PHOEG Helps Obtaining Extremal Graphs

Hadrien Mélot

Joint work with Gauvain Devillez and Pierre Hauweele

Service d'Algorithmique, Département d'Informatique

Faculté des Sciences, Université de Mons

UMONS

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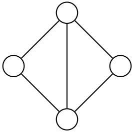
Introduction

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.

Introduction

- 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 under progress
  - PHOEG is currently a prototype
  - the problem about ECI is not fully solved

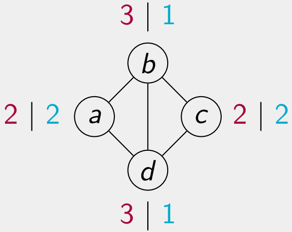
Eccentric Connectivity Index

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



$$\xi^c(G) = 2 \times (4 + 3) = 14$$

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

Problem

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

(To avoid infinite eccentricities, we restrict the problem to connected graph)

Graphs $E_{n,m}$

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

$$n = 7, m = 14$$

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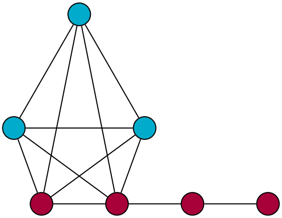
- The biggest possible clique without disconnecting the graph, leaving a path with the remaining vertices.

$n = 7, m = 14$



Graphs $E_{n,m}$

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

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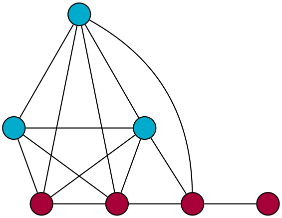

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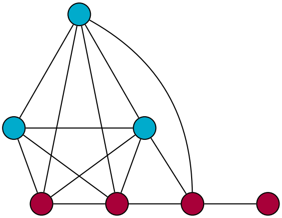


This graph is unique for given n and m.

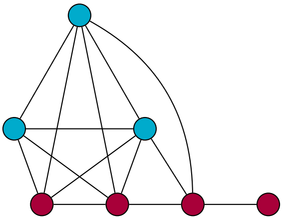
Graphs $E_{n,m}$

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

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

Remarks :

- In the following, we simply use d for $d_{n,m}$;
- d is decreasing when m increase (and n fixed);
- For $E_{n,m}$, d is its diameter.



Conjecture of Zhang, Liu and Zhou

Conjecture (Zhang, Liu and Zhou, 2014)

Let G be a connected graph of order n and size m such that $d \geq 3$. 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 exists a "proof" published in a journal of University of Isfahan (Iran, 2014) but that is obviously wrong.

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This conjecture leads to several questions:

- Is the conjecture true?
- If yes, how to prove it?
- If no, how to improve or correct it?
- What about graphs such that $d \leq 2$?

How the computer can help?

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

P $\quad$ H$_{\text{elps}}$ $\quad$ O$_{\text{btaining}}$ E$_{\text{xtremal}}$ G$_{\text{raphs}}$

Overview of PHOEG

- Former system (GraPHedron): graphs and invariant's values written sequentially in files;
- PHOEG uses a PostgreSQL DB with more than 12 millions of non-isomorphic graphs (up to order 10) and tables of corresponding invariants' values;
- Invariant's values are computed once (useful for NP-hard invariants);
- Each graph has its unique signature used as primary key (canonical form, thanks to Nauty)
- This allows complex (and fast) queries on graphs.

Database query – Points and multiplicities

```
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
     [...]
```

Database query – Polytope

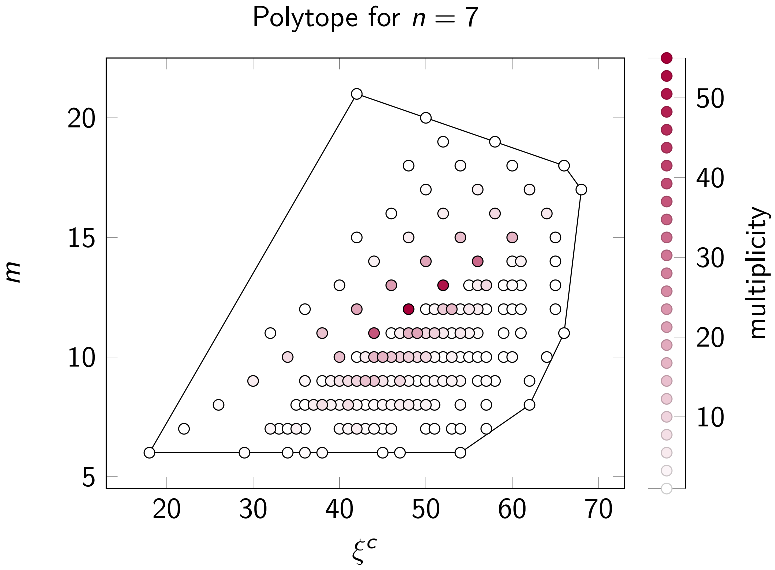
Main principle:

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

```
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



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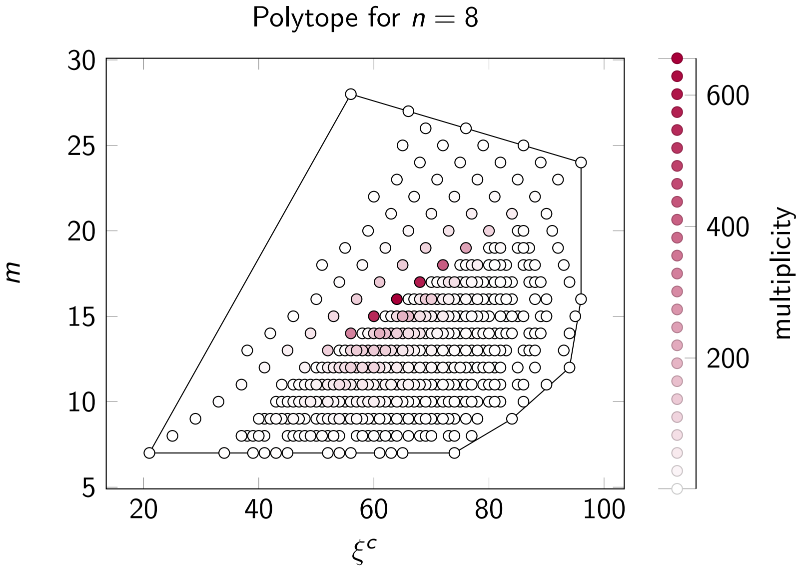

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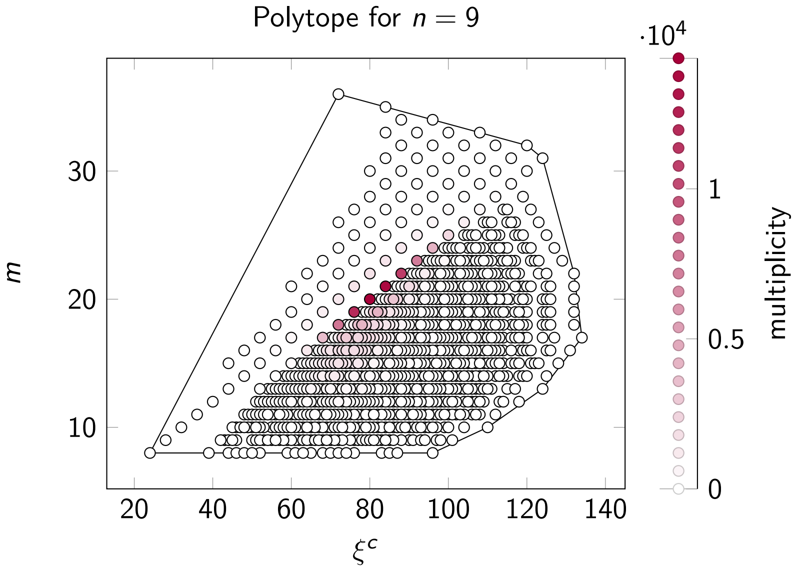

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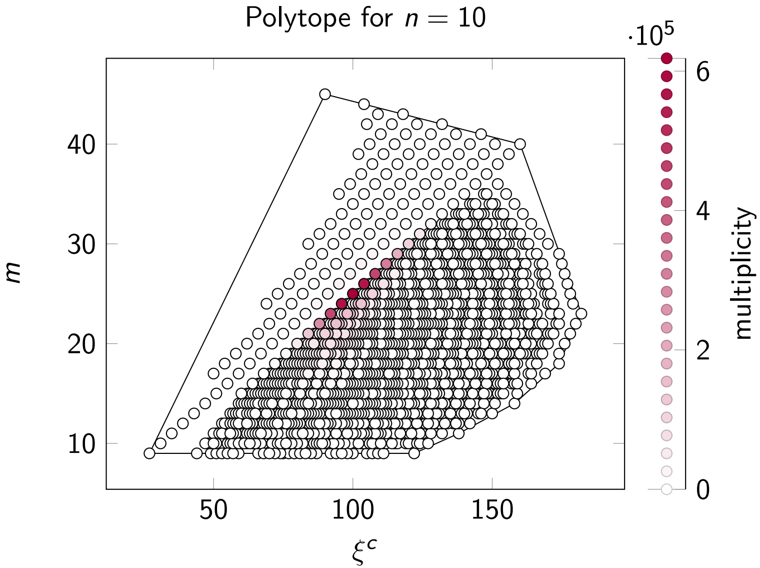
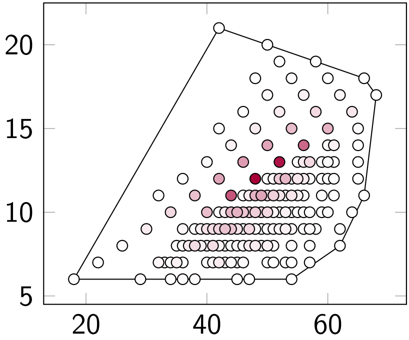


Observations and questions



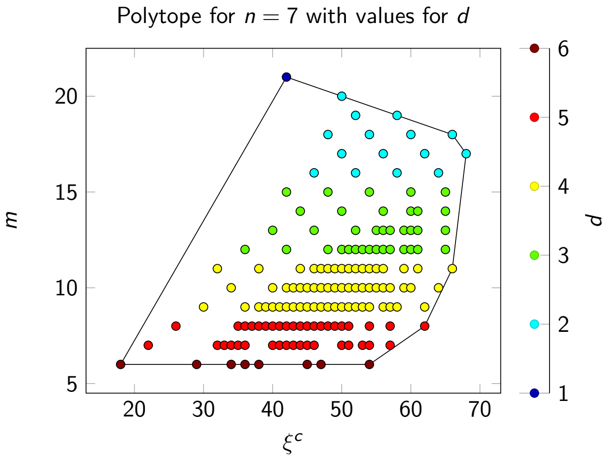
- Is the conjecture of Zhang, Liu and Zhou true when $d \geq 3$?
- Upper bound when $d \leq 2$?
- How to explain the grid?

Database query – adding 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



Is the conjecture true for $d \geq 3$?

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
```

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WITH tmp AS (
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```
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-------+---+----+-----+----
 F@IQO | 7 |  6 |  54 | 6
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 FWCYw | 7 |  9 |  62 | 4
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 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
```
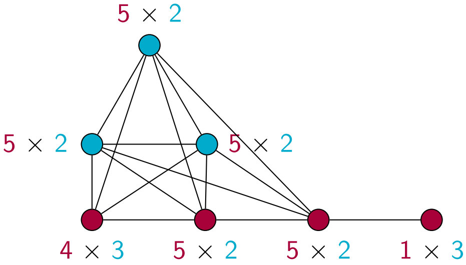

Counter-example to the conjecture: no unicity for extremal graphs

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



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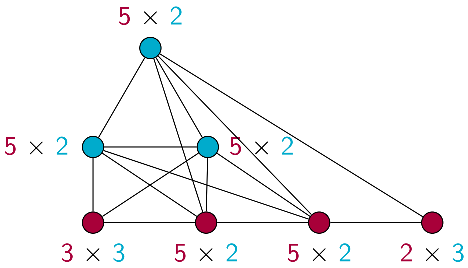

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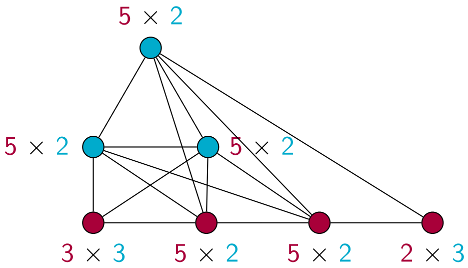
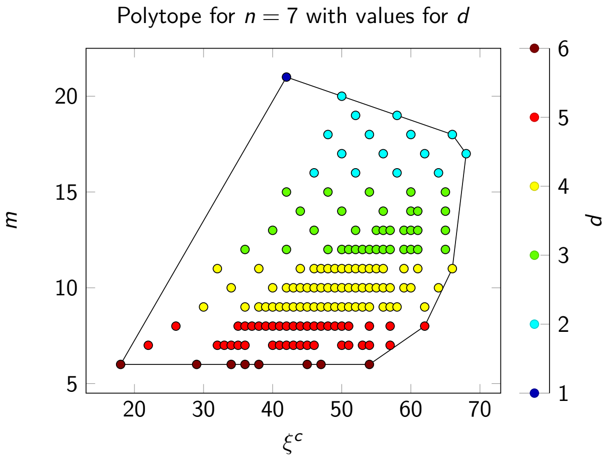


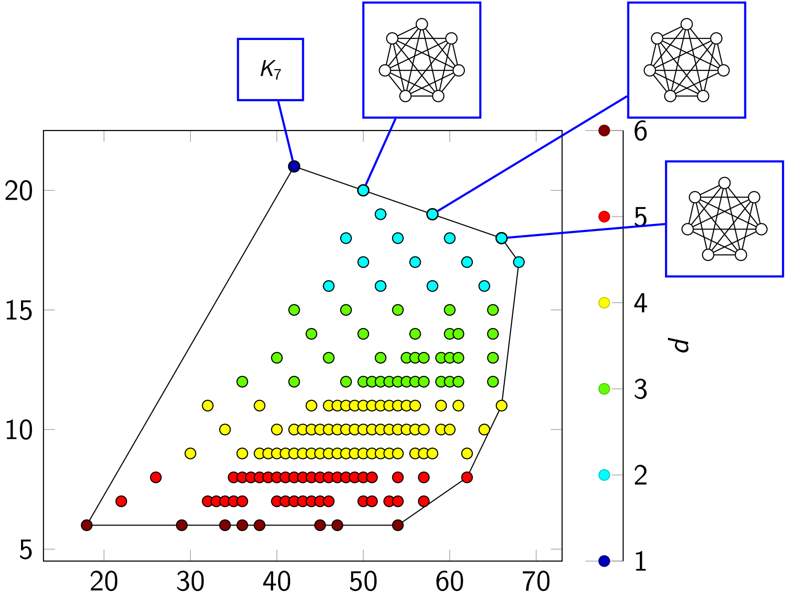
It is possible to construct counter-examples for any values of $n \geq 6$ (with $d = 3$).

Coloring points with values of d



Upper bound when $d \leq 2$?

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



A new upper bound tight when $d \leq 2$

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 $d \leq 2$).

PHOEG – Transproof

Up to this point, we have

- a tight upper bound when $d \leq 2$;
- and counter-examples for the unicity if $d = 3$.

It is also possible to have an explanation of the grid using PHOEG (skipped).

Is the conjecture true if $d \geq 4$? (actually, we believe it is).

If yes, is PHOEG able to help for a proof?

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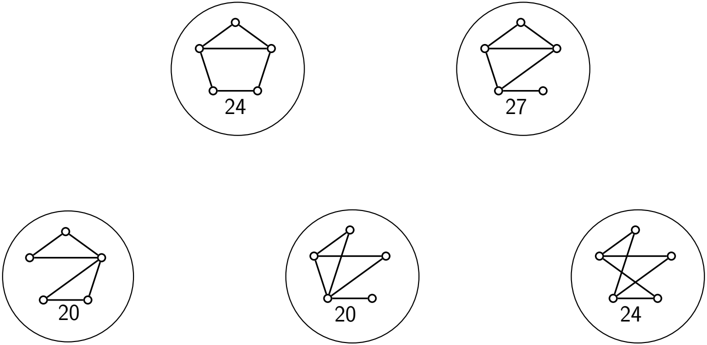
This is the purpose of the *Transproof* module:

- using graph transformations is a common proof technique;
- not always easy to find "good" transformations.

Metagraph of rotations that increase ξ^c ($n = 5$ and $m = 6$)



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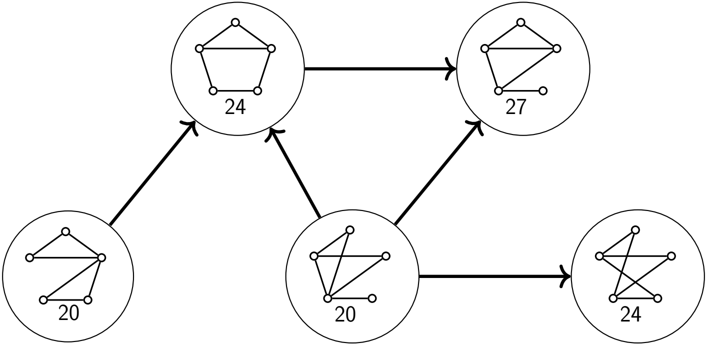


Applying only one rotation is thus not sufficient to have a proof.

Metagraph of transformations

- Idea : find an "improving path" from any graph to an extremal graph
- Metagraph stored in a graph DB (*Neo4j*)
  - for all graphs up to order 9
  - using 8 simple transformations
  - $\rightarrow$ for $n = 9$, it makes a metagraph of order 274 668 and size 380 814 904
- Useful to reject / find good transformations while searching for a proof

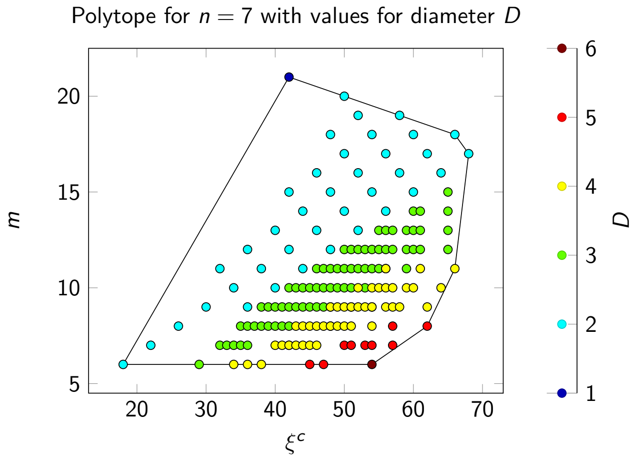
Concluding remarks

- 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)
- PHOEG is intended to be an ecosystem of useful modules (e.g., Forbidden Subgraph Characterization)

Perspectives

- Invariants' DB allows a form of dynamic programming
- Create a simple interface for queries
- Allow easy visualization and manipulation of outputs (GUI, PDF, etc.)
- Simplify the definitions of transformations
- Suggest automatically (a short list of) transformations

Coloring points with highest diameter



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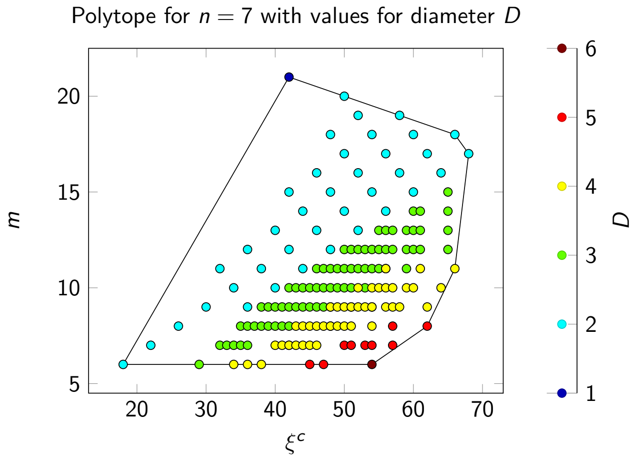
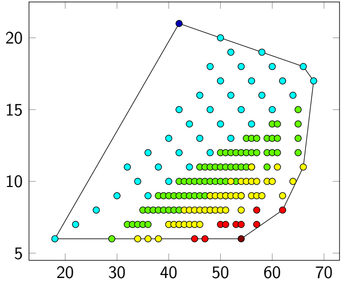


Can the diameter explain the blue grid? Actually, yes!

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 $\epsilon(v) = 2$

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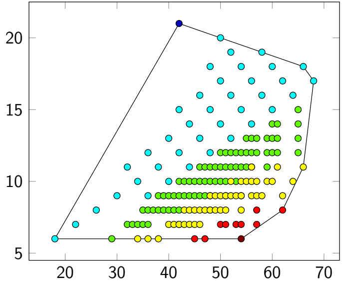

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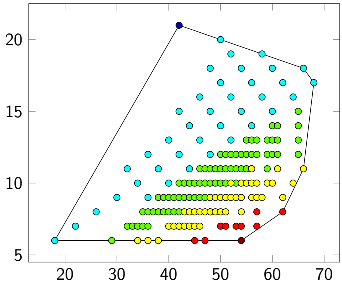

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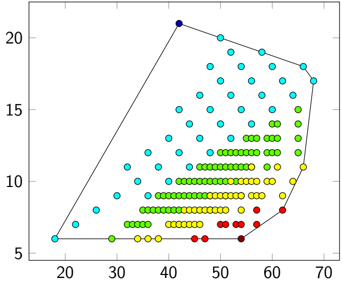

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- The sum of degrees of non dominant vertices is

$$2m - k(n-1)$$

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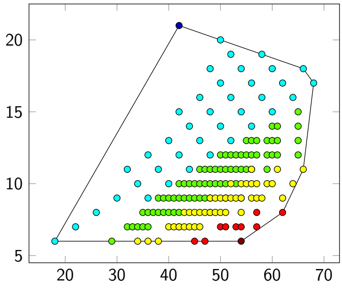

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Thus,

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

that is maximum if $k = 0$ and, moreover, explain the grid.