. We first show that the total weight of the vertices in $V_0 \cup V_{1,2}$ is at most

$$D(n - D)(n - D - 1 - n_{3}^{D-1} - n_{3}^{D}) - 2Dr^* + D \min\{1, \rho^*\}.$$ 

• If $r^* = 0$, then the largest possible weight of the vertices in $V_0 \cup V_{1,2}$ occurs when all of them have two neighbors in $P$ (i.e., $n_0 = 0$ and no vertex in $V_{1,2}$ has one neighbor on $P$). In such a case, $n_0 + n_{1,2} = n - D - 1 - n_{3}^{D-1} - n_{3}^{D}$, and all these vertices have degree $n - D$. Hence, their total weight is at most $D(n - D)(n - D - 1 - n_{3}^{D-1} - n_{3}^{D})$.

• If $r^* > 0$ and $\rho^* > 0$, then let $i$ be such that $r_i = r^*$. It follows from Lemma 3 that there is a path $w_1 - \ldots - w_{\epsilon(u_i)+1}$ such that $w_1, \ldots, w_{r_i-1}$ have no neighbor on $P$ and $w_{r_i}$ has at most one neighbor on $P$. Hence, the largest possible weight of the vertices in $V_0 \cup V_{1,2}$ occurs when $r^* - 1$ vertices have 0 neighbor on $P$, one vertex has one neighbor on $P$, and $n - D - 1 - n_{3}^{D-1} - n_{3}^{D} - r^*$ vertices have 2 neighbors in $P$. Hence, the largest possible weight for the vertices in $V_0 \cup V_{1,2}$ is

$$D(n - D - 2)(r^* - 1) + D(n - D - 1) + D(n - D)(n - D - 1 - n_{3}^{D-1} - n_{3}^{D} - r^*)$$

$$= D(n - D)(n - D - 1 - n_{3}^{D-1} - n_{3}^{D}) - 2Dr^* + D.$$

• If $r^* > 0$ and $\rho^* = 0$, then consider the same path $w_1 - \ldots - w_{\epsilon(u_i)+1}$ as in the above case. If $w_{r_i}$ has no neighbor on $P$, then there are at least $r^*$ vertices with no neighbor on $P$ and the largest possible weight for the vertices in $V_0 \cup V_{1,2}$ is

$$D(n - D - 2)(r^*) + D(n - D)(n - D - 1 - n_{3}^{D-1} - n_{3}^{D} - r^*)$$

$$= D(n - D)(n - D - 1 - n_{3}^{D-1} - n_{3}^{D}) - 2Dr^*.$$ 

Also, if there are at least two vertices in $V_{1,2}$ with only one neighbor on $P$, then the largest possible weight for the vertices in $V_0 \cup V_{1,2}$ is

$$D(n - D - 2)(r^* - 1) + 2D(n - D - 1) + D(n - D)(n - D - 1 - n_{3}^{D-1} - n_{3}^{D} - r^* - 1)$$

$$= D(n - D)(n - D - 1 - n_{3}^{D-1} - n_{3}^{D}) - 2Dr^*.$$ 

So assume $w_{r_i}$ is the only vertex in $V_{1,2}$ with only one neighbor on $P$. We thus have $d(u_i, w_{r_i}) = \delta_i + 1$. We now show that this case is impossible. We know from Lemma 4 that $w_{r_i}$ is adjacent to $u_0$ or (exclusive) to $u_D$. Since $\rho(v) = 0$ for all vertices $v$ outside $P$, we know that $u_i$ has no neighbor outside $P$. Hence, $w_{\epsilon(u_i)}$ is $u_{i-1}$ or $u_{i+1}$,
say \( u_{i+1} \) (the other case is similar). Then \( w_{r^*} \) is not adjacent to \( u_0 \) else there is \( j \) with \( r^* + 1 \leq j < \epsilon(u_i) - 1 \) such that \( w_j \) is outside \( P \) and has \( w_{j+1} \) as neighbor on \( P \), and since \( w_j \) must have a second neighbor \( u_\ell \) on \( P \) with \( \ell \geq i + 2 \), we would have

\[
i + 2 \leq \ell = d(u_0, u_\ell) \leq d(w_{r^*}, w_j) + 2 \leq (d(w_{r^*}, u_i) - 2) + 2 = i + 1.
\]

Hence, \( w_{r^*} \) is adjacent to \( u_D \). Then there is also a path linking \( u_i \) to \( w_1 \) going through \( u_{i-1} \) else \( d(u_0, w_1) = d(u_0, u_1) + d(u_1, w_1) > i + \delta_i \geq D \). Let \( Q \) be such a path of minimum length. Clearly, \( Q \) has length at least equal to \( \epsilon(u_i) \). So let \( w_1^* \) be the subpath of \( Q \) of length \( \epsilon(u_i) \) and having \( u_i \) as extremity (i.e., \( w_{\epsilon(u_i)} = u_{i-1} \) and \( w_{\epsilon(u_i)+1} = u_i \)). Applying the same argument to \( w_{r^*}^* \), as was done for \( w_{r^*} \), we conclude that \( w_{r^*}^* \) has \( u_0 \) as unique neighbor on \( P \). We thus have two vertices in \( V_{1,2} \) with a unique neighbor on \( P \), a contradiction.

The total weight of the vertices in \( V_{3}^{D-1} \cup V_{3}^{D} \) is at most \((n - D + 1)((D - 1)n_{3}^{D-1} + D n_{3}^{D})\), which gives the following upper bound \( B \) on the total weight of the vertices outside \( P \):

\[
B = D(n - D)((n - D - 1)n_{3}^{D-1} - n_{3}^{D}) + (n - D + 1)((D - 1)n_{3}^{D-1} + D n_{3}^{D})
\]

\[
- 2D r^* + D \min \{1, r^*\}
\]

\[
= (n - D - 1)D(n - D) + n_{3}^{D-1}(2D - n - 1) + D n_{3}^{D} - 2D r^* + D \min \{1, r^*\}.
\]

This bound can only be reached if all vertices outside \( P \) are pairwise adjacent. But Lemma [1] shows that this cannot happen if \( r^* > 0 \). Indeed, consider a vertex \( v \) in \( V_{1,2} \cup V_{3}^{D} \cup V_{3}^{D-1} \) with \( r(v) > 0 \). There is a vertex \( u_i \) in \( P \) adjacent to \( v \) such that \( r(v) = r_i = \epsilon(u_i) - \delta_i > 0 \). We know from Lemma [4] that there is a shortest path \( w_1 - w_2 - \ldots - w_{\epsilon(u_i)+1} = u_i \) linking \( u_i \) to a vertex \( w_1 \) with \( d(w_1, w_1) = \epsilon(u_i) \) and such that \( w_1, \ldots, w_{\epsilon(v)} \) do not belong to \( P \). In what follows, we denote \( Q^v \) such a path. If \( v \) is adjacent to a \( w_j \) with \( 1 \leq j \leq \epsilon(v) \), then the path \( u_i - v - w_j - \ldots - w_1 \) links \( u_i \) to \( w_1 \) and has length at most \( \epsilon(v) + 1 < r_i + \delta_i = \epsilon(u_i) \), a contradiction. Hence \( v \) has at least \( r(v) \) non-neighbors outside \( P \). Also, as shown in Lemma [4], \( w_1, \ldots, w_{\epsilon(v)-1} \) belong to \( V_0 \), while \( w_{\epsilon(v)} \) belongs to \( V_0 \cup V_{1,2} \). In the upper bound \( B \), we have assumed that \( \epsilon(w_1) = \ldots = \epsilon(w_{\epsilon(v)}) = D \). Hence, if \( v \in V_{1,2} \cup V_{3}^{D} \), we can gain \( 2D \) units on \( B \) for every \( w_j, j = 1, \ldots, \epsilon(v) \) (for \( v \) and \( D \) for \( w_j \), while the gain is \( 2D - 1 \) (\( D - 1 \) for \( v \) and \( D \) for \( w_j \)) if \( v \in V_{3}^{D-1} \).

We can gain an additional \( 2D \) for every \( v \in V_{3}^{D} \). Indeed, consider such a vertex \( v \) and let \( w^* \) be a vertex at distance \( D \) from \( v \). Note that \( w^* \) is not on \( P \) and has at most one neighbor on \( P \) else \( d(v, w^*) \leq D - 1 \). Hence, if \( r(v) = 0 \), we can gain \( 2D \) (one \( D \) for \( v \) and one \( D \) for \( w \)) in the above upper bound. So assume \( r(v) > 0 \), and consider again the shortest path \( Q^v = w_1 - w_2 - \ldots - w_{\epsilon(u_i)+1} = u_i \), with \( r(v) = r_i \). Also, let \( W = \{w_1, \ldots, w_{\epsilon(v)}\} \). To gain an additional \( 2D \), it is sufficient to determine a vertex in \( (V_0 \cup V_{1,2}) \setminus W \) which is not adjacent to \( v \). So assume no such vertex exists, and let us prove that such a situation cannot occur. Note that \( w^* \notin V_{3}^{D} \cup V_{3}^{D-1} \) (since it has at most one neighbor on \( P \)), which implies \( w^* \in W \).

- If a vertex \( w_j \in W \) has a neighbor \( x \in V_0 \cup V_{1,2} \) outside \( W \), then \( v \) is adjacent to \( x \), and the path \( v - x - w_j - \ldots - w^* \) has length at most \( 1 + r(v) \leq 1 + \lfloor \frac{D}{2} \rfloor < D \), a contradiction.
• If a vertex $w_j \in W$ has a neighbor $x \in V_3^D \cup V_3^{D-1}$, then $d(u_i, w_1) \leq d(u_i, x) + d(x, w_1) \leq \delta_i - 1 + r_i < \epsilon(u_i)$, a contradiction.

Since $G$ is connected and $w_1, \ldots, w_{\rho(u) - 1}$ have no neighbors outside $Q^\rho$, we know that $w_{\rho(u)}$ is adjacent to the extremity of $P$ at distance $\delta_i$ from $u_i$ (and to no other vertex on $P$). Hence, the vertices on $P$ and those in $W$ induce a path of length $D + \rho(v) > D$ in $G$, a contradiction.

In summary, the following value is a more precise upper bound on the total weight of the vertices outside $P$:

$$B - \sum_{v \in V_1,2 \cup V_3^D} 2\rho(v) - \sum_{v \in V_3^{D-1}} (2D - 1)\rho(v) - 2Dn_3^D$$

$$\leq (n - D - 1)D(n - D) + n_3^{D-1}(2D - n - 1) - Dn_3^D - 2Dr^* + D \min\{1, \rho^*\}$$

$$- \sum_{v \in V_1,2 \cup V_3^D \cup V_3^{D-1}} (2D - 1)\rho(v).$$

Let us now consider the vertices on $P$. We have $W(u_0) = D(1 + o_D)$, $W(u_D) = D(1 + o_D)$, and $W(u_i) = \epsilon(u_i)(2 + o_i)$ for $i = 1, \ldots, D - 1$. Since $\epsilon(u_i) = \delta_i + r_i$, the total weight of the vertices on $P$ is

$$2D + D(o_0 + o_D) + \sum_{i=1}^{D-1} (\delta_i + r_i)(2 + o_i)$$

$$= 2 \sum_{i=0}^{D-1} \delta_i + 2 \sum_{i=1}^{D-1} r_i + \sum_{i=1}^{D-1} r_i o_i + \delta_i o_i.$$

Each edge that links a vertex $v$ outside $P$ to a vertex $u_i$ in $P$ contributes for $r_i \leq \rho(v)$ in the sum $\sum_{i=1}^{D-1} r_i o_i$. Hence,

$$\sum_{i=1}^{D-1} r_i o_i \leq \sum_{v \in V_1,2} 2\rho(v) + \sum_{v \in V_3^D \cup V_3^{D-1}} 3\rho(v) \leq \sum_{v \in V_1,2 \cup V_3^D \cup V_3^{D-1}} 3\rho(v).$$

Since $2\sum_{i=1}^{D-1} r_i \leq 2r^*(D - 1)$, we get the following valid upper bound on the total weight of the vertices on $P$:

$$2 \sum_{i=0}^{D-1} \delta_i + \sum_{i=0}^{D} \delta_i o_i + 2r^*(D - 1) + \sum_{v \in V_1,2 \cup V_3^D \cup V_3^{D-1}} 3\rho(v).$$

Summing up the bounds for the vertices outside $P$ with those on $P$, we get the following upper bound for the total weight of the vertices in $G$:

$$(n - D - 1)D(n - D) + n_3^{D-1}(2D - n - 1) - Dn_3^D + 2 \sum_{i=0}^{D-1} \delta_i + \sum_{i=0}^{D} \delta_i o_i$$

$$- \sum_{v \in V_1,2 \cup V_3^D \cup V_3^{D-1}} (2D - 4)\rho(v) - 2r^* + D \min\{1, \rho^*\}.$$
• If $r^* = 0$, then $A_2 = 0$, which implies $A_1 + A_2 = A_1$.
• If $\rho^* > 0$, then $A_2 \leq 4 - 2D - 2r^* + D = 4 - D - 2r^* < 0$, which implies $A_1 + A_2 < A_1$.
• If $r^* > 0$ and $\rho^* = 0$, then $A_2 = -2r^* < 0$, which implies $A_1 + A_2 < A_1$.

In summary, the best possible upper bound is $A_1$ and is attained only if $r^* = 0$, $n_0 = 0$, $\epsilon(v) = D$ for all vertices in $V_{1,2}$, and the vertices outside $P$ are pairwise adjacent. We now have to compare $A_1$ with $f(n, D)$.

Let us start with $D = 3$. In that case, we have $f(n, 3) = 14 + (n - 4)(3n - 4 + \max\{0, 7 - n\})$, while $A_1 = (n - 4)3(n - 3) + n_3^3(5 - n) - 3n_3^2 + 14 + \sum_{i=0}^3 \delta_i o_i$. Hence, the difference is:

$$f(n, 3) - A_1 = (n - 4)(5 + \max\{0, 7 - n\}) - n_3^2(5 - n) + 3n_3^3 - \sum_{i=0}^3 \delta_i o_i.$$

We have

$$\sum_{i=0}^3 o_i \leq 3(n_3^3 + n_3^3) + 2(n - 4 - n_3^2 - n_3^2) = 2(n - 4) + n_3^2 + n_3^3.$$

Since $o_0 + o_3 \leq n - 4$ to avoid a path of length 2 joining $u_0$ to $u_3$, we have

$$\sum_{i=0}^3 \delta_i o_i \leq 3(n - 4) + 2(n - 4 + n_3^2 + n_3^3).$$

Hence,

$$f(n, 3) - A_1 \geq (n - 4) \max\{0, 7 - n\} - n_3^2(7 - n) + n_3^3.$$

This difference is minimized if and only if $n_3^3 = 0$, while $n_3 = 0$ if $n > 7$, $n_3 = 0, 1, 2$ or 3 if $n = 7$, and $n_3 = n - 4$ if $n < 7$. In all such cases, we get $f(n, 3) - A_1 = 0$.

• If $n = 4$, there is no vertex outside $P$, and $G \simeq E_{4,3,0}$ which is the unique graph in $C_4^3$.

• If $n = 5$, $n_3^3 = 1$, which means that the unique vertex outside $P$ is adjacent to 3 consecutive vertices on $P$. Hence, $G \simeq E_{5,3,1}$ which is the unique graph in $C_5^3$.

• If $n = 6$, $n_3^2 = 2$, which means that both vertices outside $P$ are adjacent to 3 consecutive vertices on $P$. If one of them is adjacent to $u_0, u_1, u_2$, while the other is adjacent to $u_1, u_2, u_3$, we have $G \simeq H_2$. Otherwise, we have $G \simeq E_{6,3,2}$.

• If $n = 7$, $n_3^2 \in \{0, 1, 2, 3\}$ and $n_1, 2 = 3 - n_3^2$. If $n_1, 2 > 0$ then the vertices in $V_{1,2}$ are all adjacent to $u_0$ and $u_1$ or all to $u_2$ and $u_3$, since they are pairwise adjacent, and they all have eccentricity 3. So assume without loss of generality, they are all adjacent to $u_0$ and $u_1$. Then the vertices in $V_3^2$ are all adjacent to $u_0, u_1, u_2$, else the vertices in $V_{1,2}$ would have eccentricity 2. But $G$ is then equal to $E_{7,3,0}, E_{7,3,1}$ or $E_{7,3,2}$. If $n_1 = 0$, then the three vertices outside $P$ are all adjacent to three consecutive vertices on $P$. If they are all adjacent to $u_0, u_1, u_2$, or all to $u_1, u_2, u_3$, then $G \simeq E_{7,3,3}$, else $G \simeq H_3$.

• If $n > 7$, all vertices outside $P$ are adjacent to $u_0, u_1$, or to $u_2, u_3$ (so that they all have eccentricity 3). Hence, $G \simeq E_{n,3,0}$.

Assume now $D \geq 4$. We have

$$f(n, D) = 2 \sum_{i=0}^{D-1} \delta_i + (n - D - 1) \left(2D - 1 + D(n - D) + \max\{0, 3D - n - 3\}\right)$$
and
\[ A_1 = 2 \sum_{i=0}^{D-1} \delta_i + (n - D - 1)D(n - D) + n_3^{D-1}(2D - n - 1) - Dn_3^D + \sum_{i=0}^{D} \delta_i o_i. \]

Hence, the difference is:

\[ f(n, D) - A_1 = (n - D - 1)(2D - 1 + \max \{0, 3D - n - 3\}) - n_3^{D-1}(2D - n - 1) + Dn_3^D - \sum_{i=0}^{D} \delta_i o_i. \]

We have
\[ \sum_{i=0}^{D} o_i \leq 3(n_3^{D-1} + n_3^D) + 2(n - D - 1 - n_3^{D-1} - n_3^D) = 2(n - D - 1) + n_3^{D-1} + n_3^D. \]

Let \( p \) be the number of vertices linked to both \( u_1 \) and \( u_{D-1} \).

- If \( D \geq 5 \), then \( p = 0 \), else \( d(u_0, u_D) \leq 4 < D \).
- If \( D = 4 \), then no vertex outside \( P \) linked to \( u_1 \) and \( u_{D-1} \) can also be linked to \( u_0 \) or to \( u_D \) since \( d(u_0, u_D) \) would be strictly smaller than 4. Since no vertex outside \( P \) can be linked to both \( u_0 \) and \( u_D \) (else \( d(u_0, u_D) < 3 \)) we have \( o_0 + o_D \leq n - D - 1 - p \) and \( o_1 + o_{D-1} \leq n - D - 1 + p \). Hence, \( o_2 \leq n_3^{D-1} + n_3^D \).

So,
\[ \sum_{i=0}^{D} \delta_i o_i \leq D(n - D - 1 - p) + (D - 1)(n - D - 1 + p) + (D - 2)(n_3^{D-1} + n_3^D) \]
\[ = (n - D - 1)(2D - 1) + (D - 2)(n_3^{D-1} + n_3^D) - p. \]

This value is maximized for \( p = 0 \).

Hence, in all cases, we have
\[ \sum_{i=0}^{D} \delta_i o_i \leq (n - D - 1)(2D - 1) + (D - 2)(n_3^{D-1} + n_3^D). \]

Hence,
\[ f(n, D) - A_1 \geq (n - D - 1) \max \{0, 3D - n - 3\} - n_3^{D-1}(3D - n - 3) + 2n_3^D. \]

This difference is minimized if and only if \( n_3^D = 0 \), while \( n_3^{D-1} = 0 \) if \( n > 3(D - 1) \), \( n_3^{D-1} \in \{0, \ldots, n - D - 1\} \) if \( n = 3(D - 1) \), and \( n_3^{D-1} = n - D - 1 \) if \( n < 3(D - 1) \). In all such cases, we get \( f(n, D) - A_1 = 0 \).

- If \( n < 3(D - 1) \), then all vertices outside \( P \) are adjacent to 3 consecutive vertices on \( P \). They are all adjacent to \( u_0, u_1, u_2 \), or all adjacent to \( u_{D-2}, u_{D-1}, u_D \), else \( d(u_0, u_D) \leq 3 < D \). Hence, we have \( G \simeq E_{n,D,n-1} \).
- If \( n = 3(D - 1) \), \( n_3^{D-1} \in \{0, \ldots, n - D - 1\} \) and \( n_{1,2} = 2D - 2 - n_3^{D-1} \). If \( n_{1,2} > 0 \) then the vertices in \( V_{1,2} \) are all adjacent to \( u_0 \) and \( u_1 \) or all to \( u_{D-1} \) and \( u_D \), since they are pairwise adjacent, and they all have eccentricity \( D \). So assume without loss of generality, they are all adjacent to \( u_0 \) and \( u_1 \). Then the vertices in \( V_{3}^{D-1} \) are all adjacent to \( u_0, u_1, u_2 \), else \( d(u_0, u_D) \leq 3 < D \). But \( G \) is then equal to \( E_{n,D,n_3^D} \). If \( n_{1,2} = 0 \), then all vertices outside \( P \) are adjacent to \( u_0, u_1, u_2 \), or all of them are adjacent to \( u_{D-2}, u_{D-1}, u_D \), else \( d(u_0, u_D) \leq 3 < D \). Hence, \( G \simeq E_{n,D,n-1} \).
• If \( n > 3(D - 1) \), all vertices outside \( P \) are adjacent to \( u_0, u_1 \), or to \( u_2, u_3 \) (so that they all have eccentricity \( D \)). Hence, \( G \simeq E_{n,D,0} \).

\[
\square
\]

3 Results for a fixed order and no fixed diameter

We now determine the connected graphs that maximize the eccentric connectivity index when the order \( n \) of the graph is given, while there is no fixed diameter. Clearly, \( K_3 \) and \( P_3 \) are the only connected graphs of order \( n = 3 \) and \( \xi^c(K_3) = \xi^c(P_3) = 6 \). For \( n > 3 \), \( \xi^c(M_n) = 2n^2 - 4n - 2(n \mod 2) > n^2 - n = \xi^c(K_n) \), which means that the optimal diameter is not \( D = 1 \).

- If \( n = 4 \), \( f(4, 3) = 14 < \xi^c(M_4) = 16 \), which means that \( M_4 \) has maximum eccentric connectivity among all connected graphs with 4 vertices.
- If \( n = 5 \), \( f(5, 3) = 27, f(5, 4) = 24 \) and \( \xi^c(M_5) = 30 \), which means that \( M_5 \) and \( H_1 \) have maximum eccentric connectivity index among all connected graphs with 5 vertices.
- If \( n = 6 \), \( f(6, 3) = 44, f(6, 4) = 42, f(6, 5) = 38 \) and \( \xi^c(M_6) = 48 \), which means that \( M_6 \) has maximum eccentric connectivity index among all connected graphs with 6 vertices.

Assume now \( n \geq 7 \). We first show that lollipops are not optimal. Indeed, consider a lollipop \( E_{n,D,0} \) of order \( n \) and diameter \( D \).

- If \( D = n - 1 \), then \( G \simeq P_n \) which implies

\[
\xi^c(E_{n,n-1,0}) = \sum_{i=1}^{D-1} 2 \max\{i, D - i\} + 2D = \frac{3D^2 + D \mod 2}{2} \\
\leq \frac{3D^2 + 1}{2} = \frac{3n^2}{2} - 3n + 2 < 2n^2 - 4n - 2 \leq \xi^c(M_n).
\]

- If \( D < n-1 \) then either \( n < 3(D-1) \), and we know from Corollary \([7]\) that \( \xi^c(E_{n,D,n-D-1}) > \xi^c(E_{n,D,0}) \), or \( n \geq 3(D - 1) \), in which case we show that \( \xi^c(E_{n,D+1,n-D-2}) > \xi^c(E_{n,D,0}) \). Since \( 2 \sum_{i=0}^{D-1} \max\{i, D - i\} = \frac{3D^2 + D \mod 2}{2} \), we know from Lemma \([5]\) that

\[
\xi^c(E_{n,D+1,n-D-2}) = 2 \sum_{i=0}^{D} \max\{i, D + 1 - i\} \\
+ \left( n - D - 2 \right) \left( 2(D + 1) - 1 + (D + 1)(n - D - 1) \right) \\
+ \left( n - D - 2 \right) \left( 2(D + 1) - n - 1 + (D + 1) - 2 \right) \\
= \frac{3(D + 1)^2 + (D + 1) \mod 2}{2} + \left( n - D - 2 \right) \left( 3D + D(n - D) \right)
\]

and

\[
\xi^c(E_{n,D,0}) = 2 \sum_{i=0}^{D-1} \max\{i, D - i\} + \left( n - D - 1 \right) \left( 2D - 1 + D(n - D) \right) \\
= \frac{3D^2 + D \mod 2}{2} + \left( n - D - 1 \right) \left( 2D - 1 + D(n - D) \right).
\]
Simple calculations lead to

$$\xi^c(E_{n,D+1,n-D-2}) - \xi^c(E_{n,D,0}) = n - 2D + (D - 1) \mod 2 \geq n - 2 \left(\frac{n}{3} + 1\right) = \frac{n}{3} - 2 > 0.$$ 

Hence, the remaining candidates to maximize the eccentric connectivity index when \(n \geq 7\) are \(M_n\) and \(E_{n,D,n-D-1}\). Let

$$g(n) = \max_{D=\left\lceil \frac{n+1}{3} \right\rceil} \xi^c(E_{n,D,n-D-1}).$$

We can rewrite \(\xi^c(E_{n,D,n-D-1})\) as follows:

$$\xi^c(E_{n,D,n-D-1}) = D^3 - D^2(n + \frac{5}{2}) + D(n^2 + 5n - 1) - n^2 - 3n + 4 + D \mod 2.$$ 

It is then not difficult to show that \(g(n) = \xi^c(E_{n,D^*,n-D^*-1})\) with \(D^* = \left\lceil \frac{n+1}{3} \right\rceil + 1\), and simple calculations lead to

$$g(n) = \frac{1}{54}(8n^3 + 21n^2 - 36n + \begin{cases} 
0 & \text{if } n \mod 6 = 0 \\
6n + 1 & \text{if } n \mod 6 = 1 \\
32 & \text{if } n \mod 6 = 2 \\
27 & \text{if } n \mod 6 = 3 \\
6n + 28 & \text{if } n \mod 6 = 4 \\
59 & \text{if } n \mod 6 = 5 
\end{cases}).$$

We then have \(g(7) = 66 < 68 = \xi^c(M_7)\), which means that \(M_7\) has the largest eccentric connectivity among all graphs with 7 vertices. Also, \(g(8) = 96 = \xi^c(M_8)\), which means that both \(E_{8,4,3}\) and \(M_8\) have the largest eccentric connectivity index among all graphs with 8 vertices. For graphs of order \(n \geq 9\), we have \(\frac{8n^3+21n^2-36n}{54} > 2n^2 - 4n\), which means that \(E_{n,D^*,n-D^*-1}\) is the unique graph with largest eccentric connectivity index among all graphs with \(n\) vertices. These results are summarized in Table 1, where \(\xi^c_{n*}\) stands for the largest eccentric connectivity index among all graphs with \(n\) vertices.

| \(n\) | \(\xi^c_{n*}\) | optimal graphs |
|------|-------------|---------------|
| 3    | 6           | \(K_3\) and \(P_3\) |
| 4    | 16          | \(M_4\)       |
| 5    | 30          | \(M_5\) and \(H_1\) |
| 6    | 48          | \(M_6\)       |
| 7    | 68          | \(M_7\)       |
| 8    | 96          | \(M_8\) and \(E_{8,4,3}\) |
| \(\geq 9\) | \(g(n) = E_{n,\lceil \frac{n+1}{3} \rceil +1,n-\lceil \frac{n+1}{3} \rceil -2}\) |

Note finally that Tavakoli et al. [4] state that \(g(n) = \xi^c(E_{n,D,n-D-1})\) with \(D = \left\lceil \frac{n}{3} \right\rceil + 1\) while we have shown that the best diameter for a given \(n\) is \(D = \left\lceil \frac{n+1}{3} \right\rceil + 1\). Hence for all \(n \geq 9\) with \(n \mod 3 = 0\), we get a better result. For example, for \(n = 9\), they consider \(E_{9,4,4}\) which has an eccentric connectivity index equal to 132 while \(g(9)=134\).
4 Conclusion

We have characterized the graphs with largest eccentric connectivity index among those of fixed order $n$ and fixed or non-fixed diameter $D$. It would also be interesting to get such a characterization for graphs with a given order $n$ and a given size $m$. We propose the following conjecture which is more precise than the one proposed in [5]

**Conjecture.** Let $n$ and $m$ be two integers such that $n \geq 4$ and $m \leq \left(\frac{n-1}{2}\right)$. Also, let

$$D = \left\lfloor \frac{2n + 1 - \sqrt{17 + 8(m - n)}}{2} \right\rfloor$$

and

$$k = m - \left(\frac{n - D + 1}{2}\right) - D + 1$$

Then, the largest eccentric connectivity index among all graphs of order $n$ and size $m$ is attained with $E_{n,D,k}$. Moreover,

- if $D > 3$ then $\xi^c(G) < \xi^c(E_{n,D,k})$ for all other graphs $G$ of order $n$ and size $m$.
- if $D = 3$ and $k = n - 4$, then the only other graphs $G$ with $\xi^c(G) = \xi^c(E_{n,D,k})$ are those obtained by considering a path $u_0 - u_1 - u_2 - u_3$, and by joining $1 \leq i \leq n - 3$ vertices of a clique $K_{n-4}$ to $u_0, u_1, u_2$ and the $n - 4 - i$ other vertices of $K_{n-4}$ to $u_1, u_2, u_3$.

References

[1] Diestel, R. *Graph Theory*, second edition ed. Springer-Verlag, 2000.

[2] Morgan, M.J., Mukwembi, S., and Swart, H.C. On the eccentric connectivity index of a graph. *Discrete Mathematics* 311 (2011), 1229 – 1234.

[3] Sharma, V., Goswani, R., and Madan, A.K. Eccentric Connectivity Index: A Novel Highly Discriminating Topological Descriptor for Structure Property and Structure Activity Studies. *J. Chem. Inf. Comput. Sci.* 37 (1997), 273 – 282.

[4] Tavakoli, M., Rahbarinia, F., Mirzavaziri, M., and Ashrafi, R. Complete solution to a conjecture of Zhang-Liu-Zhou. *Transactions on Combinatorics* 3 (2014), 55 – 58.

[5] Zhang, J., Liu, Z., and Zhou, B. On the maximal eccentric connectivity indices of graphs. *Appl. Math. J. Chinese Univ.* 29 (2014), 374 – 378.