Extremal results on the eccentric connectivity index

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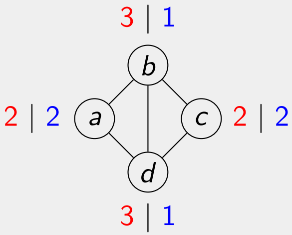
Definition

The Eccentric 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



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

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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- 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.
- 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)

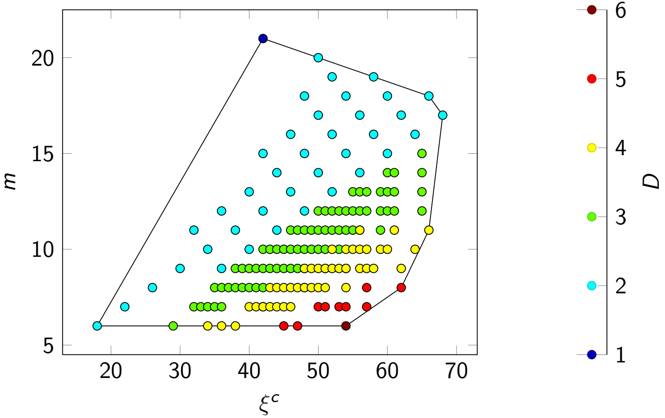
Let G be a graph of order n and size m such that $d_{n,m} \geq 3$. Then,

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

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

- The authors prove that the conjecture is true when $m = n - 1, n, \ldots, n + 4$ (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



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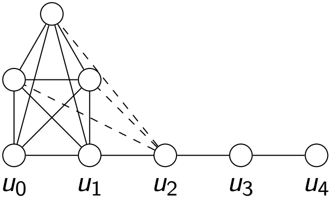
What about an exact bound ?

Definition

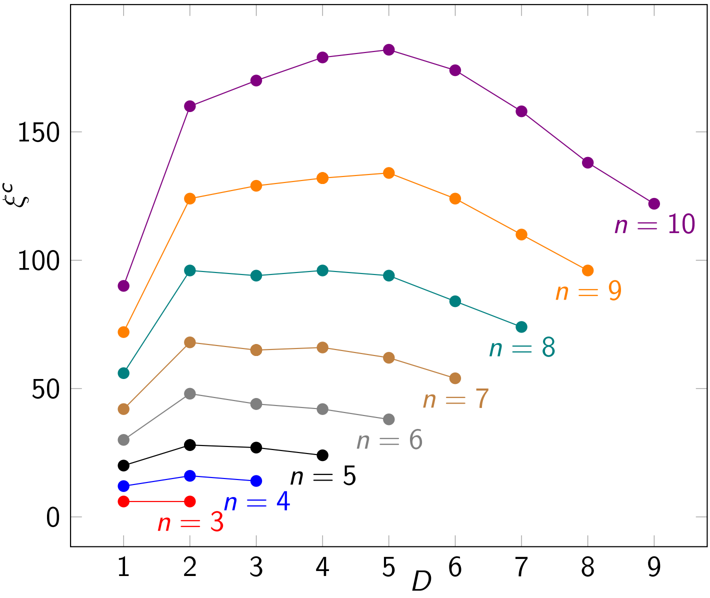
Let n, D and k be integers such that $n \geq 4$, $3 \leq D \leq n-1$ and $0 \leq k \leq n-D-1$, and let $\mathrm{E}_{n,D,k}$ be the graph (of order n and diameter D) constructed from a path $u_0 - u_1 - \ldots - u_D$ by joining each vertex of a clique K_{n-D-1} to u_0 and u_1, and k vertices of the clique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

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



$\mathrm{E}_{8,4,k}$, dashed edges depend on k.

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



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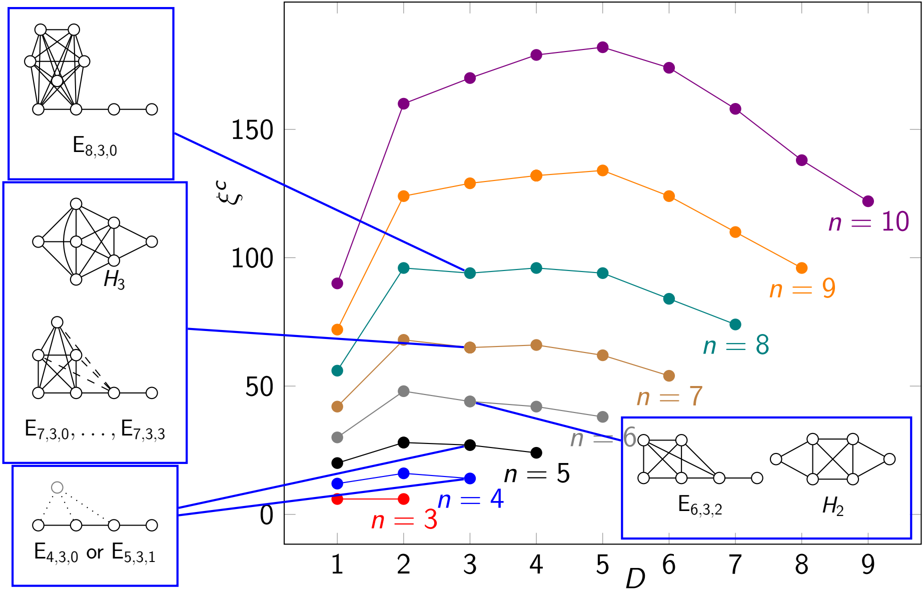
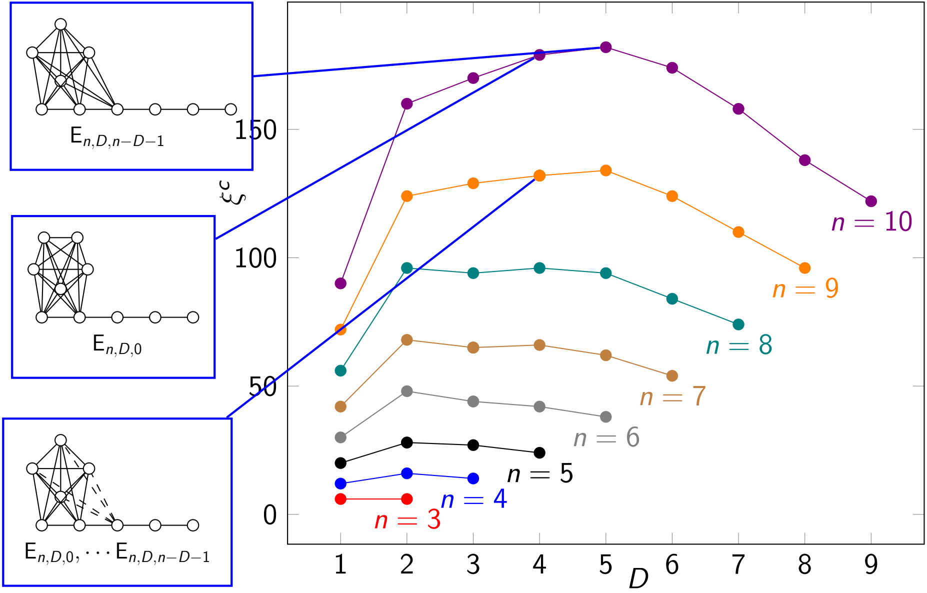


Maximum values of ξ^c for given order n and diameter D



$\max \xi^c$ 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 $f(n,D) = \max\{\xi^c(\mathsf{E}_{n,D,k}) \mid k = 0,\dots,n-D-1\}$. Then $\xi^c(G) \leq f(n,D)$ with equality if and only if G belongs to $\mathcal{C}_n^D$.

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

Proof plan

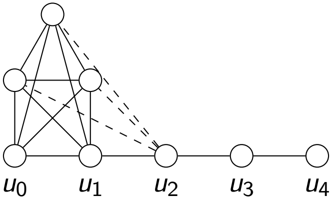
1. Compute $\xi^c(\mathrm{E}_{n,D,k})$.
2. Work out $f(n, D) = \max_k \xi^c(\mathrm{E}_{n,D,k})$ (and convince ourselves that the graphs in $\mathcal{C}_n^D$ have $\xi^c = f(n, D)$).
3. Show that, for a graph G of order n and diameter D, $\xi^c(G) \leq f(n, D)$, and if it attains the bound, then it is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

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

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

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



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$$\text{"}k \text{ term"} = \begin{cases} 2D-n+1 & \text{if } D = 3; \\ 3D-n-3 & \text{if } D \geq 4. \end{cases}$$

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

3. Last step of the proof — subplan

Theorem

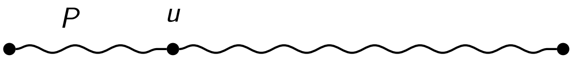
Let G be a connected graph of order $n \geq 4$ and diameter $3 \leq D \leq n-1$. Then $\xi^c(G) \leq f(n, D)$ with equality if and only if G belongs to $\mathcal{C}_n^D$.

1. Give an upper bound on the total weight of the vertices outside P.
2. Improve that bound a bit.
3. Extend to an upper bound on $\xi^c(G)$.
4. 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 $v = w_1 - w_2 - \cdots - w_{\epsilon(u)+1} = u$ be a shortest path linking v to u. 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.*



$\|P\| = D$

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$$\epsilon(u) > L$$

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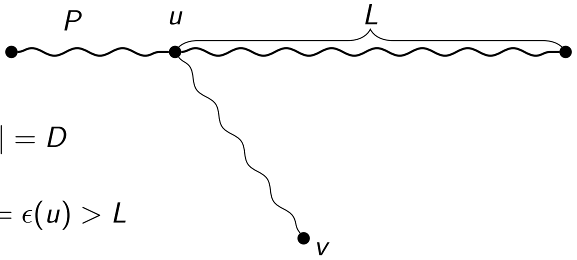

$\|P\| = D$

$d(u,v) = \epsilon(u) > L$

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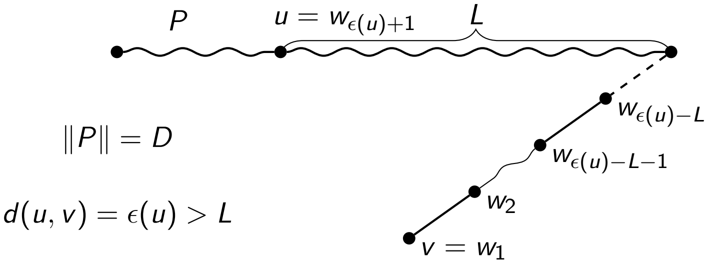


o_i number of vertices going from u_i out of P.

$$\delta_i = \max\{i, D - i\},$$
$$r_i = \epsilon(u_i) - \delta_i,$$
$$r^* = \max_{i=1}^{D-1} r_i,$$
$$V_0 = \{v \notin P \mid N(v) \cap P = \emptyset\},$$
$$V_{1,2} = \{v \notin P \mid |N(v) \cap P| \in \{1, 2\}\},$$
$$V_3^{D-1} = \{v \notin P \mid |N(v) \cap P| = 3, \epsilon(v) \leq D - 1\},$$
$$V_3^D = \{v \notin P \mid |N(v) \cap P| = 3, \epsilon(v) = D\},$$
$$\rho(v) = \max\{r_i \mid u_i \text{ is adjacent to } v\},$$
$$\rho^* = \max_{v \in V_{1,2} \cup V_3^{D-1} \cup V_3^D} \rho(v).$$

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

$$\mathcal{W}(V_0 \cup V_{1,2}) \leq D(n-D)(n-D-1-n_3^{D-1}-n_3^{D}) - 2Dr^* + D\min\{1,\rho^*\}.$$

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

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

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

Can only be reached if all vertices outside P are pairwise adjacent.
But not possible if $\rho^* > 0$.

3.2. Improving the bound on the weight outside of P

Better upper bound on the total weight of vertices outside of P

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

Which is the claim.

Claim (weight on P)

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

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.

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

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

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

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

with

$$A_1 = (n - D - 1)D(n - D) + n_3^{D-1}(2D - n - 1) - Dn_3^D + 2\sum_{i=0}^{D-1} \delta_i + \sum_{i=0}^{D} \delta_i o_i$$

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

- 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 $\mathcal{C}_n^D$

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

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

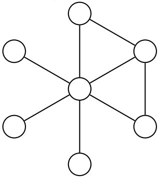
$$\max_D f(n, D).$$

Theorem (Devillez et al. 2018)

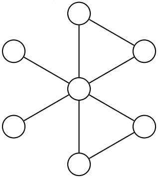
Let ${\xi^c_{n,p}}^*$ be the largest eccentric connectivity index among all graphs of order $n > 3$ with $p < n - 2$ pending vertices. The only graphs that attain ${\xi^c_{n,p}}^*$ are the following:

n	p	*optimal graphs*
> 3	> 0	$H_{n,p}$
4	0	K_4
5	0	$H_{5,0}$, $S_{5,2}$, K_5 and C_1
6	0	$S_{6,2}$
≥ 7	0	$H_{n,0}$

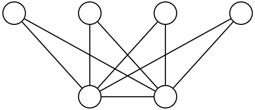
$H_{7,3}$



$H_{7,2}$



$S_{4,2}$



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 $\mathsf{E}_{n,D,k}$. 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.*

Devillez, G. et al. (2018). “Minimum Eccentric Connectivity Index for Graphs with Fixed Order and Fixed Number of Pending Vertices”. In: *arXiv preprint arXiv:1809.03158*.

H, P. et al. (2019). “Maximum eccentric connectivity index for graphs with given diameter”. In: *Discrete Applied Mathematics*. DOI: https://doi.org/10.1016/j.dam.2019.04.031.

Morgan, M.J, S. Mukwembi, and H.C Swart (2011). “On the eccentric connectivity index of a graph”. In: *Discrete Mathematics* 311, pp. 1229 –1234.

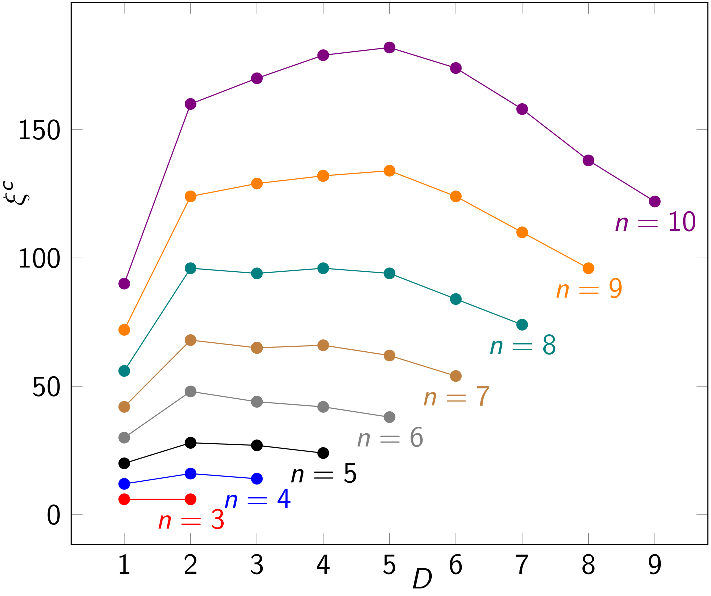
– (2012). “A lower bound on the eccentric connectivity index of a graph”. In: *Discrete Applied Mathematics* 160, pp. 248 –258.

Zhang, J., Z. Liu, and B. Zhou (2014). “On the maximal eccentric connectivity indices of graphs”. In: *Appl. Math. J. Chinese Univ.* 29, pp. 374 –378.

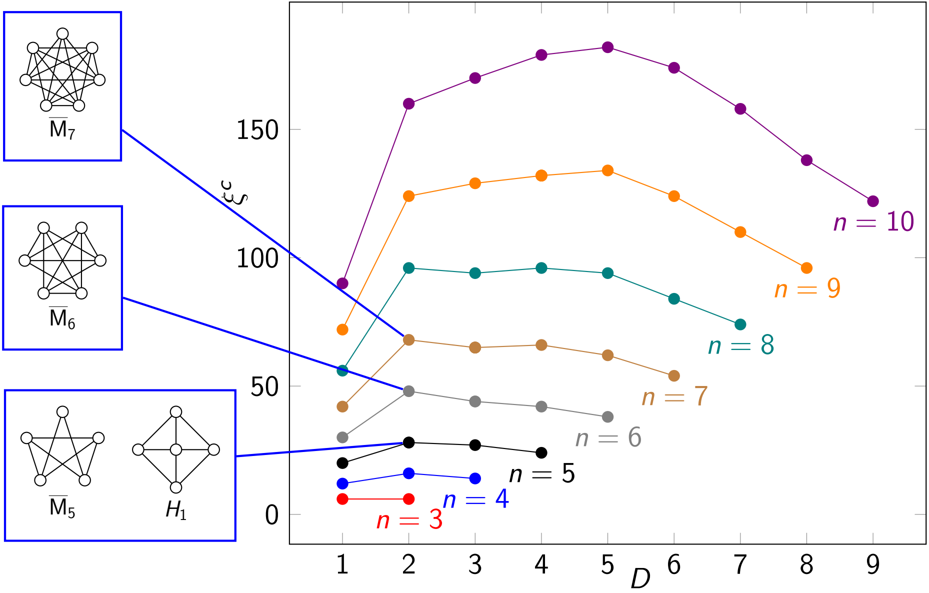
Zhou, B. and Z. Du (2010). “On Eccentric Connectivity Index”. In: *MATCH Commun. Math. Comput. Chem.* 63, pp. 181 –198.

Appendix

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



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

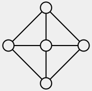


max ξ^c with given order and diameter when $D = 2$

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

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

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

$$n = 7, m = 14$$

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

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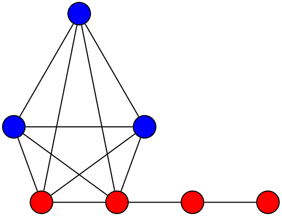
$n = 7, m = 14$

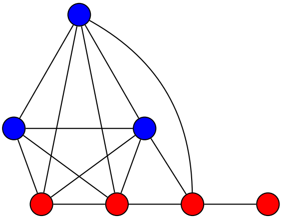


Upper bound on ξ^c for connected graphs with fixed size

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

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

$n = 7, m = 14$



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

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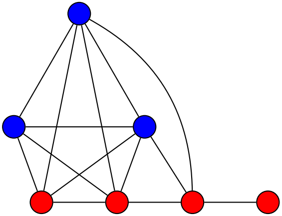

This graph is unique for given n and m. We define $d_{n,m}$ as the diameter of $E_{n,m}$.

Zhou and Du 2010

- Complete graphs: $\xi^c(\mathrm{K}_n) = n(n-1)$
- Complete bipartite graphs: $\xi^c(\mathrm{K}_{a,b}) = 4ab$ for $a, b \geq 2$
- Stars: $\xi^c(\mathrm{S}_n) = 3(n-1)$
- Cycles: $\xi^c(\mathrm{C}_n) = 2n\lfloor \frac{n}{2} \rfloor$
- Paths: $\xi^c(\mathrm{P}_n) = \lfloor \frac{3(n-1)^2+1}{2} \rfloor$

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 $G = K_n$.