

Maximizing the eccentric connectivity index for graphs with given order and diameter

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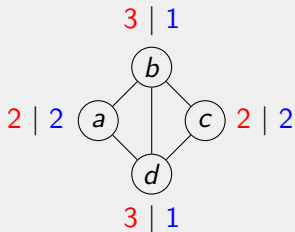
JGA — 2019

Definition

The **Eccentricity Connectivity Index** of a graph $G = (V, E)$, denoted by $\xi^c(G)$, is

$$\xi^c(G) = \sum_{v \in V} \deg(v) \epsilon(v). \quad \text{Alternatively, } \xi^c(G) = \sum_{uv \in E} (\epsilon(u) + \epsilon(v)).$$

Example



$$\xi^c(G) = 2 \cdot 2 + 3 \cdot 1 + 2 \cdot 2 + 3 \cdot 1 = 14$$

Problem

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Theorem (Morgan, Mukwembi, and Swart 2011)

Let G be a connected graph of order n and diameter D . Then,

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

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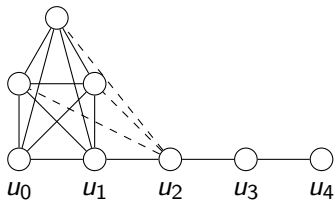
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What about an exact bound ?

Definition

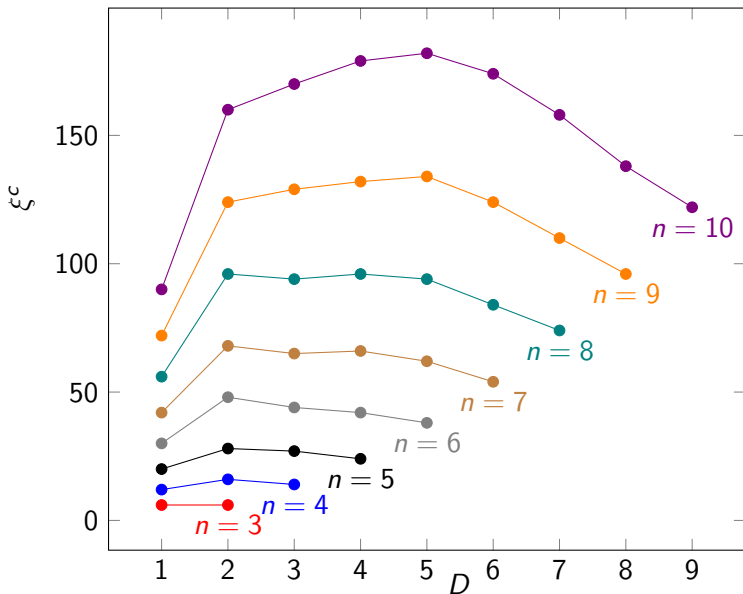
Let n, D and k be integers such that $n \geq 4$, $3 \leq D \leq n - 1$ and $0 \leq k \leq n - D - 1$, and let $E_{n,D,k}$ be the graph (of order n and diameter D) constructed from a path $u_0 - u_1 - \dots - u_D$ by joining each vertex of a clique K_{n-D-1} to u_0 and u_1 , and k vertices of the clique to u_2 .

- $E_{n,D,0} \simeq L_{n,D}$, the lollipop;
- $E_{n,D,n-D-1}$ is a lollipop $L_{n,D-1}$ missing an edge;
- if $D = n - 1$, then $k = 0$ and $E_{n,n-1,0} \simeq P_n$.

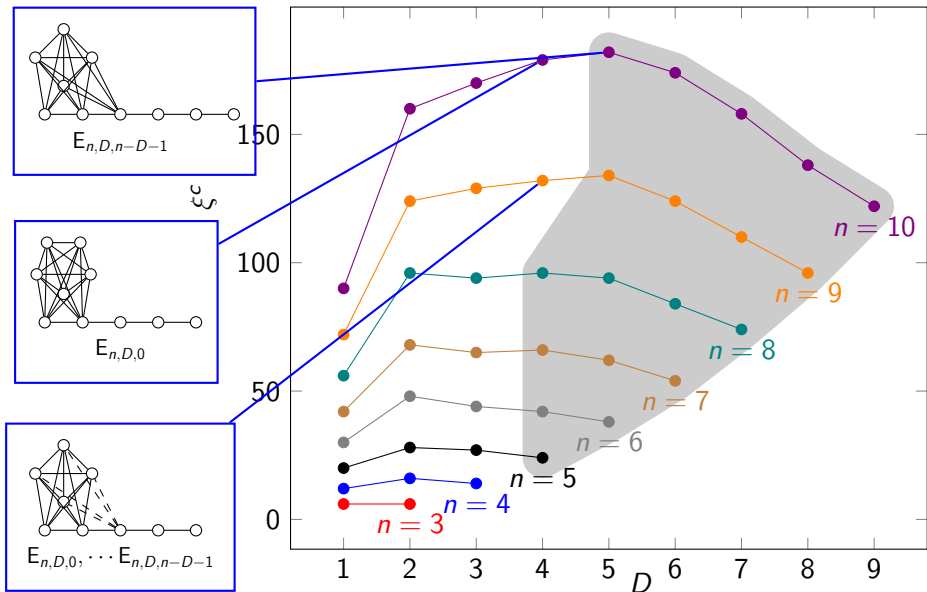


$E_{8,4,k}$, dashed edges depend on k .

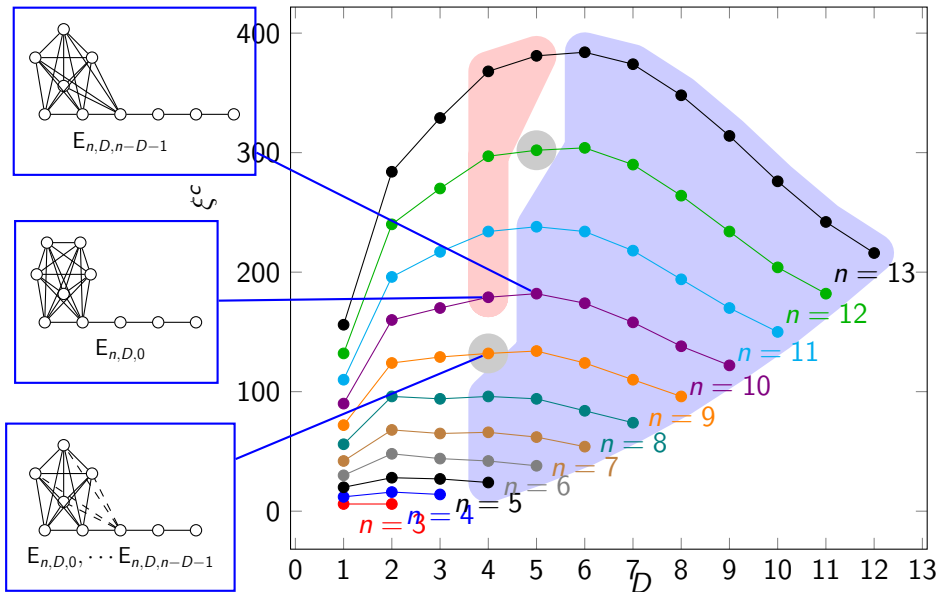
$\max \xi^c$ for given order n and diameter D



max ξ^c for given order n and diameter D



max ξ^c for given order n and diameter D



max ξ^c with order and diameter when $D \geq 3$

Theorem (H et al. 2019)

Let G be a connected graph of order $n \geq 4$ and diameter $3 \leq D \leq n - 1$. Let $f(n, D) = \max\{\xi^c(E_{n,D,k}) \mid k = 0, \dots, n - D - 1\}$. Then $\xi^c(G) \leq f(n, D)$ with equality if and only if G belongs to \mathcal{C}_n^D .

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

Proof plan

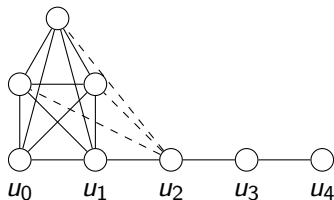
- 1 Compute $\xi^c(E_{n,D,k})$.
- 2 Work out $f(n, D) = \max_k \xi^c(E_{n,D,k})$ (and convince ourselves that the graphs in \mathcal{C}_n^D have $\xi^c = f(n, D)$).
- 3 Show that, for a graph G of order n and diameter D , $\xi^c(G) \leq f(n, D)$, and if it attains the bound, then it is isomorphic to a graph in \mathcal{C}_n^D .

1. Compute $\xi^c(E_{n,D,k})$

Lemma

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

$$\xi^c(E_{n,D,k}) = 2 \sum_{i=0}^{D-1} \max\{i, D - i\} + (n - D - 1)(2D - 1 + D(n - D)) + k(3D - n - 3).$$



2. Work out $f(n, D) = \max_k \xi^c(E_{n,D,k})$

$$\xi^c(E_{n,D,k}) = 2 \sum_{i=0}^{D-1} \max\{i, D-i\} + (n-D-1)(2D-1 + D(n-D)) \\ + k(3D-n-3).$$

$$\mathcal{C}_n^D = \begin{cases} [\dots] & \text{if } n > 3(D-1) \text{ and } D \geq 4; \\ \{E_{n,D,0}\} & \text{if } n = 3(D-1) \text{ and } D \geq 4; \\ \{E_{n,D,0}, \dots, E_{n,D,n-D-1}\} & \text{if } n < 3(D-1) \text{ and } D \geq 4. \end{cases}$$

2. Work out $f(n, D) = \max_k \xi^c(E_{n,D,k})$

$$\xi^c(E_{n,D,k}) = 2 \sum_{i=0}^{D-1} \max\{i, D-i\} + (n-D-1)(2D-1 + D(n-D)) \\ + k(3D-n-3).$$

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

3. Last step of the proof — subplan

Theorem

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 .

- 1 Give an upper bound on the total weight of the vertices outside a diametral path P .
- 2 Extend to an upper bound on $\xi^c(G)$.
- 3 Prove that this bound is attained only if G is isomorphic to one of \mathcal{C}_n^D .

Tool lemma

Let G be a connected graph of diameter $D \geq 3$. Let P be a diametral path, and u a vertex on P such that $\epsilon(u) > L$, with L the longest distance from u to an extremity of P . Finally, let v be a vertex such that $d(u, v) = \epsilon(u)$ and let $v = w_1 - w_2 - \dots - w_{\epsilon(u)+1} = u$ be a shortest path linking v to u . Then

- vertices $w_1, \dots, w_{\epsilon(u)-L}$ 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 $w_1, \dots, w_{\epsilon(u)-L-1}$ have no neighbor on P .



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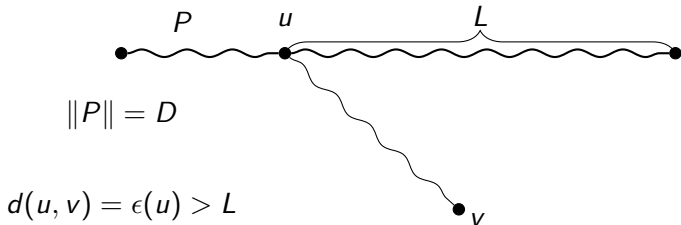
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$$\epsilon(u) > L$$

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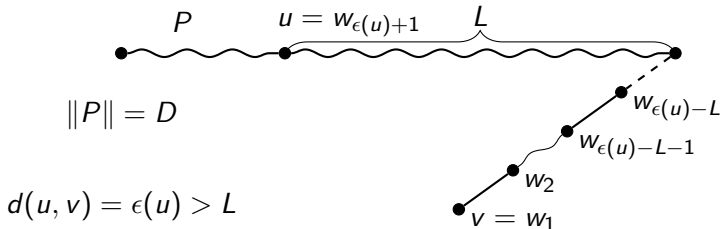
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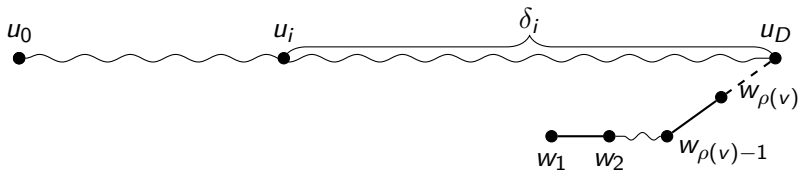


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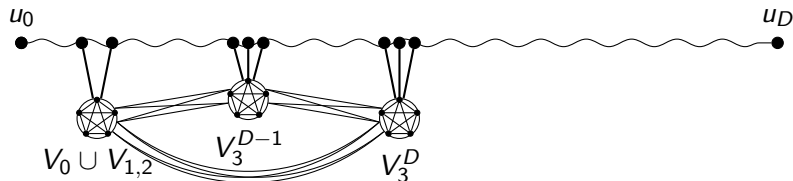
$$r_i = \epsilon(u_i) - \delta_i.$$

$$r^* = \max_{i=0}^D r_i).$$

Claim (weight outside P)

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

3.1. Bound on the weight outside P



$$\mathcal{W}(V_0 \cup V_{1,2}) \leq D(n - D)(n - D - 1 - n_3^{D-1} - n_3^D)$$

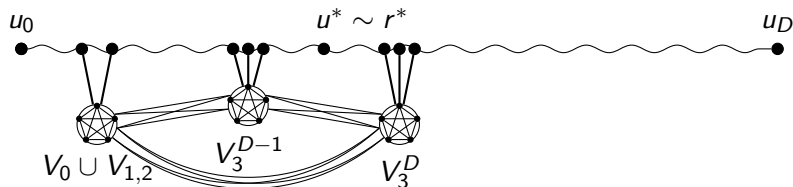
$$\mathcal{W}(V_3^{D-1} \cup V_3^D) \leq (n - D + 1)((D - 1)n_3^{D-1} + Dn_3^D)$$

$$V_{1,2} = \{v \notin P \mid |N(v) \cap P| \in \{1, 2\}\},$$

$$V_3^{D-1} = \{v \notin P \mid |N(v) \cap P| = 3, \epsilon(v) \leq D - 1\},$$

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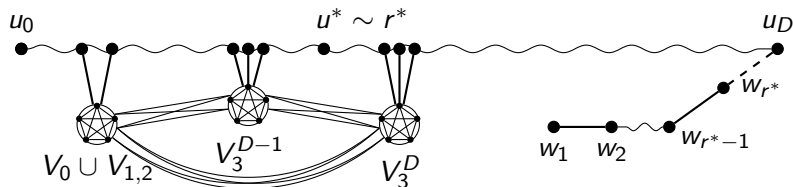
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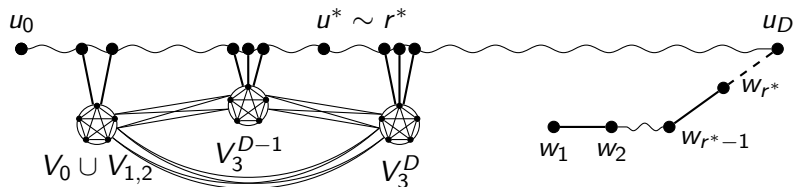
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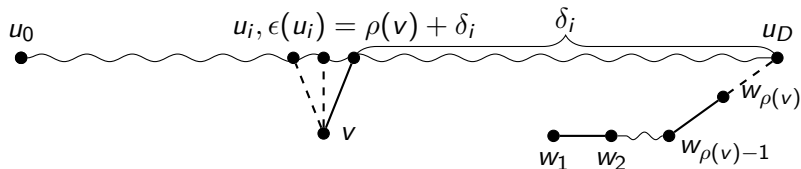
$$\mathcal{W}(V_3^{D-1} \cup V_3^D) \leq (n - D + 1)((D - 1)n_3^{D-1} + Dn_3^D)$$

We get a bound on the total weight of the vertices outside P

$$\begin{aligned} B &= \mathcal{W}(V_0 \cup V_{1,2} \cup V_3^{D-1} \cup V_3^D) \\ &= (n - D - 1)D(n - D) + n_3^{D-1}(2D - n - 1) + Dn_3^D - 2Dr^* \\ &\quad + D \min\{1, \rho^*\}. \end{aligned}$$

Can only be reached if all vertices outside P are pairwise adjacent.

3.2. Improving the bound on the weight outside of P



$$\rho(v) = \max\{r_i \mid u_i \text{ is adjacent to } v\}, r_i = \epsilon(u_i) - \delta_i.$$

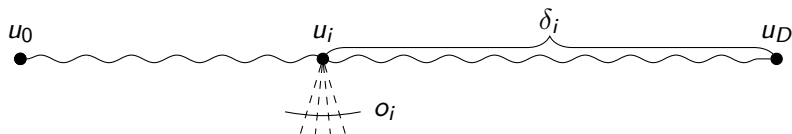
$$\begin{aligned} B &- \sum_{v \in V_{1,2} \cup V_3^D} 2D\rho(v) - \sum_{v \in V_3^{D-1}} (2D-1)\rho(v) - 2Dn_3^D \\ &\leq (n-D-1)D(n-D) + n_3^{D-1}(2D-n-1) - Dn_3^D - 2Dr^* \\ &\quad + D \min\{1, \rho^*\} - \sum_{v \in V_{1,2} \cup V_3^D \cup V_3^{D-1}} (2D-1)\rho(v). \end{aligned}$$

Which is the claim.

Claim (total weight on G)

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

Bounding the weight on P



Now we compute a bound on the total weight of P .

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

We bound this, so as to remove the r_i 's.

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

3.3. Upper bound on $\xi^c(G)$

Summing the bounds from the two claims and rewriting, we have

$$\xi^c(G) \leq A_1 + A_2,$$

$$\begin{aligned} \text{with } A_1 &= (n - D - 1)D(n - D) + n_3^{D-1}(2D - n - 1) - Dn_3^D \\ &\quad + 2 \sum_{i=0}^{D-1} \delta_i + \sum_{i=0}^D \delta_i o_i \end{aligned}$$

$$A_2 = - \sum_{v \in V_{1,2} \cup V_3^D \cup V_3^{D-1}} (2D - 4)\rho(v) - 2r^* + D \min\{1, \rho^*\}.$$

- 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 $A_1 + A_2 < A_1$.

3.4. The bound is attained only if G is one of C_n^D

In summary, the best possible bound is A_1 and this bound is attained only if the upper bound of Claim (weight outside P) is reached with $r^* = 0$. As shown in the proof of the claim, this implies $n_0 = 0$, $\epsilon(v) = D$ for all vertices in $V_{1,2}$, and all vertices in $V_{1,2} \cup V_3^{D-1}$ are pairwise adjacent.

We only need 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 C_n^D . \rightarrow bound and minimize $f(n, D) - A_1$.

Maximizing ξ^c for a fixed order

Morgan, Mukwembi, and Swart 2011 also gave an asymptotic bound for maximizing ξ^c given the order only.

Theorem (Morgan, Mukwembi, and Swart 2011)

Let G be a connected graph of order n . Then,

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

Theorem (H et al. 2019)

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	\overline{M}_4
5	30	\overline{M}_5 and H_1
6	48	\overline{M}_6
7	68	\overline{M}_7
8	96	\overline{M}_8 and $E_{8,4,3}$
≥ 9	$g(n)$	$E_{n, \lceil \frac{n+1}{3} \rceil + 1, n - \lceil \frac{n+1}{3} \rceil - 2}$.

This is obtained as a corollary of our previous results by a simple analysis of

$$\max_D f(n, D).$$

Maximizing ξ^c with given order and size

Conjecture (H et al. 2019)

Let n and m be two integers such that $n \geq 4$ and $m \leq \binom{n-1}{2}$. Also, let

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

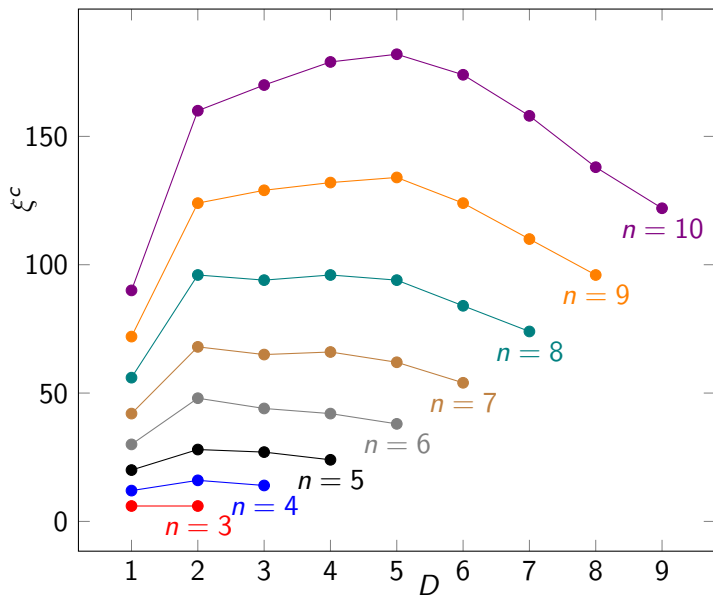
Then, the largest eccentric connectivity index among all graphs of order n and size m is attained with $E_{n,D,k}$. Moreover,

- 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 .

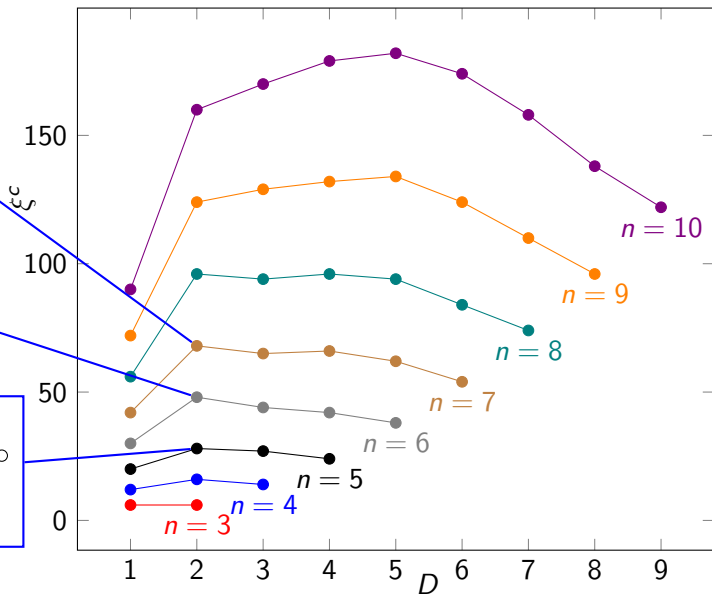
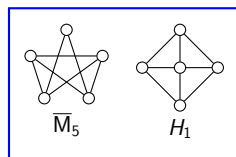
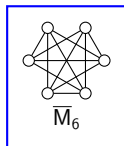
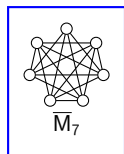
Appendix

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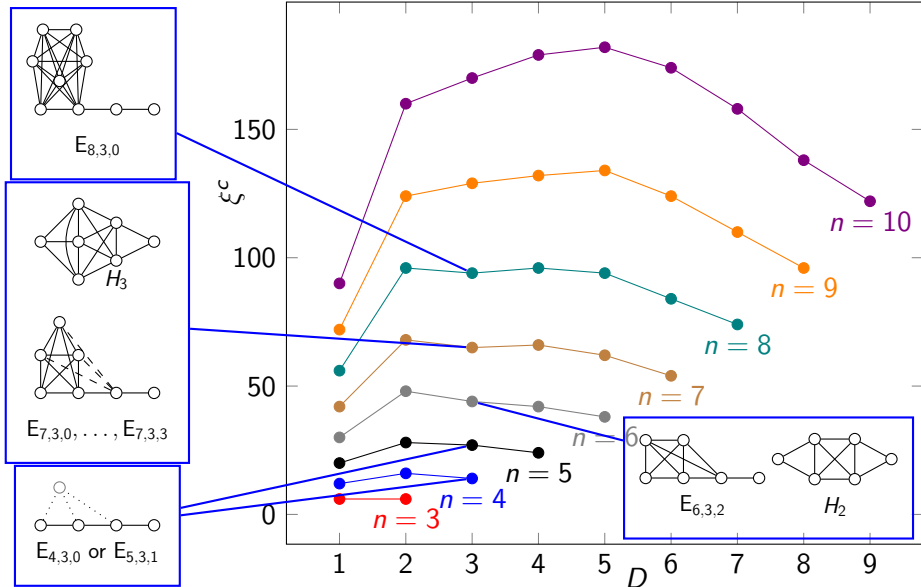
Maximum values of ξ^c for given order n and diameter D



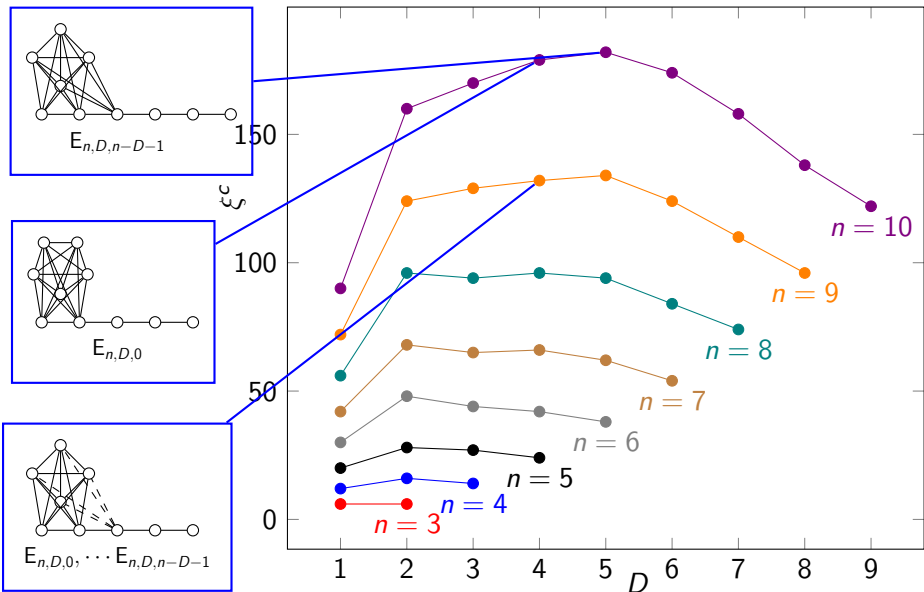
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Maximum values of ξ^c for given order n and diameter D



max ξ^c with given order and diameter when $D = 2$

Theorem (H et al. 2019)

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 $G \simeq \overline{M}_n$, or $n = 5$ and $G \simeq$



Zhou and Du 2010

- Complete graphs: $\xi^c(K_n) = n(n - 1)$
- Complete bipartite graphs: $\xi^c(K_{a,b}) = 4ab$ for $a, b \geq 2$
- Stars: $\xi^c(S_n) = 3(n - 1)$
- Cycles: $\xi^c(C_n) = 2n \lfloor \frac{n}{2} \rfloor$
- Paths: $\xi^c(P_n) = \lfloor \frac{3(n-1)^2+1}{2} \rfloor$

Theorem (Zhou and Du 2010)

Let G be a connected graph of order $n \geq 4$, then

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

with equality if and only if $G \simeq S_n$.

Theorem (Zhou and Du 2010)

Let G be an n -vertex connected graph with m edges, where

$n-1 \leq m \leq \binom{n}{2}$. Let $a = \left\lfloor \frac{2n-1-\sqrt{(2n-1)^2-8m}}{2} \right\rfloor$. Then

$$\xi^c(G) \geq 4m - a(n-1)$$

with equality if and only if $G \in \mathbf{G}_{(n,m)}$.

$\mathbf{G}_{(n,m)}$ is the set of graphs $K_a \vee H$, where H is a graph with $n-a$ vertices and $m - \binom{a}{2} - a(n-a)$ edges.

Theorem (Morgan, Mukwembi, and Swart 2012)

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

$$\xi^c(G) \geq \xi^c(V_{n,D}),$$

where $V_{n,D}$ is the volcano 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} .

Degree distance

The degree distance D' of a graph G is

$$\sum_{uv \in E} (\deg(u) + \deg(v))d(u, v).$$

Theorem (Zhou and Du 2010)

Let $G = (V, E)$ be a connected graph with $n \geq 2$ vertices. Then

$$\xi^c(G) \geq \frac{1}{n-1} D'(G),$$

with equality if and only if $G = K_n$.

Eccentric Connectivity Index

- Sharma, Goswani and Madan introduced ξ^c in 1997 in Chemistry;
- Useful as a discriminating topological descriptor for Structure Properties and Structure Activity studies;
- Since 1997, more than 200 chemical papers about ξ^c : applications in drug design, prediction of anti-HIV activities, etc.

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- Since 1997, more than 200 chemical papers about ξ^c : applications in drug design, prediction of anti-HIV activities, etc.
- However, the first mathematical paper with extremal properties on ξ^c was published only in 2010;
- Since 2010, about a dozen papers containing bounds on ξ^c .

Problem

Among connected graphs of order n and size m , what is the maximum possible value for ξ^c ?

Maximizing ξ^c given order and size

Conjecture (Zhang, Liu, and Zhou 2014)

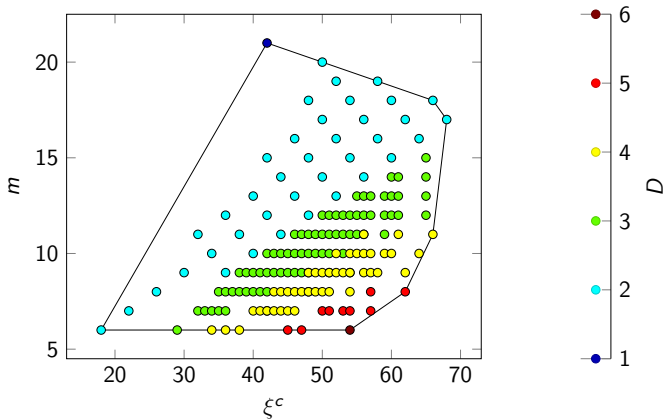
Let G be a graph of order n and size m such that $d_{n,m} \geq 3$. Then,

$$\xi^c(G) \leq \xi^c(E_{n,m}),$$

with equality if and only if $G \simeq E_{n,m}$.

- The authors prove that the conjecture is true when $m = n - 1, n, \dots, n + 4$ (if n is large enough).
- It misses some corner cases (we'll come to it later).

Polytope for $n = 7$ with points colored by the diameter D



Upper bound on ξ^c for connected graphs with fixed size

We define $E_{n,m}$ as follows :

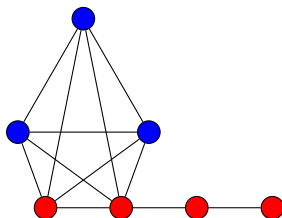
$$n = 7, m = 14$$

Upper bound on ξ^c for connected graphs with fixed size

We define $E_{n,m}$ as follows :

- The biggest possible clique without disconnecting the graph, leaving a path with the remaining vertices.

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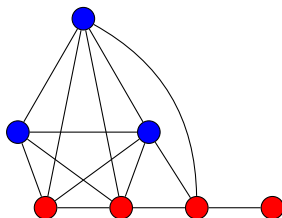


Upper bound on ξ^c for connected graphs with fixed size

We define $E_{n,m}$ as follows :

- The biggest possible clique without disconnecting the graph, leaving a path with the remaining vertices.
- Add remaining edges between vertices of the clique and the first vertex of the path.

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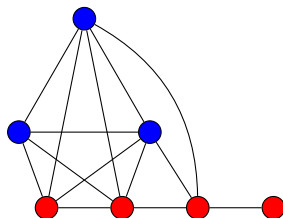


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This graph is unique for given n and m . We define $d_{n,m}$ as the diameter of $E_{n,m}$.

Bounds for connected graphs

Invariant(s)	Lower bound	Upper bound
—	✓	✗
m (size)	✓	✓
D (diameter)	✓	✓
p (number of pending vertices)	✓	✗
δ (minimum degree)	✗	✓
D (diameter) and m (size)	✓ (with conditions on m and D)	
D' (degree distance)	✓	✗
M_1 (Zagreb index) and m	✗	✓
W (Wiener index)	✗	✓

Bounds for trees

Invariant(s)	Lower bound	Upper bound
—	✓	✓
D (diameter)	✓	✓
r (radius)	✗	✓
p (number of pending vertices)	✓	✓
Δ (maximum degree)	✓	✓
β (matching number)	✓	✓
α (stability number)	✓	✓
W (Wiener index)	✗	✓

Bounds for other graph classes

Unicyclic graphs

Invariant(s)	Lower bound	Upper bound
—	✓	✓
g (girth)	✓	✓

Bicyclic graphs

Invariant(s)	Lower bound	Upper bound
—	✓	✗

k -regular graphs

Invariant(s)	Lower bound	Upper bound
$k \geq 3$ fixed	✓	✓