PHOEG Helps Obtaining Extremal Graphs

Pierre Hauweele
Joint work with Gauvain Devillez and Hadrien Mélot

Algorithms Lab, Computer Science Departement
Faculty of Sciences, University of Mons

UMONS

CSD8, Mons, August 23, 2017
Introduction

We consider simple undirected graphs.

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

- its order $|V|$ is denoted by $n$;
- its size $|E|$ is denoted by $m$.

A graph invariant is a function on graphs that is constant on isomorphism classes.

Examples: order $n$, size $m$, chromatic number $\chi$, maximum degree $\Delta$, diameter $D$, planarity, ...
Extremal Graph Theory aims to find bounds on a graph invariant under some constraints. Generally, those constraints are of two types:

- restricting class of graphs (e.g., connected graphs, trees);
- fixing (and restricting) values of other invariants (e.g., size, maximum degree).

Results in Extremal Graph Theory mainly consists in

- giving bounds;
- characterizing graphs achieving these bounds.
Computer-assisted discovery

- **Context**: Computer-assisted Discovery in Extremal Graph Theory
- **Several existing systems**: Graph, Graffiti, AutoGraphiX, GraPHedron, ...
  - exploit different ideas to help graph theorists
- **Objectives of this talk**:
  - presentation of PHOEG, a successor of GraPHedron
  - use of an illustrative problem (Eccentric Connectivity Index, ECI)
- **Remark**: work in progress
  - PHOEG is currently a prototype
  - the problem about ECI is not fully solved
Overview of PHOEG

PHOEG

CoreLib
- Representation of graphs
- Invariants computation
- Various tools

Forbidden subGraph Characterization

Invariants Database
- Convex Hull Computation
- Using PostGIS

Relational Database - PostgreSQL

Transproof
- Graph transformations
- Graph Database - Neo4J

P. Hauweele — UMONS

PHOEG Helps Obtaining Extremal Graphs

CSD8 – 2017
Eccentric Connectivity Index

Let \( v \) be a vertex of a graph \( G \), recall that:
- **degree** \( d(v) \) = number of adjacent vertices of \( v \);
- **eccentricity** \( \epsilon(v) \) = maximal distance between \( v \) and any other vertex.

**Example**

```
<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
</tr>
</tbody>
</table>
```

```
<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
</tr>
</tbody>
</table>
```
Eccentric Connectivity Index

Definition

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

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

Example

\[
\begin{array}{c|c}
3 & 1 \\
\end{array}
\]

\[
\begin{array}{c|c|c}
2 & 2 & \text{2 | 2} \\
\end{array}
\]

\[
\begin{array}{c|c|c}
3 & 1 & \text{3 | 1} \\
\end{array}
\]

\[
\begin{array}{c}
\text{b} \\
\end{array}
\]

\[
\begin{array}{c}
\text{a} \\
\end{array}
\]

\[
\begin{array}{c}
\text{c} \\
\end{array}
\]

\[
\begin{array}{c}
\text{d} \\
\end{array}
\]

$$\xi^c(G) = (2 \times 2 + 3 \times 1) \times 2 = 14$$
Eccentric Connectivity Index

History and motivation

- 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.
- 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 $\xi^c$. 
Some Extremal Theory problem about $\xi^c$

Now, let’s make extremal graph theory about $\xi^c$ with the help of a computer.

First step: define a problem by choosing constraints.
Some Extremal Theory problem about $\xi^c$

Now, let’s make extremal graph theory about $\xi^c$ with the help of a computer.

First step: define a problem by choosing constraints.

Several papers containing bounds on $\xi^c$ — using various invariants as constraints — have been published (since 2010).
Some Extremal Theory problem about $\xi^c$

Now, let’s make extremal graph theory about $\xi^c$ with the help of a computer.

**First step**: define a problem by choosing constraints.

Several papers containing bounds on $\xi^c$ — using various invariants as constraints — have been published (since 2010).

**Problem**

Among connected graphs of order $n$ and size $m$, what is the maximum possible value for $\xi^c$?
Upper bound on $\xi^c$ for connected graphs with fixed size

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

$$\begin{align*}
    n &= 7, \\
    m &= 14
\end{align*}$$
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.

$n = 7, m = 14$

![Graph Diagram]
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 $E_{n,m}$.

$n = 7, m = 14$
Conjecture of Zhang, Liu and Zhou

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).
- There exists a “proof” published in a journal of University of Isfahan (Iran, 2014) but that is obviously wrong.
Conjecture of Zhang, Liu and Zhou

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 $G \cong E_{n,m}$.

- Is the conjecture true?
- If yes, how to prove it?
- If no, how to improve or correct it?
- What about graphs such that $d_{n,m} < 3$?
How can the computer help?

In the following, we will show how PHOEG can help to study all of the preceding questions and to raise new ones.

PHOEG Helps Obtaining Extremal Graphs
PHOEG — the database part

- Former system (GraPHedron): graphs and invariant's values written sequentially in files;
- PHOEG uses a PostgreSQL DB with tens of millions of non-isomorphic graphs and invariants’ values;
- Invariant’s values are computed once (useful for NP-hard invariants);
Database of the invariants

- Each graph has its unique signature used as primary key (canonical form, thanks to Nauty by Brendan McKay), $\text{sig}(C_5) = "DqK"$, $\text{sig}(K_3) = "Bw"$.
- 12 millions simple graphs up to order 10, 8 millions cubic graphs up to order 22.

<table>
<thead>
<tr>
<th>Graphs signature</th>
<th>NumVertices signature</th>
<th>NumVertices val</th>
<th>NumEdges signature</th>
<th>NumEdges val</th>
<th>ECI signature</th>
<th>ECI val</th>
</tr>
</thead>
<tbody>
<tr>
<td>A_</td>
<td>A_</td>
<td>2</td>
<td>A_</td>
<td>1</td>
<td>A_</td>
<td>2</td>
</tr>
<tr>
<td>A?</td>
<td>A?</td>
<td>2</td>
<td>A?</td>
<td>0</td>
<td>BW</td>
<td>6</td>
</tr>
<tr>
<td>B?</td>
<td>B?</td>
<td>3</td>
<td>B?</td>
<td>0</td>
<td>Bw</td>
<td>6</td>
</tr>
<tr>
<td>BG</td>
<td>BG</td>
<td>3</td>
<td>BG</td>
<td>1</td>
<td>C~</td>
<td>14</td>
</tr>
<tr>
<td>Bw</td>
<td>Bw</td>
<td>3</td>
<td>BW</td>
<td>2</td>
<td>CF</td>
<td>9</td>
</tr>
<tr>
<td>BW</td>
<td>BW</td>
<td>3</td>
<td>BW</td>
<td>2</td>
<td>CN</td>
<td>13</td>
</tr>
<tr>
<td>C'</td>
<td>C'</td>
<td>4</td>
<td>C'</td>
<td>2</td>
<td>Cr</td>
<td>16</td>
</tr>
<tr>
<td>C~</td>
<td>C~</td>
<td>4</td>
<td>C~</td>
<td>5</td>
<td>CR</td>
<td>14</td>
</tr>
<tr>
<td>C?</td>
<td>C?</td>
<td>4</td>
<td>C?</td>
<td>0</td>
<td>D' [</td>
<td>25</td>
</tr>
<tr>
<td>C@</td>
<td>C@</td>
<td>4</td>
<td>C@</td>
<td>1</td>
<td>D' {</td>
<td>20</td>
</tr>
</tbody>
</table>
GraPHedron’s main principle

- view graphs as points in the space of invariants;

Polytope for $n = 7$
GraPHedron’s main principle

- view graphs as points in the space of invariants;
- compute the convex hull of these points (for small values of $n$).

Polytope for $n = 7$
SELECT P.val AS eci, num_edges.val AS m, COUNT(*) AS mult
FROM eci P
JOIN num_vertices USING(signature)
JOIN num_edges USING(signature)
WHERE num_vertices.val = 7
GROUP BY m, eci;

<table>
<thead>
<tr>
<th>eci</th>
<th>m</th>
<th>mult</th>
</tr>
</thead>
<tbody>
<tr>
<td>47</td>
<td>8</td>
<td>5</td>
</tr>
<tr>
<td>46</td>
<td>8</td>
<td>3</td>
</tr>
<tr>
<td>40</td>
<td>8</td>
<td>3</td>
</tr>
<tr>
<td>32</td>
<td>7</td>
<td>3</td>
</tr>
<tr>
<td>48</td>
<td>12</td>
<td>55</td>
</tr>
<tr>
<td>48</td>
<td>18</td>
<td>1</td>
</tr>
<tr>
<td>61</td>
<td>14</td>
<td>4</td>
</tr>
<tr>
<td>59</td>
<td>13</td>
<td>1</td>
</tr>
<tr>
<td>48</td>
<td>11</td>
<td>17</td>
</tr>
</tbody>
</table>

SELECT ST_AsText(ST_ConvexHull(ST_Collect(ST_Point(eci, m))))
FROM poly;

<table>
<thead>
<tr>
<th>st_astext</th>
</tr>
</thead>
<tbody>
<tr>
<td>POLYGON((18 6, 42 21, 66 18, 68 17, 66 11, 62 8, 54 6, 18 6))</td>
</tr>
</tbody>
</table>

[...]
Exploring $\xi^c$ with PHOEG: polytopes

Polytope for $n = 5$
Exploring $\xi^c$ with PHOEG: polytopes

Polytope for $n = 6$
Exploring $\xi^c$ with PHOEG: polytopes

Polytope for $n = 7$
Exploring $\xi^c$ with PHOEG: polytopes

Polytope for $n = 8$
Exploring $\xi^c$ with PHOEG: polytopes

Polytope for $n = 9$
Exploring $\xi^c$ with PHOEG: polytopes

Polytope for $n = 10$
Observations and questions

- How to explain the grid?
- Is the conjecture of Zhang, Liu and Zhou true when $d_{n,m} \geq 3$?
- Upper bound when $d_{n,m} < 3$?
### Database query – Polytope with some other information

```sql
SELECT num_edges.val AS m, 
    p.val AS eci, d.val AS d, 
    diam.val AS diam 
FROM eci p 
    JOIN num_vertices USING(signature) 
    JOIN num_edges USING(signature) 
    JOIN d USING(signature) 
    JOIN diam USING(signature) 
WHERE num_vertices.val = 7 
ORDER BY diam, d, m, eci;
```

<table>
<thead>
<tr>
<th>m</th>
<th>eci</th>
<th>d</th>
<th>diam</th>
</tr>
</thead>
<tbody>
<tr>
<td>21</td>
<td>42</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>16</td>
<td>46</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>16</td>
<td>52</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>16</td>
<td>52</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>16</td>
<td>52</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>16</td>
<td>52</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>16</td>
<td>52</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>16</td>
<td>52</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>16</td>
<td>52</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>16</td>
<td>52</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>16</td>
<td>52</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>16</td>
<td>52</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>16</td>
<td>52</td>
<td>2</td>
<td>2</td>
</tr>
</tbody>
</table>

[...]

P. Hauweele — UMONS

PHOEG Helps Obtaining Extremal Graphs

CSD8 – 2017 19 / 34
Recall that the conjecture is stated for $d_{n,m} \geq 3$. Is it true for $n = 7$?
WITH tmp AS (  
    SELECT n.val AS n, m.val AS m,  
        P.signature, P.val AS eci, d.val AS d,  
        rank() OVER (  
            PARTITION BY n.val, m.val  
            ORDER BY P.val DESC  
        ) AS pos  
    FROM num_vertices n  
    JOIN num_edges m USING(signature)  
    JOIN d USING(signature)  
    JOIN eci P USING(signature)  
    WHERE n.val = 7  
)  
SELECT signature AS sig, n, m, eci, d  
FROM tmp  
WHERE pos = 1 AND d >= 3  
ORDER BY n, m, d, eci;

<table>
<thead>
<tr>
<th>sig</th>
<th>n</th>
<th>m</th>
<th>eci</th>
<th>d</th>
</tr>
</thead>
<tbody>
<tr>
<td>F@IQO</td>
<td>7</td>
<td>6</td>
<td>54</td>
<td>6</td>
</tr>
<tr>
<td>F@‘J_</td>
<td>7</td>
<td>7</td>
<td>57</td>
<td>5</td>
</tr>
<tr>
<td>FgCXW</td>
<td>7</td>
<td>8</td>
<td>62</td>
<td>5</td>
</tr>
<tr>
<td>FWCYw</td>
<td>7</td>
<td>9</td>
<td>62</td>
<td>4</td>
</tr>
<tr>
<td>FgCwxw</td>
<td>7</td>
<td>10</td>
<td>64</td>
<td>4</td>
</tr>
<tr>
<td>F‘Kyw</td>
<td>7</td>
<td>11</td>
<td>66</td>
<td>4</td>
</tr>
<tr>
<td>F‘Kzw</td>
<td>7</td>
<td>12</td>
<td>65</td>
<td>3</td>
</tr>
<tr>
<td>F‘Lzw</td>
<td>7</td>
<td>13</td>
<td>65</td>
<td>3</td>
</tr>
<tr>
<td>F‘\zw</td>
<td>7</td>
<td>14</td>
<td>65</td>
<td>3</td>
</tr>
<tr>
<td>FJ]\w</td>
<td>7</td>
<td>15</td>
<td>65</td>
<td>3</td>
</tr>
<tr>
<td>FJ\w</td>
<td>7</td>
<td>15</td>
<td>65</td>
<td>3</td>
</tr>
</tbody>
</table>
WITH tmp AS (  
    SELECT n.val AS n, m.val AS m,  
          P.signature, P.val AS eci, d.val AS d,  
          rank() OVER (  
            PARTITION BY n.val, m.val  
            ORDER BY P.val DESC  
          ) AS pos  
    FROM num_vertices n  
    JOIN num_edges m USING(signature)  
    JOIN d USING(signature)  
    JOIN eci P USING(signature)  
    WHERE n.val = 7  
  )  
SELECT signature AS sig, n, m, eci, d  
FROM tmp  
WHERE pos = 1 AND d >= 3  
ORDER BY n, m, d, eci;

<table>
<thead>
<tr>
<th>sig</th>
<th>n</th>
<th>m</th>
<th>eci</th>
<th>d</th>
</tr>
</thead>
<tbody>
<tr>
<td>F@IQO</td>
<td>7</td>
<td>6</td>
<td>54</td>
<td>6</td>
</tr>
<tr>
<td>F@‘J_</td>
<td>7</td>
<td>7</td>
<td>57</td>
<td>5</td>
</tr>
<tr>
<td>FgCXW</td>
<td>7</td>
<td>8</td>
<td>62</td>
<td>5</td>
</tr>
<tr>
<td>FWCYw</td>
<td>7</td>
<td>9</td>
<td>62</td>
<td>4</td>
</tr>
<tr>
<td>FgCwxw</td>
<td>7</td>
<td>10</td>
<td>64</td>
<td>4</td>
</tr>
<tr>
<td>F‘Kyw</td>
<td>7</td>
<td>11</td>
<td>66</td>
<td>4</td>
</tr>
<tr>
<td>F‘Kzw</td>
<td>7</td>
<td>12</td>
<td>65</td>
<td>3</td>
</tr>
<tr>
<td>F‘Lzw</td>
<td>7</td>
<td>13</td>
<td>65</td>
<td>3</td>
</tr>
<tr>
<td>F‘\zw</td>
<td>7</td>
<td>14</td>
<td>65</td>
<td>3</td>
</tr>
<tr>
<td>FJ|w</td>
<td>7</td>
<td>15</td>
<td>65</td>
<td>3</td>
</tr>
</tbody>
</table>

⇒ counter-example to the conjecture!  
Extremal graphs are not always unique
Counter-example \((n = 7 \text{ and } m = 15)\)
Counter-example \((n = 7 \text{ and } m = 15)\)
Counter-example ($n = 7$ and $m = 15$)

It is possible to construct counter-examples for any values of $n \geq 6$ (with $d_{n,m} = 3$).
Coloring points with values of $d_{n,m}$

Polytope for $n = 7$ with values for $d_{n,m}$

Upper bound when $d_{n,m} < 3$?
Upper facet of the polytope \((n = 7)\)
Coloring points with values of the diameter

Polytope for $n = 7$ with values for diameter $D$

Can the diameter explain the blue grid? Actually, yes!
Coloring points with values of the diameter

Polytope for $n = 7$ with values for diameter $D$

Can the diameter explain the blue grid? Actually, yes!
A new tight upper bound when $d_{n,m} < 3$

**Theorem**

Let $G$ be a graph of order $n$ and size $m$. Then,

$$\xi^c(G) \leq n(n-1)(n-2) - 2m(n-3),$$

with equality if and only if $G$ is the complement of a matching.

Note that the bound is valid for all graphs but can be tight only if

$$m \geq \binom{n}{2} - \left\lfloor \frac{n}{2} \right\rfloor,$$

(and thus $d_{n,m} < 3$).
We note $P(G, k)$ the number of non-equivalent colorings of $G$ that use exactly $k$ colors.

$P(P_3, 2) = 1$

$P(P_3, 3) = 1$
Total number of non-equivalent colorings

Definition

The total number of non-equivalent colorings $\mathcal{P}(G)$ of a graph $G$ is

$$\mathcal{P}(G) = \sum_{k=0}^{n} P(G, k) = \sum_{k=\chi(G)}^{n} P(G, k),$$

where $\chi(G)$ is the chromatic number of $G$.

Example: $\mathcal{P}(P_3) = P(P_3, 2) + P(P_3, 3) = 1 + 1 = 2$

$\mathcal{P}(G)$ is the value of the $\sigma$-polynomial when $x = 1$ and is also known as the Bell number of a graph [Duncan & Peele, 2009].
### Problem

What is minimum possible value of $P$ for graphs of fixed order $n$ and size $m$ and what are the graphs attaining those bounds?
Some extremal graphs

\[(n, m) = (5, 4)\]

\[(n, m) = (5, 4)\]

\[(n, m) = (5, 5)\]

\[(n, m) = (5, 6)\]

\[(n, m) = (6, 10)\]

\[(n, m) = (6, 11)\]

\[(n, m) = (6, 12)\]

\[(n, m) = (6, 13)\]

\[(n, m) = (8, 15)\]

\[(n, m) = (8, 16)\]

\[(n, m) = (8, 16)\]

\[(n, m) = (8, 17)\]
The extremal(?) graphs

Given \( n \) the order and \( m \) the size of graphs. Let \( t_k \) be the biggest triangular number such that \( t_k \leq m \). We call \( r_m = m - t_k \) the remainder.

We define \( G^*(n, m) \) as the unique graph formed from \( K_{k+1} \cup \overline{K}_{n-k-1} \), where one (if any) vertex of \( \overline{K}_{n-k-1} \) is connected to \( r_m \) vertices of the clique.

If \( r_m = 1 \), and \( n - k - 1 \geq 2 \), we define \( G'(n, m) \) as \( K_{k+1} \cup \overline{K}_{n-k-1} \), where two vertices of \( K_{k+1} \cup \overline{K}_{n-k-1} \) are connected.
Forbidden Graph Characterization

In this tool, we want a necessary and sufficient characterization of our graphs.

\[ S_1 \quad S_2 \quad S_3 \quad S_4 \quad S_5 \quad S_6 \quad S_7 \]
Concluding remarks

- Not only extremal graphs are useful to study extremal properties of an invariant
- Exact approach limited to small graphs \((n \leq 10)\)
- However, dealing with small graphs has already shown to be very useful and led to numerous results (AutoGraphiX, GraPHedron)
Perspectives

- Invariants’ DB allows a form of dynamic programming;
- Create a simple interface for queries, define a domain specific language;
- Allow easy visualization and manipulation of outputs (GUI, PDF, etc.);
- Go up in the order of graphs, relaxing the exact constraint.
Appendix
Understanding the grid of blue points

- Suppose $D(G) = 2$ (light blue points)
- For each vertex $v$, since $D(G) = 2$, either $\epsilon(v) = 1$ or $\epsilon(v) = 2$
- If $\epsilon(v) = 1$, then $v$ is dominant and $d(v) = n - 1$
- Let $k$ be the number of dominant vertices of $G$
- The sum of degrees of non dominant vertices is $2m - k(n - 1)$

Thus,

$$\xi^c(G) = k(n - 1) + 2(2m - k(n - 1)) = 4m - k(n - 1),$$

that is maximum if $k = 0$ and, moreover, explain the grid.
Upper bound on $\xi^c$ for connected graphs with fixed size

**Definition**

For positive integers $n$ and $m$ with $n - 1 \leq m \leq \binom{n}{2}$, let

$$d_{n,m} = \left\lfloor \frac{2n + 1 - \sqrt{17 + 8(m - n)}}{2} \right\rfloor.$$  

In the following, we simply use $d$ for $d_{n,m}$.

**Definition**

Let $E_{n,m}$ be the graph obtained from a clique $K_{n-d-1}$ and a path $P_{d+1} = v_0v_1\ldots v_d$ by joining each vertex of the clique to both $v_d$ and $v_{d-1}$, and by joining

$$m - n + 1 - \binom{n - d}{2}$$

vertices of the clique to $v_{d-2}$.
Upper bound on $\xi^c$ for connected graphs with fixed size

Example ($n = 5$)

<table>
<thead>
<tr>
<th>$m$</th>
<th>$4$</th>
<th>$5$</th>
<th>$6$</th>
<th>$7$</th>
<th>$8$</th>
<th>$9$</th>
<th>$10$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d$</td>
<td>$4$</td>
<td>$3$</td>
<td>$3$</td>
<td>$2$</td>
<td>$2$</td>
<td>$2$</td>
<td>$1$</td>
</tr>
<tr>
<td>$n - d - 1$</td>
<td>$0$</td>
<td>$1$</td>
<td>$1$</td>
<td>$2$</td>
<td>$2$</td>
<td>$2$</td>
<td>$3$</td>
</tr>
<tr>
<td>$#$ edges to $v_{d-2}$</td>
<td>$0$</td>
<td>$0$</td>
<td>$1$</td>
<td>$0$</td>
<td>$1$</td>
<td>$2$</td>
<td>$0$</td>
</tr>
</tbody>
</table>

![Graph diagram]
**Upper bound on** $\xi^c$ **for connected graphs with fixed size**

**Example** ($n = 5$)

<table>
<thead>
<tr>
<th>$m$</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d$</td>
<td>4</td>
<td>3</td>
<td>3</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>$n - d - 1$</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td># edges to $v_{d-2}$</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>0</td>
</tr>
</tbody>
</table>

Diagram:

- A blue circle connected to four red circles.
- The red circles are arranged in a line with one circle connected to the first and fourth circle, and another circle connected to the second and third circle.
Upper bound on $\xi^c$ for connected graphs with fixed size

Example ($n = 5$)

<table>
<thead>
<tr>
<th>$m$</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d$</td>
<td>4</td>
<td>3</td>
<td>3</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>$n - d - 1$</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>$#$ edges to $v_{d-2}$</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>0</td>
</tr>
</tbody>
</table>

![Diagram of a graph with 5 vertices and edges connecting them]
Upper bound on $\xi^c$ for connected graphs with fixed size

Example ($n = 5$)

<table>
<thead>
<tr>
<th>$m$</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d$</td>
<td>4</td>
<td>3</td>
<td>3</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>$n - d - 1$</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td># edges to $v_{d-2}$</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>0</td>
</tr>
</tbody>
</table>

Diagram:

![Graph diagram](image-url)
Upper bound on $\xi^c$ for connected graphs with fixed size

Example ($n = 5$)

<table>
<thead>
<tr>
<th>$m$</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d$</td>
<td>4</td>
<td>3</td>
<td>3</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>$n - d - 1$</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td># edges to $v_{d-2}$</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>0</td>
</tr>
</tbody>
</table>

Diagram: A graph with nodes labeled and connections showing the number of edges to each node.
Upper bound on $\xi^c$ for connected graphs with fixed size

Example ($n = 5$)

<table>
<thead>
<tr>
<th>$m$</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d$</td>
<td>4</td>
<td>3</td>
<td>3</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>$n - d - 1$</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td># edges to $v_{d-2}$</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>0</td>
</tr>
</tbody>
</table>
Upper bound on $\xi^c$ for connected graphs with fixed size

Example ($n = 5$)

<table>
<thead>
<tr>
<th>$m$</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d$</td>
<td>4</td>
<td>3</td>
<td>3</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>$n - d - 1$</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td># edges to $v_{d-2}$</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>0</td>
</tr>
</tbody>
</table>

Diagram of a connected graph with $n = 5$ vertices.
What about other classes of graphs?

Let’s try to maximize $\xi^c$ on cubic (3-regular) graphs.

```sql
SELECT t.n, t.signature, t.eci
FROM (SELECT n.val AS n, eci.signature, eci.val as eci,
       DENSE_RANK() OVER (PARTITION BY n.val
                     ORDER BY eci.val DESC
       ) AS pos
    FROM cubic
    JOIN num_vertices n USING(signature)
    JOIN eccentric_connectivity_index eci USING(signature)
  ) t
WHERE t.pos = 1
ORDER BY t.n;
```
Maximize $\xi^c$ on cubic graphs

<table>
<thead>
<tr>
<th>n</th>
<th>signature</th>
<th>eci</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>C~</td>
<td>12</td>
</tr>
<tr>
<td>6</td>
<td>Es\o</td>
<td>36</td>
</tr>
<tr>
<td>6</td>
<td>E{Sw</td>
<td>36</td>
</tr>
<tr>
<td>8</td>
<td>Gv?IXW</td>
<td>72</td>
</tr>
<tr>
<td>8</td>
<td>Gs@ipo</td>
<td>72</td>
</tr>
<tr>
<td>10</td>
<td>Iv?GOKFY?</td>
<td>126</td>
</tr>
<tr>
<td>12</td>
<td>Kt?GOKFOAOeA</td>
<td>177</td>
</tr>
<tr>
<td>14</td>
<td>Mt?GO?@_KgKOWM??</td>
<td>270</td>
</tr>
</tbody>
</table>