PHOEG Helps Obtaining Extremal Graphs

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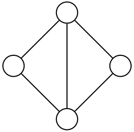
Introduction

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 χ, maximum degree Δ, diameter D, planarity, ...

Extremal Graph Theory

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).

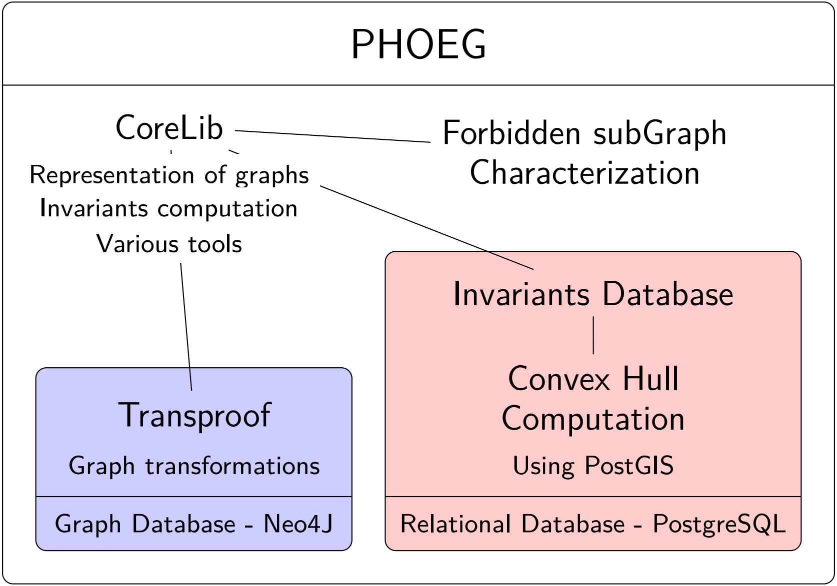
Results in Extremal Graph Theory mainly consists in

- 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

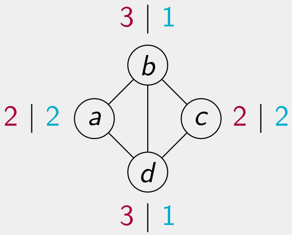


Eccentric Connectivity Index

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



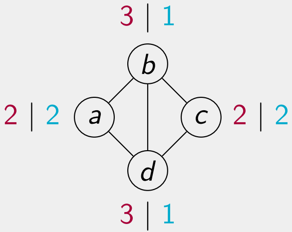
Eccentric Connectivity Index

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



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

Eccentric Connectivity Index

History and motivation

- 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.

Some Extremal Theory problem about ξ^c

Now, let's make extremal graph theory about ξ^c with the help of a computer.

First step: define a problem by choosing constraints.

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

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Problem

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

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

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

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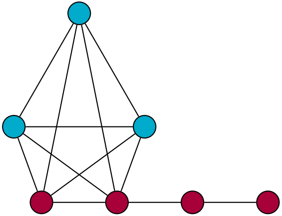

Upper bound on ξ^c for connected graphs with fixed size

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

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- Add remaining edges between vertices of the clique and the first vertex of the path.

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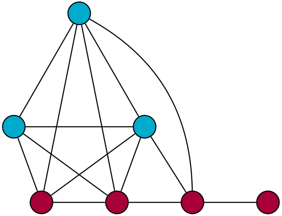

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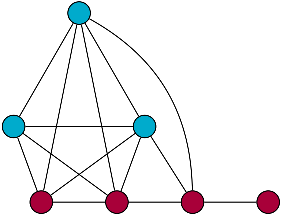

This graph is unique for given n and m. We define $d_{n,m}$ as the diameter of $E_{n,m}$.

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

- The authors prove that the conjecture is true when $m = n - 1, n, \ldots, n + 4$ (if n is large enough).
- There exists a "proof" published in a journal of University of Isfahan (Iran, 2014) but that is obviously wrong.

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

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

- 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.

P 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), $sig(C_5) = "DqK"$, $sig(K_3) = "Bw"$.
- 12 millions simple graphs up to order 10, 8 millions cubic graphs up to order 22.

Graphs
signature
A_
A?
B?
BG
Bw
BW
C`
C^
C~
C?
C@

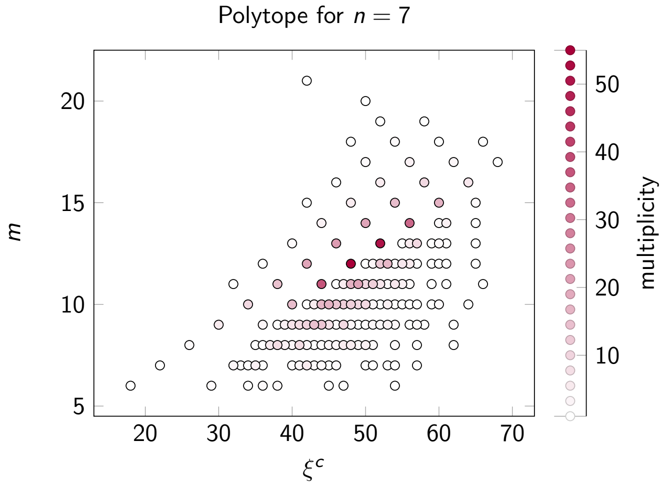
NumVertices	
signature	val
A_	2
A?	2
B?	3
BG	3
Bw	3
BW	3
C`	4
C^	4
C~	4
C?	4
C@	4

NumEdges	
signature	val
A_	1
A?	0
B?	0
BG	1
Bw	3
BW	2
C`	2
C^	5
C~	6
C?	0
C@	1

ECI	
signature	val
A_	2
BW	6
Bw	6
C^	14
C~	12
CF	9
CN	13
Cr	16
CR	14
D`[	25
D`{	20

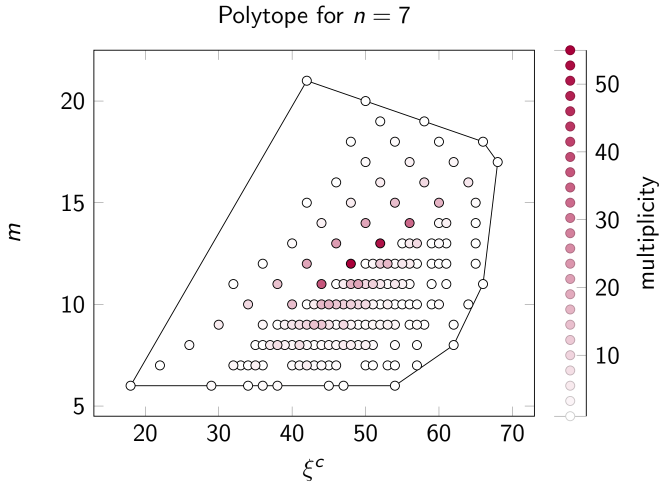
GraPHedron's main principle

- view graphs as points in the space of invariants;



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).



Database query – Points, multiplicities and polytope

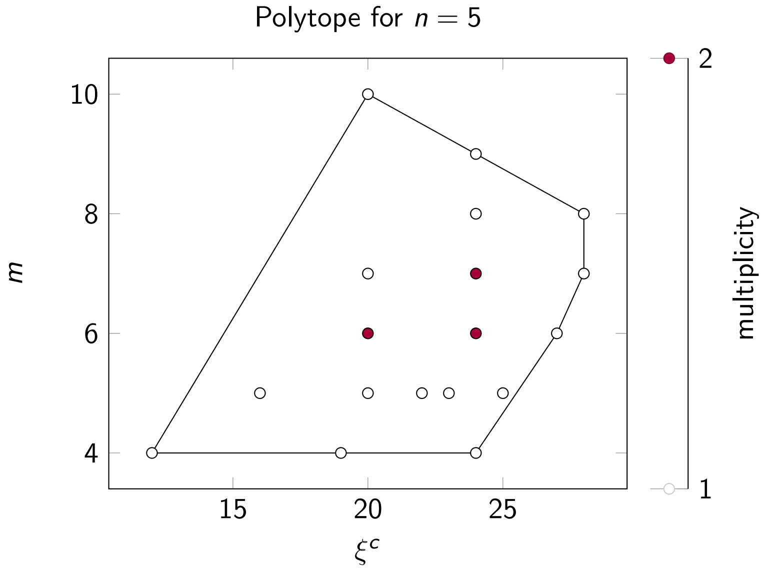
```
SELECT P.val AS eci, num_edges.val AS m,
  COUNT(*) AS mult
FROM eci P
  JOIN num_vertices USING(signature)
  JOIN num_edges USING(signature)
WHERE num_vertices.val = 7
GROUP BY m, eci;
```

```
 eci | m  | mult
-----+----+------
  47 |  8 |    5
  46 |  8 |    3
  40 |  8 |    3
  32 |  7 |    3
  48 | 12 |   55
  48 | 18 |    1
  61 | 14 |    4
  59 | 13 |    1
  48 | 11 |   17
  43 |  9 |   14
  47 |  6 |    1
  64 | 10 |    1
  59 | 11 |    1
  45 |  9 |    7
  38 |  6 |    2
         [...]
```

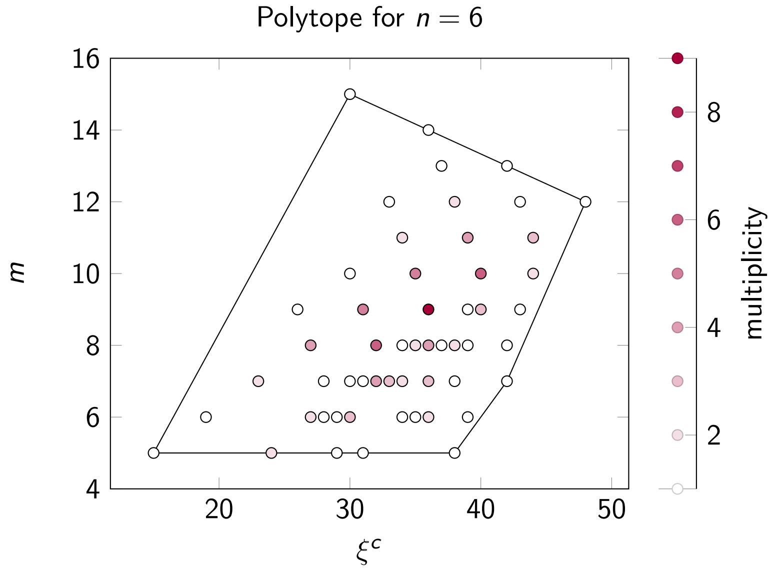
```
SELECT ST_AsText(ST_ConvexHull(
  ST_Collect(ST_Point(eci, m))))
FROM poly;
```

```
                     st_astext
-----------------------------------------------------------
 POLYGON((18 6,42 21,66 18,68 17,66 11,62 8,54 6,18 6))
```

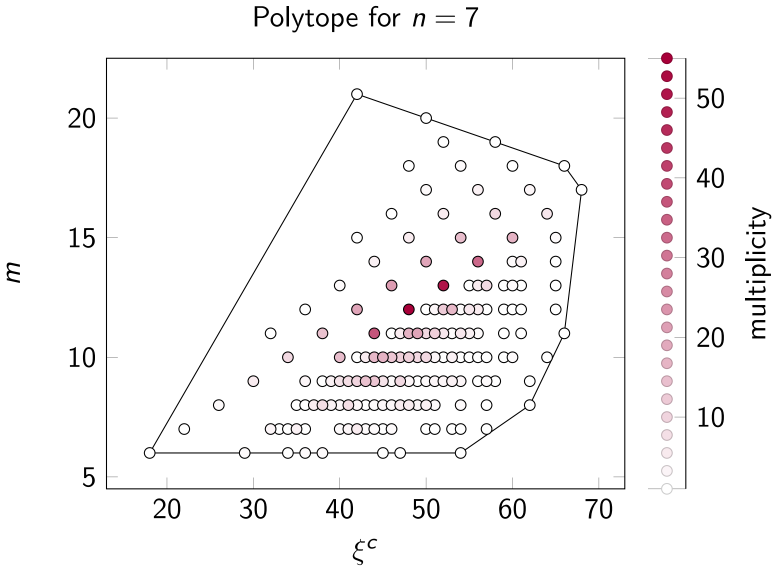
Exploring ξ^c with PHOEG: polytopes



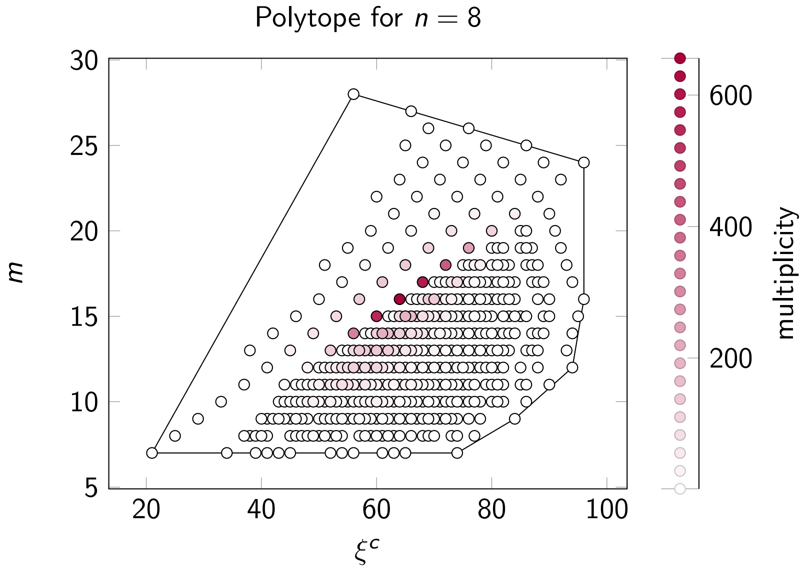
Exploring ξ^c with PHOEG: polytopes



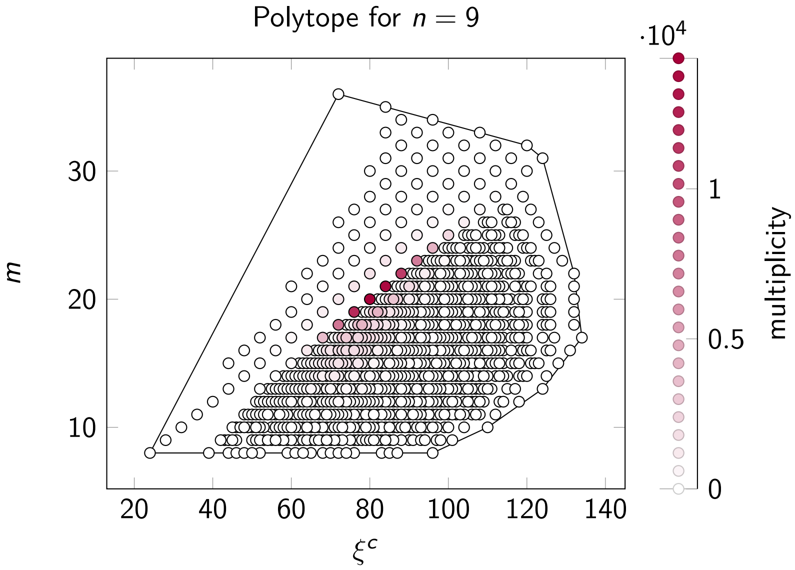
Exploring ξ^c with PHOEG: polytopes



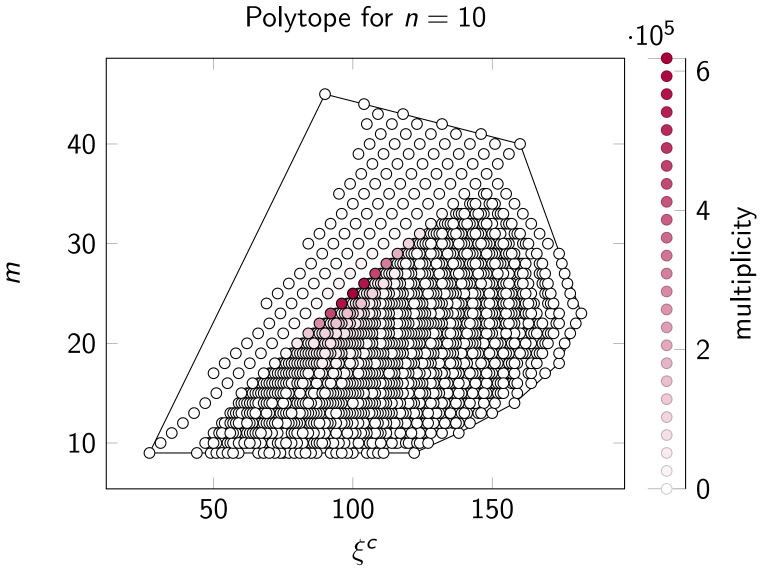
Exploring ξ^c with PHOEG: polytopes



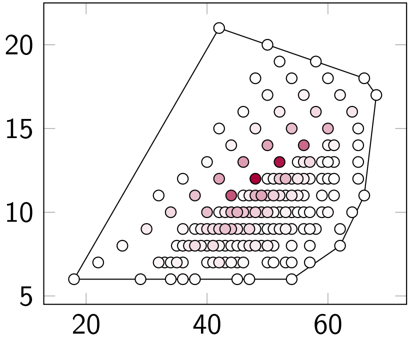
Exploring ξ^c with PHOEG: polytopes



Exploring ξ^c with PHOEG: polytopes



Observations and questions



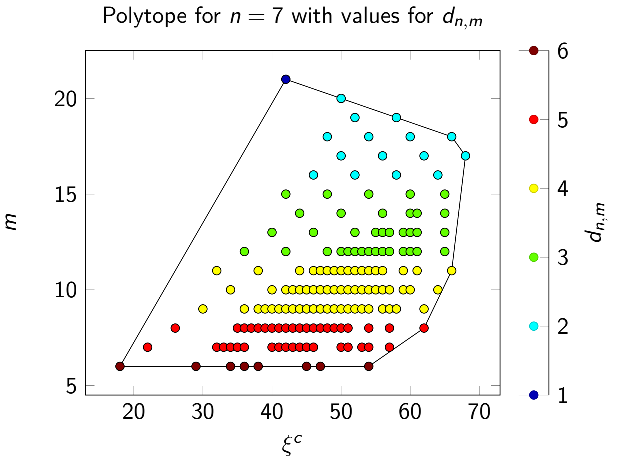
- How to explain the grid?
- Is the conjecture of Zhang, Liu and Zhou true when $d_{n,m} \geq 3$?
- Upper bound when $d_{n,m} < 3$?

Database query – Polytope with some other information

```
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;
```

```
m   | eci | d | diam
---+-----+---+------
21 |  42 | 1 |    1
16 |  46 | 2 |    2
16 |  52 | 2 |    2
16 |  52 | 2 |    2
16 |  52 | 2 |    2
16 |  52 | 2 |    2
16 |  52 | 2 |    2
16 |  58 | 2 |    2
16 |  58 | 2 |    2
16 |  58 | 2 |    2
16 |  58 | 2 |    2
16 |  58 | 2 |    2
16 |  58 | 2 |    2
16 |  58 | 2 |    2
16 |  58 | 2 |    2
           [...]
```

Coloring points with values of $d_{n,m}$



Recall that the conjecture is stated for $d_{n,m} \geq 3$. Is it true for $n = 7$?

Database query – Extremal graphs

```
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;
```

```
 sig   | n | m  | eci | d
-------+---+----+-----+----
F@IQO  | 7 |  6 |  54 | 6
F@`J_  | 7 |  7 |  57 | 5
FgCXW  | 7 |  8 |  62 | 5
FWCYw  | 7 |  9 |  62 | 4
FgCxw  | 7 | 10 |  64 | 4
F`Kyw  | 7 | 11 |  66 | 4
F`Kzw  | 7 | 12 |  65 | 3
F`Lzw  | 7 | 13 |  65 | 3
F`\zw  | 7 | 14 |  65 | 3
FJ]|w  | 7 | 15 |  65 | 3
FJ\|w  | 7 | 15 |  65 | 3
```

Database query – Extremal graphs

```
WITH tmp AS (
  SELECT n.val AS n, m.val AS m,
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    rank() OVER (
      PARTITION BY n.val, m.val
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  JOIN eci P USING(signature)
  WHERE n.val = 7
)
SELECT signature AS sig, n, m, eci, d
FROM tmp
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ORDER BY n, m, d, eci;
```
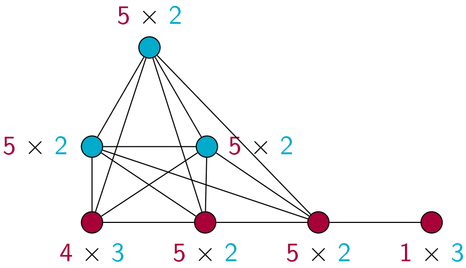
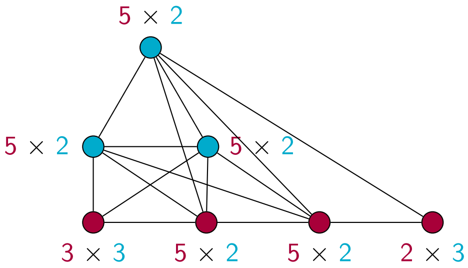

```
 sig   | n | m  | eci | d
-------+---+----+-----+----
F@IQO  | 7 |  6 |  54 | 6
F@‘J_  | 7 |  7 |  57 | 5
FgCXW  | 7 |  8 |  62 | 5
FWCYw  | 7 |  9 |  62 | 4
FgCxw  | 7 | 10 |  64 | 4
F‘Kyw  | 7 | 11 |  66 | 4
F‘Kzw  | 7 | 12 |  65 | 3
F‘Lzw  | 7 | 13 |  65 | 3
F‘\zw  | 7 | 14 |  65 | 3
FJ]|w  | 7 | 15 |  65 | 3
FJ\|w  | 7 | 15 |  65 | 3
```

⇒ counter-example to the conjecture !
Extremal graphs are not always unique

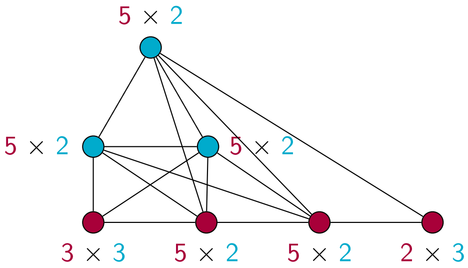
Counter-example ($n = 7$ and $m = 15$)



Counter-example ($n = 7$ and $m = 15$)

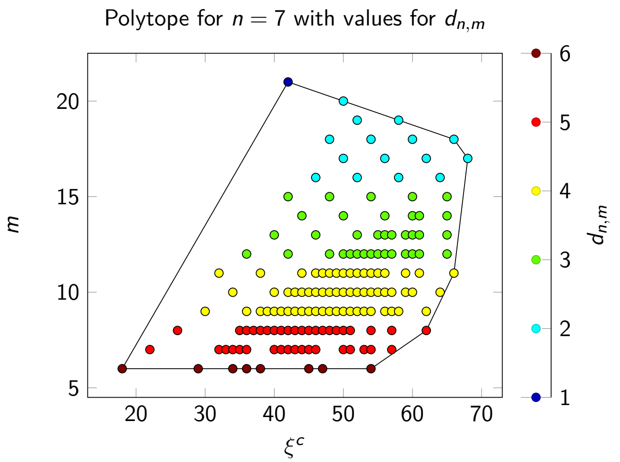


Counter-example ($n = 7$ and $m = 15$)



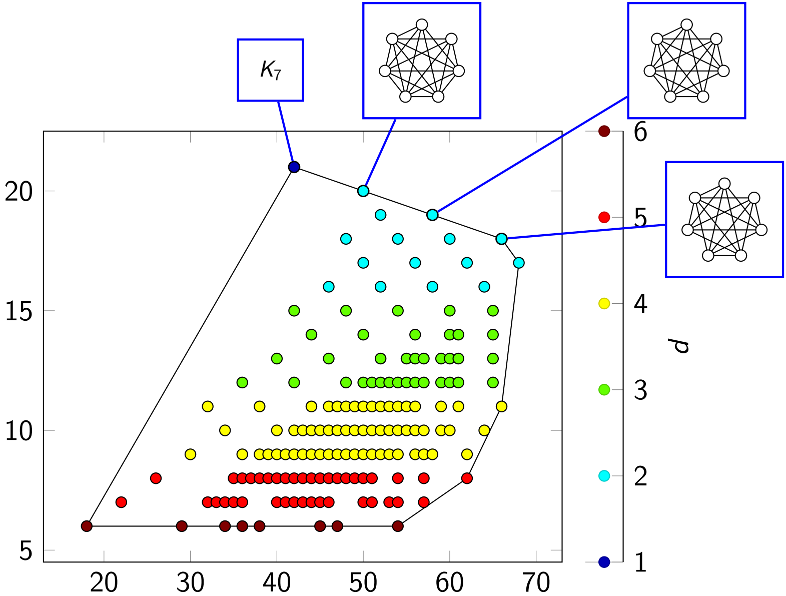
It is possible to construct counter-examples for any values of $n \geq 6$ (with $d_{n,m} = 3$).

Coloring points with values of $d_{n,m}$

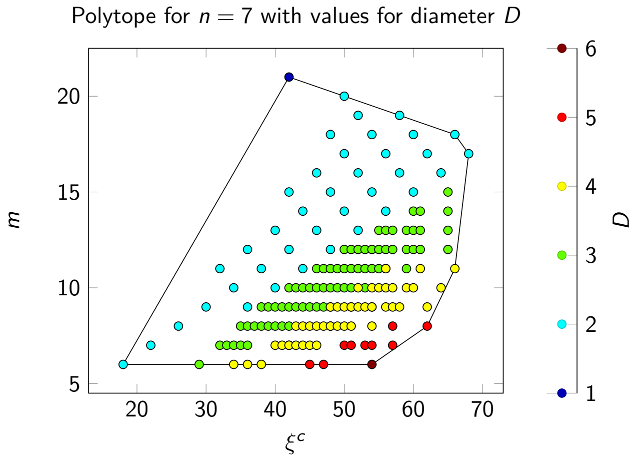


Upper bound when $d_{n,m} < 3$?

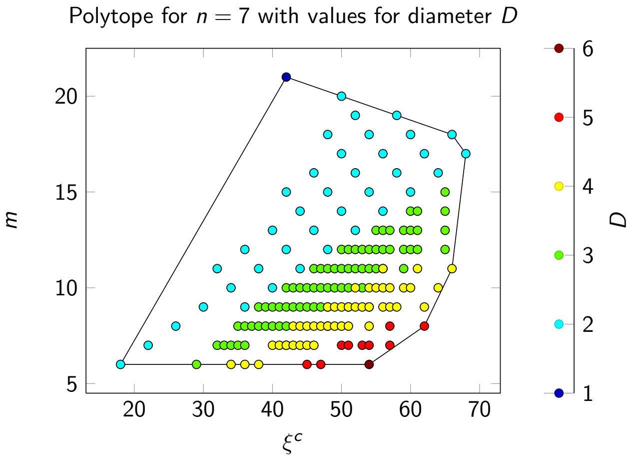
Upper facet of the polytope ($n = 7$)



Coloring points with values of the diameter



Coloring points with values of the diameter



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 $d_{n,m} < 3$).

Number of non-equivalent colorings

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

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

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

Example: $\mathcal{P}(\mathrm{P}_3) = \mathrm{P}(\mathrm{P}_3, 2) + \mathrm{P}(\mathrm{P}_3, 3) = 1 + 1 = 2$

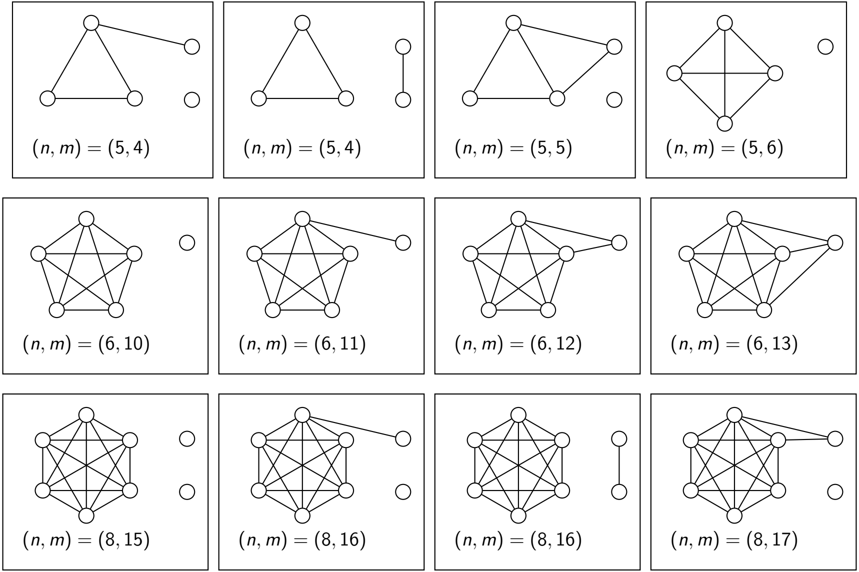
$\mathcal{P}(G)$ is the value of the σ-polynomial when $x = 1$ and is also known as the Bell number of a graph [Duncan & Peele, 2009].

The Min-NumCol-NumEdges Problem

Problem

What is minimum possible value of $\mathcal{P}$ for graphs of fixed order n and size m and what are the graphs attaining those bounds ?

Some extremal graphs



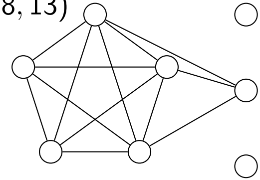
The extremal(?) graphs

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.

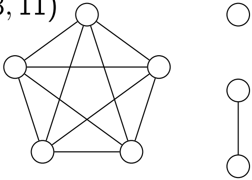
We define $G^*(n, m)$ as the unique graph formed from $K_{k+1} \bigcup \overline{K}_{n-k-1}$, where one (if any) vertex of $\overline{K}_{n-k-1}$ is connected to r_m vertices of the clique.

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

$G^*(8, 13)$

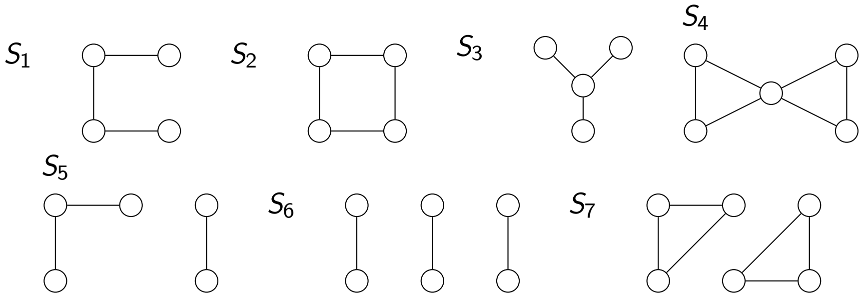


$G'(8, 11)$



Forbidden Graph Characterization

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



Concluding remarks

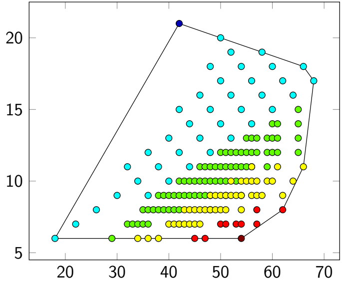
- Not only extremal graphs are useful to study extremal properties of an invariant
- Exact approach limited to small graphs ($n \leq 10$)
- However, dealing with small graphs has already shown to be very useful and led to numerous results (AutoGraphiX, GraPHedron)

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 ξ^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 $P_{d+1} = v_0 v_1 \ldots v_d$ 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 ξ^c for connected graphs with fixed size

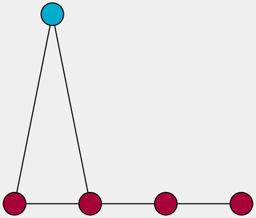
Example ($n = 5$)

m	**4**	5	6	7	8	9	10
d	**4**	3	3	2	2	2	1
$n - d - 1$	**0**	1	1	2	2	2	3
# edges to v_{d-2}	**0**	0	1	0	1	2	0

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

Example ($n = 5$)

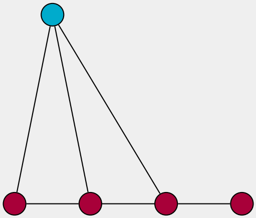
m	4	**5**	6	7	8	9	10
d	4	**3**	3	2	2	2	1
$n-d-1$	0	**1**	1	2	2	2	3
# edges to v_{d-2}	0	**0**	1	0	1	2	0



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

Example ($n = 5$)

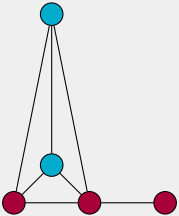
m	4	5	**6**	7	8	9	10
d	4	3	**3**	2	2	2	1
$n - d - 1$	0	1	**1**	2	2	2	3
# edges to v_{d-2}	0	0	**1**	0	1	2	0



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

Example ($n = 5$)

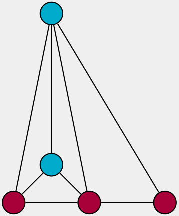
m	4	5	6	**7**	8	9	10
d	4	3	3	**2**	2	2	1
$n - d - 1$	0	1	1	**2**	2	2	3
# edges to v_{d-2}	0	0	1	**0**	1	2	0



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

Example ($n = 5$)

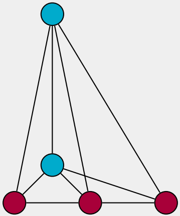
m	4	5	6	7	**8**	9	10
d	4	3	3	2	**2**	2	1
$n - d - 1$	0	1	1	2	**2**	2	3
# edges to v_{d-2}	0	0	1	0	**1**	2	0



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

Example ($n = 5$)

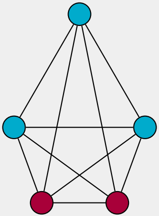
m	4	5	6	7	8	**9**	10
d	4	3	3	2	2	**2**	1
$n - d - 1$	0	1	1	2	2	**2**	3
# edges to v_{d-2}	0	0	1	0	1	**2**	0



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

Example ($n = 5$)

m	4	5	6	7	8	9	**10**
d	4	3	3	2	2	2	**1**
$n - d - 1$	0	1	1	2	2	2	**3**
# edges to v_{d-2}	0	0	1	0	1	2	**0**



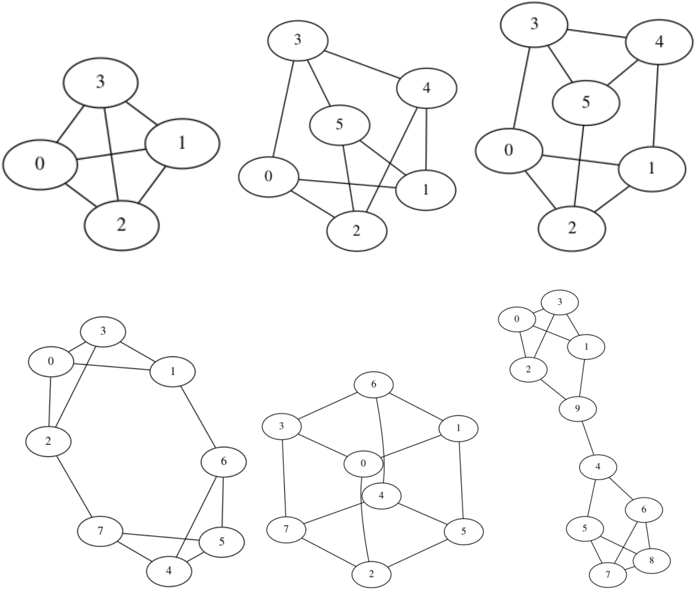
What about other classes of graphs ?

Let's try to maximize ξ^c on cubic (3-regular) graphs.

```
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 ξ^c on cubic graphs

n	signature	eci
4	C~	12
6	Es\o	36
6	E{Sw	36
8	Gv?IXW	72
8	Gs@ipo	72
10	Iv?GOKFY?	126
12	Kt?GOKFOAOeA	177
14	Mt?GO?@@_KgKOWM??	270
16	Ot?G?CA?WB`oO?O?b_@?E	348
18	Qv??W[K?G??@?B?B?A??`G?p??o	474
20	Sv?GW?@?W??@?B????G?J??w?w?M?BO??	573
22	Uv?G?CK?oE@_?H?E??G?C??C??W?@??@C_?KO??o	726


3 0 1 2
3 4 5 0 1 2
3 4 5 0 1 2
3 0 1 2 6 7 5 4
6 3 1 0 4 7 5 2
3 0 1 2 9 4 6 5 8 7