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

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

Alternatively,

\[
\xi^c(G) = \sum_{uv \in E} (\epsilon(u) + \epsilon(v)).
\]

Example

\[
\begin{align*}
\xi^c(G) &= 2 \cdot 2 + 3 \cdot 1 + 2 \cdot 2 + 3 \cdot 1 = 14
\end{align*}
\]
Eccentric Connectivity Index

- Sharma, Goswani and Madan introduced $\xi^c$ 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 $\xi^c$: applications in drug design, prediction of anti-HIV activities, etc.
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- Useful as a discriminating topological descriptor for Structure Properties and Structure Activity studies;
- Since 1997, more than 200 chemical papers about $\xi^c$: applications in drug design, prediction of anti-HIV activities, etc.
- However, the first mathematical paper with extremal properties on $\xi^c$ was published only in 2010;
- Since 2010, about a dozen papers containing bounds on $\xi^c$. 
Problem

Among connected graphs of order $n$ and size $m$, what is the maximum possible value for $\xi^c$?
Maximizing \( \xi_c \) 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 \( G \cong E_{n,m} \).

- 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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Theorem (Morgan, Mukwembi, and Swart 2011)
Let $G$ be a connected graph of order $n$ and diameter $D$. Then,

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

The lollipops $L_{n,D}$ attain this bound.
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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 $u_0 - u_1 - \ldots - u_D$ by joining each vertex of a clique $K_{n-D-1}$ to $u_0$ and $u_1$, and $k$ vertices of the clique to $u_2$.

- $E_{n,D,0} \simeq L_{n,D}$, 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 $k$. 
Maximum values of $\xi^c$ for given order $n$ and diameter $D$
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Maximum values of $\xi^c$ 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 $f(n, D) = \max\{\xi^c(E_{n,D,k}) \mid k = 0, \ldots, n - D - 1\}$. Then $\xi^c(G) \leq f(n, D)$ with equality if and only if $G$ belongs to $C^D_n$.

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

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

$$+ k\left(2D - n - 1 + \max\{2, D - 2\}\right).$$
2. Work out \( f(n, D) = \max_k \xi^c(E_{n,D,k}) \)

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\]

"k term" = \[\begin{cases} 
2D - n + 1 & \text{if } D = 3; \\
3D - n - 3 & \text{if } D \geq 4.
\end{cases}\]
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\{E_{n,3,0}, \ldots, E_{n,3,3}, H_3\} & \text{if } n = 7 \text{ and } D = 3; \\
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[\ldots] & \\
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2. Work out \( f(n, D) = \max_k \xi^c(E_{n,D,k}) \)

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

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

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

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 $P$.
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\[ \| P \| = D \]

\[ \epsilon(u) > L \]
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\[ \|P\| = D \]
\[ d(u, v) = \epsilon(u) > L \]
\( o_i \): 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 $P$)

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

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

\[
\mathcal{W}(V_3^{D-1} \cup V_3^D) \leq (n - D + 1)\left((D - 1)n_3^{D-1} + Dn_3^D\right)
\]

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

\[
B = D(n - D)(n - D - 1 - n_3^{D-1} - n_3^D) + (n - D + 1)\left((D - 1)n_3^{D-1} + Dn_3^D\right) - 2Dr^* + D \min\{1, \rho^*\}
\]

\[
= (n - D - 1)D(n - D) + n_3^{D-1}(2D - n - 1) + Dn_3^D - 2Dr^* + D \min\{1, \rho^*\}.
\]

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 $P$

$$B - \sum_{v \in V_1,2 \cup V_3^D} 2D\rho(v) - \sum_{v \in V_3^{D-1}} (2D - 1)\rho(v) - 2Dn_3^D \leq (n - D - 1)D(n - D) + n_3^{D-1}(2D - n - 1) - Dn_3^D - 2Dr^* + D \min\{1, \rho^*\} - \sum_{v \in V_1,2 \cup V_3^D \cup V_3^{D-1}} (2D - 1)\rho(v).$$

Which is the claim.
Claim (weight on $P$)

$$\xi^c(G) \leq (n - D - 1)D(n - D) + n^{D-1}_3(2D - n - 1) - Dn^D_3 + 2 \sum_{i=0}^{D-1} \delta_i + \sum_{i=0}^{D} \delta_i o_i.$$
Bounding the weight on $P$

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

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

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

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 $C_n^D$

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 $\xi^c$ for a fixed order

Morgan, Mukwembi, and Swart 2011 also gave an asymptotic bound for maximizing $\xi^c$ 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 \( \xi_n^{c*} \) be the largest eccentric connectivity index among all graphs of order \( n \). The only graphs that attain \( \xi_n^{c*} \) are the following:

<table>
<thead>
<tr>
<th>( n )</th>
<th>( \xi_n^{c*} )</th>
<th>( \text{optimal graphs} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>6</td>
<td>( K_3 ) and ( P_3 )</td>
</tr>
<tr>
<td>4</td>
<td>16</td>
<td>( \overline{M}_4 )</td>
</tr>
<tr>
<td>5</td>
<td>30</td>
<td>( \overline{M}_5 ) and ( H_1 )</td>
</tr>
<tr>
<td>6</td>
<td>48</td>
<td>( \overline{M}_6 )</td>
</tr>
<tr>
<td>7</td>
<td>68</td>
<td>( \overline{M}_7 )</td>
</tr>
<tr>
<td>8</td>
<td>96</td>
<td>( \overline{M}<em>8 ) and ( E</em>{8,4,3} )</td>
</tr>
</tbody>
</table>

\[ \geq 9 \quad g(n) \quad E_n, \left\lceil \frac{n+1}{3} \right\rceil + 1, n - \left\lceil \frac{n+1}{3} \right\rceil - 2. \]

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

<table>
<thead>
<tr>
<th>$n$</th>
<th>$p$</th>
<th>optimal graphs</th>
</tr>
</thead>
<tbody>
<tr>
<td>$&gt; 3$</td>
<td>$&gt; 0$</td>
<td>$H_{n,p}$</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>$K_4$</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
<td>$H_{5,0}$, $S_{5,2}$, $K_5$ and $C_1$</td>
</tr>
<tr>
<td>6</td>
<td>0</td>
<td>$S_{6,2}$</td>
</tr>
<tr>
<td>$\geq 7$</td>
<td>0</td>
<td>$H_{n,0}$</td>
</tr>
</tbody>
</table>

\[H_7,3\] \[H_7,2\] \[S_{4,2}\]
Maximizing \( \xi^c \) 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

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

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 \( u_1, u_2, u_3 \).


Appendix
Maximum values of $\xi^c$ for given order $n$ and diameter $D$
Maximum values of $\xi^c$ for given order $n$ and diameter $D$
max $\xi^c$ 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,

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

with equality if and only if $G \simeq \overline{M}_n$, or $n = 5$ and $G \simeq \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc$.
Upper bound on $\xi^c$ for connected graphs with fixed size

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

$n = 7, m = 14$
Upper bound on $\xi^c$ 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.

$n = 7, m = 14$
Upper bound on $\xi^c$ 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 $\xi^c$ 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.

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: \( \xi^c(K_n) = n(n - 1) \)
- 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: \( \xi^c(P_n) = \left\lfloor \frac{3(n-1)^2+1}{2} \right\rfloor \)
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 $G \cong S_n$.

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 $G \in \mathcal{G}_{(n,m)}$.

$\mathcal{G}_{(n,m)}$ 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 $G = K_n$. 