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Maximum eccentric connectivity index for graphs with given diameter

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A B S T R A C T

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.

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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* $\xi^c(G)$ of G is defined by

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

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

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

We define the weight of a vertex by $\mathcal{W}(v) = deg(v)\epsilon(v)$, and we thus have $\xi^c(G) = \sum_{v \in V} \mathcal{W}(v)$. Morgan et al. [2] gave 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,*

$$\xi^c(G) \leq D(n-D)^2 + \mathcal{O}(n^2).$$

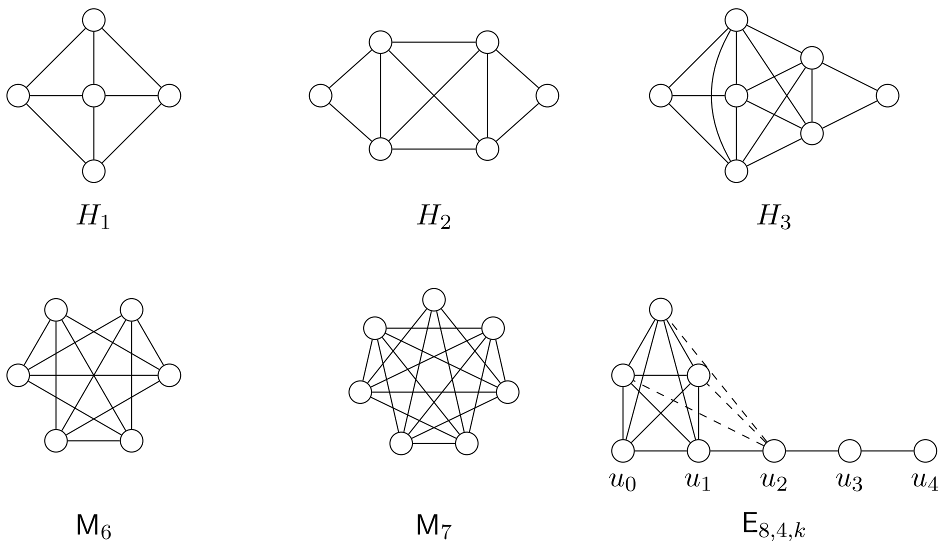

Fig. 1. Graphs H_1, H_2, H_3, M_6, M_7 and $\mathsf{E}_{8,4,k}$ (dashed edges depend on k).

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] stated that the above asymptotic bound is best possible by showing that $\xi^c(L_{n,D}) = D(n-D)^2 + \mathcal{O}(n^2)$. 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 gave an asymptotic upper bound on $\xi^c(G)$ for graphs G of order n (but without a fixed diameter), and showed that this bound is sharp by observing that it is attained by $L_{n,\frac{n}{3}}$.

Theorem 2 (*Morgan, Mukwembi and Swart, 2011 [2]*)**.** *Let G be a connected graph of order n. Then,*

$$\xi^c(G) \leq \frac{4}{27}n^3 + \mathcal{O}(n^2).$$

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, $\xi^c(\mathsf{K}_n) = n(n-1)$. Also, the only connected graph with 3 vertices and diameter 2 is P_3, and $\xi^c(\mathsf{P}_3) = \xi^c(\mathsf{K}_3) = 6$. 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 Fig. 1.

Theorem 3. *Let G be a connected graph of order $n \geq 4$ and diameter 2. Then,*

$$\xi^c(G) \leq 2n^2 - 4n - 2(n \bmod 2)$$

with equality if and only if $G \simeq \mathsf{M}_n$ or $n = 5$ and $G \simeq H_1$ (see Fig. 1).

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, $\mathcal{W}(v) = n-1$ for all vertices v of degree $n-1$, while $\mathcal{W}(v) \leq 2(n-2)$ 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,

$$\begin{aligned}\xi^c(G) &\leq x(n-1) + 2(n-x)(n-2) - 2((n-x) \bmod 2)\\ &= 2n^2 - 4n + x(3-n) - 2((n-x) \bmod 2).\end{aligned}$$

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.*, $G \simeq \mathsf{M}_5$) give the maximum value $28 = 2n^2 - 4n + (3 - n) - 2((n-1) \bmod 2) = 2n^2 - 4n - 2(n \bmod 2)$. $\square$

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 $v = w_1 - w_2 - \cdots - w_{\epsilon(u)+1} = u$ 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 $\mathsf{E}_{n,D,k}$ be the graph (of order n and diameter D) constructed from a path $u_0 - u_1 - \cdots - u_D$ 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 Fig. 1). Observe that $\mathsf{E}_{n,D,0}$ is the lollipop $L_{n,D}$ and that $\mathsf{E}_{n,D,n-D-1}$ 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 $\mathsf{E}_{n,n-1,0} \simeq \mathsf{P}_n$.

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*

$$\xi^c(\mathsf{E}_{n,D,k}) = 2\sum_{i=0}^{D-1} \max\{i, D-i\} + \Big(n - D - 1\Big)\Big(2D - 1 + D(n-D)\Big)$$
$$+ \, k\Big(2D - n - 1 + \max\{2, D-2\}\Big).$$

Proof. The sum of the weights of the vertices outside P is

$$\sum_{v \in V \setminus V(P)} \mathcal{W}(v) = k\,(n - D + 1)\,(D - 1) + (n - D - 1 - k)\,(n - D)\,D$$
$$= k\,(2D - n - 1) + (n - D - 1)(n - D)D.$$

We now consider the weights of the vertices on 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

$$\begin{aligned}
&(n-D)D + (n-D+1)(D-1) + (k+2)\max\{2, D-2\} + 2\sum_{i=3}^{D-1} \max\{i, D-i\} + D \\
&= \Big((n-D-1)D + D\Big) + \Big((n-D-1)(D-1) + 2(D-1)\Big) \\
&\quad + \Big(k\max\{2, D-2\} + 2\max\{2, D-2\}\Big) + 2\sum_{i=3}^{D-1} \max\{i, D-i\} + D \\
&= 2\sum_{i=0}^{D-1} \max\{i, D-i\} + (n-D-1)(2D-1) + k\max\{2, D-2\}.
\end{aligned}$$

By summing up all weights in G, we obtain the desired result. $\square$

In what follows, we denote $f(n, D) = \max\{\xi^c(\mathsf{E}_{n,D,k}) \mid 0 \leq k \leq n - D - 1\}$. It follows from the above lemma that

$$f(n, D) = \begin{cases} 14 + \Big(n-4\Big)\Big(3n - 4 + \max\{0, 2D - n + 1\}\Big) & \text{if } D = 3; \\ 2\displaystyle\sum_{i=0}^{D-1} \max\{i, D-i\} & \\ \quad + \Big(n - D - 1\Big)\Big(2D - 1 + D(n-D) + \max\{0, 3D - n - 3\}\Big) & \text{if } D \geq 4. \end{cases}$$

Lemma 5 allows to know for which values of k we have $\xi^c(\mathsf{E}_{n,D,k}) = f(n, D)$.

Corollary 6. *Let n and k be integers such that $n \geq 4$ and $0 \leq k \leq n-4$.*

- *If $n < 7$, then $\xi^c(\mathsf{E}_{n,3,k}) \leq f(n,3) = 2n^2 - 5n + 2$ with equality if and only if $k = n-4$.*
- *If $n > 7$, then $\xi^c(\mathsf{E}_{n,3,k}) \leq f(n,3) = 3n^2 - 16n + 30$ with equality if and only if $k = 0$.*
- *If $n = 7$, then all $\xi^c(\mathsf{E}_{n,3,k})$ 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 $\xi^c(\mathsf{E}_{n,D,k}) = f(n,D)$ if and only if $k = n-D-1$.*
- *If $n > 3(D-1)$, then $\xi^c(\mathsf{E}_{n,D,k}) = f(n,D)$ if and only if $k = 0$.*
- *If $n = 3(D-1)$, then $\xi^c(\mathsf{E}_{n,D,k}) = f(n,D)$ if and only if $k \in \{0, \ldots, n-D-1\}$.*

The graph H_2 of Fig. 1 has 6 vertices, diameter 3, and is not isomorphic to $\mathsf{E}_{6,3,k}$, while $\xi^c(H_2) = f(6,3) = 44$. Similarly, the graph H_3 of Fig. 1 has 7 vertices, diameter 3, and is not isomorphic to $\mathsf{E}_{7,3,k}$, 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 $\mathsf{E}_{n,D,k}$, then equality can only occur if $G \simeq H_2$ or $G \simeq H_3$. So, for every $n \geq 4$ and $3 \leq D \leq n-1$, let us consider the following graph class $\mathcal{C}_n^D$:

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

Note that while Morgan et al. [2] stated 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 $i = 0, \ldots, D$:

- o_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 $r^* = \max\{r_i \mid 1 \leq i \leq D-1\}$. Note that $\delta_i \geq 2$ and $r_i \leq \lfloor \frac{D}{2} \rfloor$ 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 on P. We consider the following partition of the vertices outside P in 4 disjoint sets $V_0, V_{1,2}, V_3^{D-1}, V_3^D$, and denote by $n_0, n_{1,2}, n_3^{D-1}, n_3^D$ 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 on P;
- V_3^{D-1} is the set of vertices v outside P with three neighbors on P and $\epsilon(v) \leq D-1$;
- V_3^D is the set of vertices v outside P with three neighbors on 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, $r^* \geq \rho^*$. The rest of the proof is organized as follows. We first give an upper bound on the total weight of the vertices outside P (Claim 1), which will lead to an upper bound on $\xi^c(G)$ (Claim 2). We finally prove that this bound is attained if and only if G belongs to $\mathcal{C}_n^D$.

Claim 1.
$$\sum_{v \notin P} \mathcal{W}(v) \leq (n-D-1)D(n-D) + n_3^{D-1}(2D-n-1) - Dn_3^D - 2Dr^* + D\min\{1, \rho^*\} - \sum_{v \in V_{1,2} \cup V_3^D \cup V_3^{D-1}} (2D-1)\rho(v).$$

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 on 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 4 that there is a path $w_1 - \cdots - w_{\epsilon(u_i)+1}$ such that $w_1, \ldots, w_{r^*-1}$ have no neighbor on P and w_{r^*} 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

$$\begin{aligned}&D(n-D-2)(r^*-1) + D(n-D-1) + D(n-D)(n-D-1-n_3^{D-1}-n_3^D-r^*)\\ &= D(n-D)(n-D-1-n_3^{D-1}-n_3^D) - 2Dr^* + D.\end{aligned}$$

- If $r^* > 0$ and $\rho^* = 0$, then consider the same path $w_1 - \cdots - w_{\epsilon(u_i)+1}$ as in the above case. If w_{r^*} 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

$$\begin{aligned}&D(n-D-2)(r^*) + D(n-D)(n-D-1-n_3^{D-1}-n_3^D-r^*)\\ &= D(n-D)(n-D-1-n_3^{D-1}-n_3^D) - 2Dr^*.\end{aligned}$$

  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

$$\begin{aligned}&D(n-D-2)(r^*-1) + 2D(n-D-1) + D(n-D)(n-D-1-n_3^{D-1}-n_3^D-r^*-1)\\ &= D(n-D)(n-D-1-n_3^{D-1}-n_3^D) - 2Dr^*.\end{aligned}$$

  So assume w_{r^*} is the only vertex in $V_{1,2}$ with only one neighbor on P. We thus have $d(u_i, w_{r^*}) = \delta_i + 1$. We now show that this case is impossible. We know from Lemma 4 that w_{r^*} 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 $r^*+1 \le j \le \epsilon(u_i)-1$ 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_ℓ on P with $\ell \ge i+2$, we would have

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

  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 $d(u_0, w_1) = d(u_0, u_i) + d(u_i, w_1) > i + \delta_i \ge D$. Let Q be such a path of minimum length. Clearly, Q has length at least equal to $\epsilon(u_i)$. So let $w'_1 - \cdots - w'_{\epsilon(u_i)+1}$ 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 $(n-D+1)\Big((D-1)n_3^{D-1} + Dn_3^D\Big)$, which gives the following upper bound B on the total weight of the vertices outside P:

$$\begin{aligned}B &= D(n-D)(n-D-1-n_3^{D-1}-n_3^D) + (n-D+1)\Big((D-1)n_3^{D-1} + Dn_3^D\Big)\\ &\quad - 2Dr^* + D\min\{1, \rho^*\}\\ &= (n-D-1)D(n-D) + n_3^{D-1}(2D-n-1) + Dn_3^D - 2Dr^* + D\min\{1, \rho^*\}.\end{aligned}$$

This bound can only be reached if all vertices outside P are pairwise adjacent. But Lemma 4 shows that this cannot happen if $\rho^* > 0$. Indeed, consider a vertex v in $V_{1,2} \cup V_3^D \cup V_3^{D-1}$ with $\rho(v) > 0$. There is a vertex u_i on P adjacent to v such that $\rho(v) = r_i = \epsilon(u_i) - \delta_i > 0$. We know from Lemma 4 that there is a shortest path $w_1 - w_2 - \cdots - w_{\epsilon(u_i)+1} = u_i$ linking u_i to a vertex w_1 with $d(u_i, w_1) = \epsilon(u_i)$ and such that $w_1, \ldots, w_{\rho(v)}$ do not belong to P. In what follows, we denote Q^v such a path. If v is adjacent to a w_j with $1 \le j \le \rho(v)$, then the path $u_i - v - w_j - \cdots - w_1$ links u_i to w_1 and has length at most $\rho(v) + 1 < r_i + \delta_i = \epsilon(u_i)$, a contradiction. Hence v has at least $\rho(v)$ non-neighbors outside P. Also, as shown in Lemma 4, $w_1, \ldots, w_{\rho(v)-1}$ belong to V_0, while $w_{\rho(v)}$ belongs to $V_0 \cup V_{1,2}$. In the upper bound B, we have assumed that $\epsilon(w_1) = \cdots = \epsilon(w_{\rho(v)}) = D$. Hence, if $v \in V_{1,2} \cup V_3^D$, we can gain $2D$ units on B for every w_j, $j = 1, \ldots, \rho(v)$ (D 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 $d(v, w^*) \le D-1$. Hence, if $\rho(v) = 0$, we can gain $2D$ (one D for v and one D for w) in the above upper bound. So assume $\rho(v) > 0$, and consider again the shortest path $Q^v = w_1 - w_2 - \cdots - w_{\epsilon(u_i)+1} = u_i$, with $\rho(v) = r_i$. Also, let $W = \{w_1, \ldots, w_{\rho(v)}\}$. 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 $v - x - w_j - \cdots - w^*$ has length at most $1 + \rho(v) \leq 1 + \lfloor \frac{D}{2} \rfloor < D$, 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 $w_1, \ldots, w_{\rho(v)-1}$ have no neighbors outside Q^v, we know that $w_{\rho(v)}$ is adjacent to the extremity of P at distance δ_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, which proves Claim 1:

$$\begin{aligned} &B - \sum_{v \in V_{1,2} \cup V_3^D} 2D\rho(v) - \sum_{v \in V_3^{D-1}} (2D-1)\rho(v) - 2Dn_3^D \\ &\leq (n-D-1)D(n-D) + n_3^{D-1}(2D-n-1) - Dn_3^D - 2Dr^* + D\min\{1, \rho^*\} \\ &\quad - \sum_{v \in V_{1,2} \cup V_3^D \cup V_3^{D-1}} (2D-1)\rho(v). \end{aligned}$$

Claim 2. $\xi^c(G) \leq (n-D-1)D(n-D) + n_3^{D-1}(2D-n-1) - Dn_3^D + 2\sum_{i=0}^{D-1} \delta_i + \sum_{i=0}^{D} \delta_i o_i.$

We have $\mathcal{W}(u_0) = D(1 + o_0)$, $\mathcal{W}(u_D) = D(1 + o_D)$, and $\mathcal{W}(u_i) = \epsilon(u_i)(2 + o_i)$ for $i = 1, \ldots, D-1$. Since $\epsilon(u_i) = \delta_i + r_i$, the total weight of the vertices on P is

$$\begin{aligned} &2D + D(o_0 + o_D) + \sum_{i=1}^{D-1} (\delta_i + r_i)(2 + o_i) \\ &= 2\sum_{i=0}^{D-1} \delta_i + 2\sum_{i=1}^{D-1} r_i + \sum_{i=1}^{D-1} r_i o_i + \sum_{i=0}^{D} \delta_i o_i. \end{aligned}$$

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

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

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:

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

Summing up the bounds for the vertices outside P with those on P, we get from Claim 1 the following upper bound for the total weight of the vertices in G:

$$\begin{aligned} &(n-D-1)D(n-D) + n_3^{D-1}(2D-n-1) - Dn_3^D + 2\sum_{i=0}^{D-1} \delta_i + \sum_{i=0}^{D} \delta_i o_i \\ &\quad - \sum_{v \in V_{1,2} \cup V_3^D \cup V_3^{D-1}} (2D-4)\rho(v) - 2r^* + D\min\{1, \rho^*\}. \end{aligned}$$

Let us decompose this bound into two parts $A_1 + A_2$ with A_1 being equal to the sum of the first terms of the above upper bound, and A_2 being equal to the sum of the last ones:

$$\begin{aligned} A_1 &= (n-D-1)D(n-D) + n_3^{D-1}(2D-n-1) - Dn_3^D + 2\sum_{i=0}^{D-1} \delta_i + \sum_{i=0}^{D} \delta_i o_i, \\ A_2 &= -\sum_{v \in V_{1,2} \cup V_3^D \cup V_3^{D-1}} (2D-4)\rho(v) - 2r^* + D\min\{1, \rho^*\}. \end{aligned}$$

- If $r^* = 0$, then $A_2 = 0$, which implies $A_1 + A_2 = A_1$.
- If $\rho^* > 0$, then $A_2 \le 4 - 2D - 2r^* + D = 4 - D - 2r^* < 0$, 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, which proves Claim 2.

It follows from Claim 2 that A_1 is the best possible upper bound on $\xi^c(G)$, and this bound is attained only if the upper bound in Claim 1 is reached with $r^* = 0$ (and hence $\rho^* = 0$). As shown in the proof of Claim 1, this implies $n_0 = 0$, $\epsilon(v) = D$ for all vertices in $V_{1,2}$, $\epsilon(v) = D - 1$ for all vertices in V_3^{D-1}, and all vertices in $V_{1,2} \cup V_3^{D-1}$ are pairwise adjacent.

It remains to prove that $A_1 = f(n, D)$ and that the graphs G with $\xi^c(G) = A_1 = f(n, D)$ are exactly those in $\mathcal{C}_n^D$. Let us start with $D = 3$. In that case, we have $f(n, 3) = 14 + (n-4)(3n - 4 + \max\{0, 7 - n\})$, while $A_1 = (n-4)3(n-3) + n_3^2(5-n) - 3n_3^3 + 14 + \sum_{i=0}^{3} \delta_i o_i$. 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

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

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

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

Hence,

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

This difference is minimized if and only if $n_3^3 = 0$, while $n_3^2 = 0$ if $n > 7$, $n_3^2 = 0, 1, 2$ or 3 if $n = 7$, and $n_3^2 = n - 4$ 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 $G \simeq \mathsf{E}_{4,3,0}$ which is the unique graph in $\mathcal{C}_4^3$.
- If $n = 5$, $n_3^2 = 1$, which means that the unique vertex outside P is adjacent to 3 consecutive vertices on P. Hence, $G \simeq \mathsf{E}_{5,3,1}$ which is the unique graph in $\mathcal{C}_5^3$.
- 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 $G \simeq \mathsf{E}_{6,3,2}$.
- 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 $\mathsf{E}_{7,3,0}$, $\mathsf{E}_{7,3,1}$ or $\mathsf{E}_{7,3,2}$. If $n_{1,2} = 0$, 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 $G \simeq \mathsf{E}_{7,3,3}$, 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, $G \simeq \mathsf{E}_{n,3,0}$.

Assume now $D \ge 4$. We have

$$f(n,D) = 2\sum_{i=0}^{D-1} \delta_i + \Big(n - D - 1\Big)\Big(2D - 1 + D(n-D) + \max\{0, 3D - n - 3\}\Big)$$

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

$$\sum_{i=0}^{D} o_i \le 3(n_3^{D-1} + n_3^D) + 2(n - D - 1 - n_3^{D-1} - n_3^D) = 2(n-D-1) + n_3^{D-1} + n_3^D.$$

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 $n > 3(D-1)$, $n_3^{D-1} \in \{0, \dots, n-D-1\}$ 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 $G \simeq \mathsf{E}_{n,D,n-D-1}$.
- If $n = 3(D - 1)$, $n_3^{D-1} \in \{0, \dots, n - D - 1\}$ 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, $G \simeq \mathsf{E}_{n,D,n-D-1}$.
- 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, $G \simeq \mathsf{E}_{n,D,0}$. □

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.

Theorem 9. *Let ξ_n^{c*} be the largest eccentric connectivity index among all graphs of order n. The only graphs that attain ξ_n^{c*} are the following:*

n	ξ_n^{c*}	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 $\mathsf{E}_{8,4,3}$
≥ 9	$g(n)$	$\mathsf{E}_{n,\lceil \frac{n+1}{3} \rceil + 1, n - \lceil \frac{n+1}{3} \rceil - 2}$.

Proof. Clearly, K_3 and P_3 are the only connected graphs of order $n = 3$ and $\xi^c(\mathsf{K}_3) = \xi^c(\mathsf{P}_3) = 6$. For $n > 3$, $\xi^c(\mathsf{M}_n) = 2n^2 - 4n - 2(n \bmod 2) > n^2 - n = \xi^c(\mathsf{K}_n)$, which means that the optimal diameter is not $D = 1$.

- If $n = 4$, $f(4, 3) = 14 < \xi^c(\mathsf{M}_4) = 16$, 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 $\xi^c(\mathsf{M}_5) = 30$, 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 $\xi^c(\mathsf{M}_6) = 48$, 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 $\mathsf{E}_{n,D,0}$ of order n and diameter D.

- If $D = n-1$, then $G \simeq \mathsf{P}_n$ which implies

$$\xi^c(\mathsf{E}_{n,n-1,0}) = \sum_{i=1}^{D-1} 2\max\{i, D-i\} + 2D = \frac{3D^2 + D \bmod 2}{2}$$
$$\leq \frac{3D^2+1}{2} = \frac{3n^2}{2} - 3n + 2 < 2n^2 - 4n - 2 \leq \xi^c(\mathsf{M}_n).$$

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

$$\begin{aligned}
\xi^c(\mathsf{E}_{n,D+1,n-D-2}) &= 2\sum_{i=0}^{D}\max\{i, D+1-i\} \\
&\quad + \Big(n-D-2\Big)\Big(2(D+1) - 1 + (D+1)(n-D-1)\Big) \\
&\quad + \Big(n-D-2\Big)\Big(2(D+1) - n - 1 + (D+1) - 2\Big) \\
&= \frac{3(D+1)^2 + (D+1) \bmod 2}{2} + \Big(n-D-2\Big)\Big(3D + D(n-D)\Big)
\end{aligned}$$

and

$$\begin{aligned}
\xi^c(\mathsf{E}_{n,D,0}) &= 2\sum_{i=0}^{D-1}\max\{i, D-i\} + \Big(n-D-1\Big)\Big(2D - 1 + D(n-D)\Big) \\
&= \frac{3D^2 + D \bmod 2}{2} + \Big(n-D-1\Big)\Big(2D-1+D(n-D)\Big).
\end{aligned}$$

Simple calculations lead to

$$\xi^c(\mathsf{E}_{n,D+1,n-D-2}) - \xi^c(\mathsf{E}_{n,D,0}) = n - 2D + (D-1) \bmod 2 \geq n - 2\Big(\frac{n}{3}+1\Big) = \frac{n}{3} - 2 > 0.$$

Hence, the remaining candidates to maximize the eccentric connectivity index when $n \geq 7$ are M_n and $\mathsf{E}_{n,D,n-D-1}$. Let

$$g(n) = \max_{D=\lceil \frac{n}{3}+2\rceil}^{n-D-1} \xi^c(\mathsf{E}_{n,D,n-D-1}).$$

We can rewrite $\xi^c(\mathsf{E}_{n,D,n-D-1})$ as follows:

$$\xi^c(\mathsf{E}_{n,D,n-D-1}) = D^3 - D^2(n+\frac{5}{2}) + D(n^2+5n-1) - n^2 - 3n + 4 + D \bmod 2.$$

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

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

We then have $g(7) = 66 < 68 = \xi^c(\mathsf{M}_7)$, which means that M_7 has the largest eccentric connectivity among all graphs with 7 vertices. Also, $g(8) = 96 = \xi^c(\mathsf{M}_8)$, which means that both $\mathsf{E}_{8,4,3}$ 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 $\mathsf{E}_{n,D^*,n-D^*-1}$ is the unique graph with largest eccentric connectivity index among all graphs with n vertices. $\square$

Note that Tavakoli et al. [4] stated that $g(n) = \xi^c(\mathsf{E}_{n,D,n-D-1})$ with $D = \lceil\frac{n}{3}\rceil + 1$ while we have shown that the best diameter for a given n is $D = \lceil\frac{n+1}{3}\rceil + 1$. Hence for all $n \geq 9$ with $n \bmod 3 = 0$, we get a better result. For example, for $n = 9$, they consider $\mathsf{E}_{9,4,4}$ 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 $m \leq \binom{n-1}{2}$. Also, let*

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

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

- *if $D > 3$, then $\xi^c(G) < \xi^c(\mathsf{E}_{n,D,k})$ 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 $\xi^c(G) = \xi^c(\mathsf{E}_{n,D,k})$ 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.*

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