Minimizing the eccentric connectivity index with fixed number of pending vertices

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JGA 2019
We consider simple undirected graphs. Let $v$ be a vertex of a graph $G$, recall that:

- **degree** $d_G(v)$ = number of adjacent vertices of $v$;

**Example**

![Graph diagram with vertices labeled and edges connecting them.](image)

G. Devillez

Minimizing $\xi^c$ with $p$ pending vertices

JGA 2019 1 / 20
We consider simple undirected graphs. Let $v$ be a vertex of a graph $G$, recall that:

- **degree** $d_G(v) =$ number of adjacent vertices of $v$;
- **eccentricity** $\epsilon_G(v) =$ maximal distance between $v$ and any other vertex.

**Example**

![Graph](image)

<table>
<thead>
<tr>
<th>Vertex</th>
<th>Degree</th>
<th>Eccentricity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>$b$</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>$c$</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$d$</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>$e$</td>
<td>1</td>
<td>2</td>
</tr>
</tbody>
</table>
Introduction

We consider simple undirected graphs. Let \( v \) be a vertex of a graph \( G \), recall that:

- **degree** \( d_G(v) \) = number of adjacent vertices of \( v \);
- **eccentricity** \( \epsilon_G(v) \) = maximal distance between \( v \) and any other vertex.

We also define \( w_G(v) = \epsilon_G(v)d_G(v) \).

**Example**

```
   a --- c --- e
   |     |     |
   3/2  4/1  1/2
   b --- d
   2/2
```

G. Devillez
Minimizing \( \xi^c \) with \( p \) pending vertices
JGA 2019
Introduction

For a graph $G = (V, E)$,

- its order $|V|$ is denoted by $n$;
- its number of pending vertices $P = |\{v \in V | d_G(v) = 1\}|$ is denoted by $p$.  

\[ \]
Eccentric Connectivity Index

Definition

The Eccentric Connectivity Index (ECI) of a graph $G$, denoted by $\xi^c(G)$, is

$$\xi^c(G) = \sum_{v \in V} d_G(v) e_G(v) = \sum_{v \in V} w_G(v).$$

Example

$$\xi^c(G) = 3 \times 4 + 2 + 6 = 20$$
Eccentric Connectivity Index

- Introduced by Sharma et al. in 1997 as a novel topological descriptor for molecules.
- Used in studies about anti-inflammatory properties, soil sorption of pesticides, anti-HIV activity of molecules, . . . .
- Not many extremal results about $\xi^c$.
- The first extremal results appears in 2010.
We want to solve the following problem:

**Problem**

*Among all connected graphs with $n$ vertices and $p$ pending vertices, what are the graphs with minimum value of $\xi^c$?*

Note: in this talk, we only consider graphs with $n > 3$ and $p < n - 2$. 
The graphs $H_{n,p}$

**Definition**

We define $H_{n,p}$ as the graph with $n$ vertices and $p$ pending vertices obtained from a star on $n$ vertices by adding a maximal matching between $n - p - 1$ pending vertices. If $n - p - 1$ is odd, we add an edge between one of the remaining pending vertices and a vertex covered by the matching.

**Example**

![Graphs $H_{7,3}$ and $H_{7,2}$](image)
The graphs $H_{n,p}$

We can compute $\xi^c(H_{n,p})$ using the following formulae:

- If $n - p - 1$ is even, $\xi^c(H_{n,p}) = 5n - 2p - 5$
- If $n - p - 1$ is odd, $\xi^c(H_{n,p}) = 5n - 2p - 3$

Note: this doesn’t work if $n = 4$ and $p = 0$ since $H_{4,0}$ has two dominant vertices. In this case, $\xi^c(H_{4,0}) > \xi^c(K_4)$.

\[ \xi^c(H_{4,0}) = 14 \quad \text{and} \quad \xi^c(K_4) = 12 \]
One dominant vertex

At least a star on $n$ vertices.
One dominant vertex

- At least a star on $n$ vertices.
- We keep degrees as small as possible.
One dominant vertex

- At least a star on $n$ vertices.
- We keep degrees as small as possible.
- We might need one additional edge.
One dominant vertex

- At least a star on $n$ vertices.
- We keep degrees as small as possible.
- We might need one additional edge.
- This is $H_{n,p}$. 
With more than one dominant vertex, no pending vertex.

Let $G$ be such a graph:

$$\xi^c(G) \geq (n - 1)x + (n - x)2x = -2x^2 + x(3n - 1)$$

Minimized when $x = 2$ or $x = n$.

$x = 2$:

![Graph $S_{n,2}$](image)

$$\xi^c(G) \geq 6n - 10$$

$x = n$:

![Graph $K_n$](image)

$$\xi^c(G) \geq n^2 - n$$
No dominant vertex

- Let $G = (V, E)$ be a graph with no dominant vertex, can it be as good as a graph with at least one dominant vertex?

- We can show that $\exists u \in V$ such that $d_G(u) = \epsilon_G(u) = 2$

- Let $v$ and $w$ be the neighbors of $u$.

- We first suppose that $v$ is adjacent to $w$.

- Let
  
  - $A = N(v) \setminus N(w) \setminus \{u, w\}$,
  - $C = N(w) \setminus N(v) \setminus \{u, v\}$,
  - $B = N(w) \cap N(v) \setminus \{u\}$,
  - $B' = \{x \in B | d_G(x) = 2\}$,
  - $B'' = B \setminus B'$.
$v$ and $w$ are adjacent

We obtain $G'$ by applying the following transformation:

$$\begin{array}{c}
\text{A} & \text{B} & \text{C} \\
\text{v} & \text{w} & \\
\text{u} & \\
\end{array} \Rightarrow \begin{array}{c}
\text{A} & \text{B} & \text{C} \\
\text{v} & \text{w} & \\
\text{u} & \\
\end{array}$$
$v$ and $w$ are adjacent

We can show that

$$\sum_{z \in A \cup B \cup C \cup \{u\}} w_G(z) \geq \sum_{z \in A \cup B \cup C \cup \{u\}} w_{G'}(z)$$

Thus, to prove that $G$ is not optimal, we have to show that

$$w_G(v) + w_G(w) - w_{G'}(v) - w_{G'}(w) = \alpha - \beta > 0$$
$v$ and $w$ are adjacent

- $w_G(v) = 2(|A| + |B| + 2)$
- $w_G(w) = 2(|B| + |C| + 2)$
- $\alpha = 2|A| + 4|B| + 2|C| + 8$
- $\alpha - \beta = |A| + 3|B| - 2|B'| + |C| + 2 = |A| + |B'| + 3|B''| + |C| + 2 > 0$
- Thus $G$ is not optimal.
v and w are not adjacent

If $A \cup B^\prime$ and $C \cup B^\prime$ are not empty, we obtain $G'$ by applying the following transformation:

$$\begin{align*}
A & \quad B^\prime & \quad B^\prime & \quad C \\
B & \quad v & \quad - & \quad w
\end{align*}$$

$\Rightarrow$

$$\begin{align*}
A & \quad B^\prime & \quad B^\prime & \quad C \\
B & \quad v & \quad w
\end{align*}$$
If \( A \cup B'' \) and \( C \cup B'' \) are not empty, we obtain \( G' \) by applying the following transformation:

![Diagram]

- Just like before, we only need to show that \( \alpha - \beta > 0 \).
- But, \( \alpha - \beta \geq |A| + |B'| + 3|B''| + |C| - 2 \geq 0 \)
When could $G$ be optimal?

$$\alpha - \beta \geq |A| + |B'| + 3|B''| + |C| - 2$$
When could $G$ be optimal?

$$\alpha - \beta \geq |A| + |B'| + 3 |B''| + |C| - 2$$

- The set $B''$ must be empty.
When could $G$ be optimal?

\[ \alpha - \beta \geq |A| + |B'| + 3|B''| + |C| - 2 \]

- The set $B''$ must be empty.
- $B'$ must be empty too.
When could $G$ be optimal?

\[ \alpha - \beta \geq |A| + |B'| + 3|B''| + |C| - 2 \]

- The set $B''$ must be empty.
- $B'$ must be empty too.
- $|A| = |C| = 1$
When could $G$ be optimal?

$$\alpha - \beta \geq |A| + |B'| + 3|B''| + |C| - 2$$

- The set $B''$ must be empty.
- $B'$ must be empty too.
- $|A| = |C| = 1$
- Two possible non-improving situations:

$$\xi^c(P_5) = 24 > \xi^c(H_{5,2}) = 16$$
When could $G$ be optimal?

$$\alpha - \beta \geq |A| + |B'| + 3|B''| + |C| - 2$$

- The set $B''$ must be empty.
- $B'$ must be empty too.
- $|A| = |C| = 1$
- Two possible non-improving situations:

\[\xi^c(C_5) = 20\]

\[\xi^c(K_5) = 20\]
$u$ and $v$ are not adjacent

$A \cup B''$ (or $C \cup B''$) is empty

- If $B'$ is empty, $C$ is not empty since $n > 3$ and $\exists r \in C$ s.t. $d_G(r) \geq 2$ since $p \leq n - 3$.
- We can then apply the following transformation to obtain $G'$:
Changes in $\xi^c$

- $w_G(r) - w_{G'}(r) = 3d_G(r) - 2(d_G(r) + 1) = d_G(r) - 2$
- $\forall z \in C\setminus\{r\}, w_G(z) > w_{G'}(z)$
- There is at least one such vertex $z$ such that $w_G(z) - w_{G'}(z) \geq 2$.
- Thus, $\xi^c(G) - \xi^c(G') \geq 2 - 1 + n - 3 + d_G(r) - 2 + 2 > 0$
  \[\geq 0\] \[\geq 0\]
- And $G$ is not optimal.
$u$ and $v$ are not adjacent

$A \cup B''$ (or $C \cup B''$) is empty

- If $B'$ is not empty, we transform $G$ as follows:

\begin{align*}
\begin{array}{c}
\begin{array}{c}
\begin{array}{c}
\text{Before transformation:}
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\begin{array}{c}
\text{After transformation:}
\end{array}
\end{array}
\end{array}
\end{array}
\end{align*}
Conditions for optimality

- Again, we need to show that $\alpha - \beta > 0$ and again,
  \[ \alpha - \beta \geq 3|B'| + |C| - 4 \geq 0 \]

- For $G$ to be optimal, we need $|B'| = 1$ and $|C| \leq 1$.
- In these situations, the bound is actually too low and $G'$ is still better:
- $|C| = 0$:

![Diagram]

\begin{align*}
16 & > 14
\end{align*}
Conditions for optimality

- Again, we need to show that $\alpha - \beta > 0$ and again,
  \[ \alpha - \beta \geq 3|B'| + |C| - 4 \geq 0 \]

- For $G$ to be optimal, we need $|B'| = 1$ and $|C| \leq 1$.
- In these situations, the bound is actually too low and $G'$ is still better:
  - $|C| = 1 :$

\[
\begin{array}{c}
\begin{array}{c}
|C| = 1 : \quad 23 > 20
\end{array}
\end{array}
\]
Conditions for optimality

- Again, we need to show that \( \alpha - \beta > 0 \) and again,
  \[
  \alpha - \beta \geq 3|B'| + |C| - 4 \geq 0
  \]
- For \( G \) to be optimal, we need \(|B'| = 1\) and \(|C| \leq 1\).
- In these situations, the bound is actually too low and \( G' \) is still better:
- \(|C| = 1:\)

\[
\begin{array}{c}
23 \\
\end{array} \quad > \quad \begin{array}{c}
20 \\
\end{array}
\]

- In this case, \( G \) is again not optimal.
Comparison of results

- When $p > 0$, we saw that only $H_{n,p}$ is optimal.
- When $p = 0$, we can compare the different candidates we found numerically via the formulae:
J. Zhang, Z. Liu, and B. Zhou. 
On the maximal eccentric connectivity indices of graphs. 

Vikas Sharma, Reena Goswami, and AK Madan. 
Eccentric connectivity index: a novel highly discriminating topological descriptor for structure- property and structure- activity studies. 

S Gupta, M Singh, and AK Madan. 
Application of graph theory: Relationship of eccentric connectivity index and wiener’s index with anti-inflammatory activity. 

The graphs $S_{n,2}$

**Definition**

We define $S_{n,2}$ as the graph with $n$ vertices obtained from two adjacent vertices $u$ and $v$ by adding $n - 2$ new vertices only adjacent to $u$ and $v$.

**Example**

![Diagram of $S_{4,2}$]
big values of $p$

- If $p = n - 1$, the graph can only be a star on $n$ vertices.

Example

![Diagram of a star graph with $n$ vertices]
big values of \( p \)

- If \( p = n - 2 \), the only possible graphs are obtained by adding \( n - 2 \) pending vertices randomly between the extremities of an edge with at least one pending vertex on each side.

Example

![Graphs with pending vertices](image.png)
big values of $p$

In the rest of this talk, we suppose $p \leq n - 3$. Note that if $n = 3$, we can only have $p = 0$ which is $K_3$.

We thus also suppose that $n \geq 4$. 
No dominant vertex

- Let $G$ be an extremal graph with no dominant vertex.
- Let $Q \subseteq V$ be the set of vertices of degree 2 and eccentricity 2.
- If $Q = \emptyset$, $G$ is not extremal:
  - Every non-pending vertex $v$ has $d_G(v) \geq 2$ and $\epsilon_G(v) \geq 2$. And $d_G(v) \geq 3$ or $\epsilon_G(v) \geq 3$.
  - Every pending vertex $v$ has $\epsilon_G(v) \geq 3$.
- Thus,

$$\xi^c(G) \geq 6(n - p) + 3p \geq 5n - 2p + 3 > \xi^c(H_{n,p})$$

- And $G$ is not extremal.
- Also true when $n = 4$ and $p = 0$. 
$A \cup B''$ and $C \cup B''$ are not empty

\[ w_G(v) \geq 2(|A| + |B| + 1) \]
\[ w_G(w) \geq 2(|B| + |C| + 1) \]
\[ \alpha \geq 2|A| + 4|B| + 2|C| + 4 \]
\[ \alpha - \beta \geq |A| + 3|B| - 2|B'| + |C| + 2 = |A| + |B'| + 3|B''| + |C| - 2 \]
Changes in $\xi^c$

- $\forall z \in B' \cup C \cup \{u\}, w_G(z) \leq w_{G'}(z)$

- $w_G(v) \geq 2(|B'| + 1)$
- $w_G(w) = 2(|B'| + |C| + 1)$
- $\alpha \geq 4|B'| + 2|C| + 4$
- $\alpha - \beta \geq 3|B'| + |C| - 4$

- $w_{G'}(v) \leq 6$
- $w_{G'}(w) = |B'| + |C| + 2$
- $\beta \leq |B'| + |C| + 8$
Comparison of results

We have the following results:

- If $p > 0$, $H_{n,p}$ is the extremal graph.
- If $n = 4$ and $p = 0$, the extremal graph is $K_4$.
- If $n = 5$ and $p = 0$, there are four extremal graphs: $K_5$, $H_{5,0}$, $C_5$ and $S_{5,2}$.
- If $n = 6$ and $p = 0$, the extremal graph is $S_{n,2}$. 
## Bounds for connected graphs

<table>
<thead>
<tr>
<th>Invariant(s)</th>
<th>Lower bound</th>
<th>Upper bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>—</td>
<td>✓</td>
<td>✗</td>
</tr>
<tr>
<td>$m$ (size)</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>$D$ (diameter)</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>$p$ (number of pending vertices)</td>
<td>✓</td>
<td>✗</td>
</tr>
<tr>
<td>$\delta$ (minimum degree)</td>
<td>✗</td>
<td>✓</td>
</tr>
<tr>
<td>$D$ (diameter) and $m$ (size)</td>
<td>✓ (with conditions on $m$ and $D$)</td>
<td></td>
</tr>
<tr>
<td>$D'$ (degree distance)</td>
<td>✓</td>
<td>✗</td>
</tr>
<tr>
<td>$M_1$ (Zagreb index) and $m$</td>
<td>✗</td>
<td>✓</td>
</tr>
<tr>
<td>$W$ (Wiener index)</td>
<td>✗</td>
<td>✓</td>
</tr>
</tbody>
</table>
### Bounds for trees

<table>
<thead>
<tr>
<th>Invariant(s)</th>
<th>Lower bound</th>
<th>Upper bound</th>
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<tbody>
<tr>
<td>_</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td><strong>D</strong> (diameter)</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td><strong>r</strong> (radius)</td>
<td>X</td>
<td>✓</td>
</tr>
<tr>
<td><strong>p</strong> (number of pending vertices)</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td><strong>Δ</strong> (maximum degree)</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td><strong>β</strong> (matching number)</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td><strong>α</strong> (stability number)</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td><strong>W</strong> (Wiener index)</td>
<td>X</td>
<td>✓</td>
</tr>
</tbody>
</table>
**Bounds for other graph classes**

**Unicyclic graphs**

<table>
<thead>
<tr>
<th>Invariant(s)</th>
<th>Lower bound</th>
<th>Upper bound</th>
</tr>
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<tbody>
<tr>
<td>—</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>g (girth)</td>
<td>✓</td>
<td>✓</td>
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</table>

**Bicyclic graphs**

<table>
<thead>
<tr>
<th>Invariant(s)</th>
<th>Lower bound</th>
<th>Upper bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>—</td>
<td>✓</td>
<td>X</td>
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**k-regular graphs**

<table>
<thead>
<tr>
<th>Invariant(s)</th>
<th>Lower bound</th>
<th>Upper bound</th>
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</thead>
<tbody>
<tr>
<td>k ≥ 3 fixed</td>
<td>✓</td>
<td>✓</td>
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