Lower bounds on the maximal number of realizations

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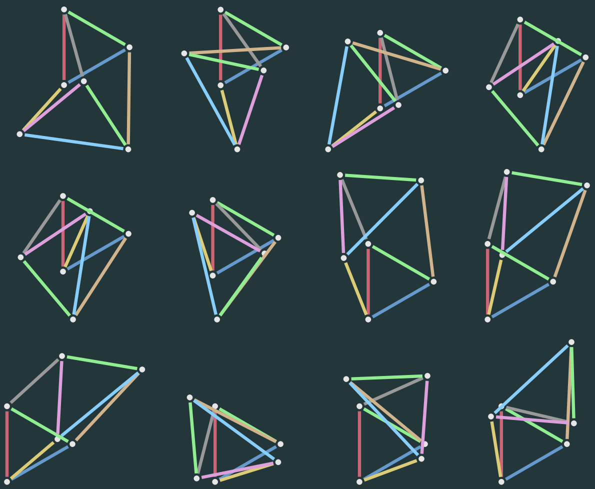
Bond-node structures: rigidity, combinatorics and chemistry
Lancaster

Lower bounds on the maximal number of realizations

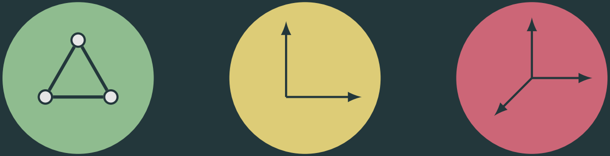
This presentation is based on the following articles:

- G. Grasegger, C. Koutschan, and E. Tsigaridas, *Lower bounds on the number of realizations of rigid graphs*, Experimental Mathematics, pages 1-12, 2018.
- E. Bartzos, I.Z. Emiris, J. Legerský, E. Tsigaridas, *On the maximal number of real embeddings of spatial minimally rigid graphs*, arXiv:1802.05860 (accepted for ISSAC 2018).

Number of Realizations



Outline of the Talk



Methods

Plane

Space

Notation

$c_d(G) \dots$ Number of complex realizations of G in $\mathbb{C}^d$

$r_d(G) \dots$ Maximal number of real realizations of G in $\mathbb{R}^d$

Object of interest: maximal r_d, c_d for graphs with n vertices

- $c_2(G) \leq \binom{2n-4}{n-2}$, $c_3(G) \leq \frac{2^{n-3}}{n-2}\binom{3n-6}{n-3}$ (Borcea, Streinu)
- Lower bounds
  - Graphs with $r_2(G) \approx 2.29^n$ (Borcea, Streinu)
  - Graphs with $r_2(G) \approx 2.3^n$ (Emiris, Moroz)
  - Graphs with $c_2(G) \approx 2.41^n$ (Jackson, Owen)
  - Graphs with $r_3(G) \approx 2.52^n$ (Emiris, Tsigaridas, Varvitsiotis)

Methods — Algebraic Equation Solving

Sphere equations

- Fix x_i, y_i, z_i for $i = 1, 2, 3$ to remove rigid motions
- $x_v^2 + y_v^2 + z_v^2 = s_v$ for $v \in V$ (magnitude equations)
- $s_u + s_v - 2(x_u x_v + y_u y_v + z_u z_v) = \lambda_{uv}^2$ for $uv \in E$

Methods — Algebraic Equation Solving

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Distance Geometry

$$CM = \begin{pmatrix} 0 & 1 & 1 & \cdots & 1 \\ 1 & 0 & d_{12}^2 & \cdots & d_{1n}^2 \\ 1 & d_{12}^2 & 0 & \ddots & \ldots \\ \ldots & \ldots & \ddots & \ddots & \ldots \\ 1 & d_{1n}^2 & d_{2n}^2 & \cdots & 0 \end{pmatrix}$$

- $\mathrm{rank}(CM) = d + 2$
- $(-1)^k \det(CM') \geq 0$, for every submatrix CM' with size $k + 1 \leq d + 2$

Methods — Algebraic Equation Solving

Gröbner basis

- FGb (Maple)
- Non-zero characteristic to accelerate computations

Homotopy Continuation

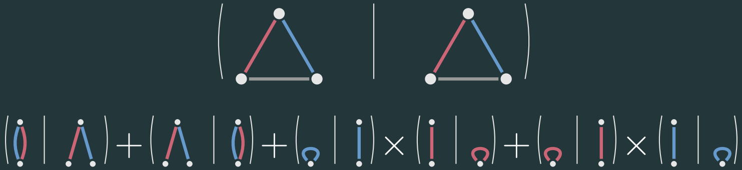
- PHCpack (Python,Sage)
- Faster computations/ less accurate
- Structure of equations is used to define the starting system

Isolation & Cell decomposition

- Isolate/Parametric (Maple)
- (Semi-)Algebraic sets over $\mathbb{R}$
- Very slow/ more accurate

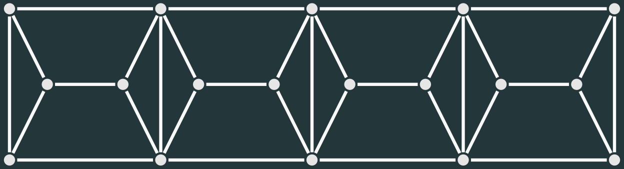
Methods — Combinatorial Algorithm

$$\mathrm{Lam}(B) = \mathrm{Lam}\left({}^{\{\bar{e}\}}B\right) + \mathrm{Lam}\left(B^{\{\bar{e}\}}\right) + \sum_{\substack{\mathcal{M}\cup\mathcal{N}=\mathcal{E}\\ \mathcal{M}\cap\mathcal{N}=\{\bar{e}\}}} \mathrm{Lam}\left({}^{\mathcal{M}}B\right)\cdot\mathrm{Lam}\left(B^{\mathcal{N}}\right)$$



- Proof: Tropical geometry
- Faster than Gröbner basis
- Computed c_2 for all graphs up to 12 vertices

Fan Constructions



$c_2(G') = c_2(G)^k \qquad (k \ldots \# \text{ copies of } G)$

Fan Constructions

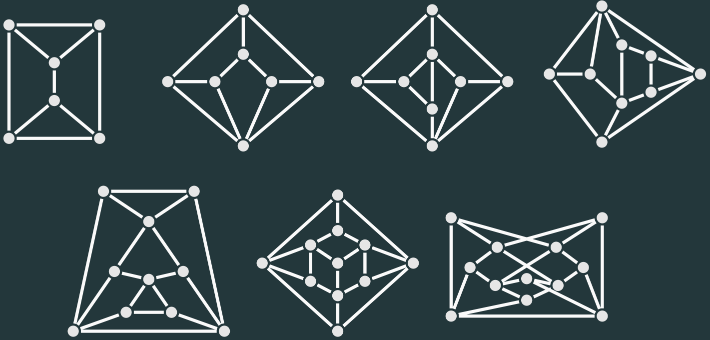
$$c_2(G') = 2 \cdot \left(\frac{c_2(G)}{2}\right)^k \qquad (k \ldots \# \text{ copies of } G)$$

$$c_2(G') = c_2(H) \cdot \left(\frac{c_2(G)}{c_2(H)}\right)^k \qquad (k \ldots \# \text{ copies of } G)$$

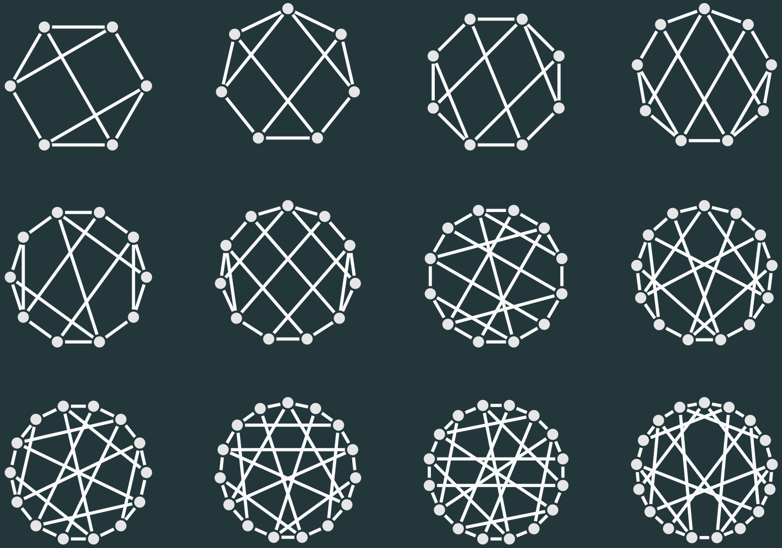
Plane

Graphs with Maximal Number of Realizations

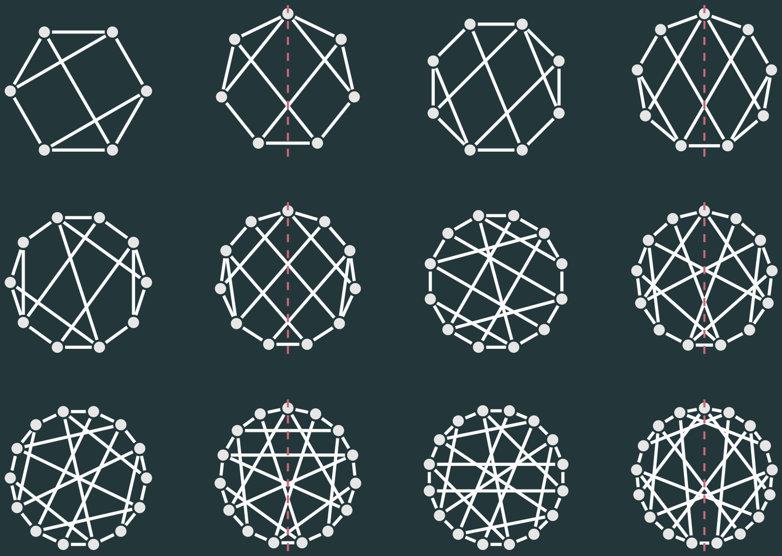
n	6	7	8	9	10	11	12		21
	24	56	136	344	880	2 288	6 180	...	$\geq$ 34 772 936



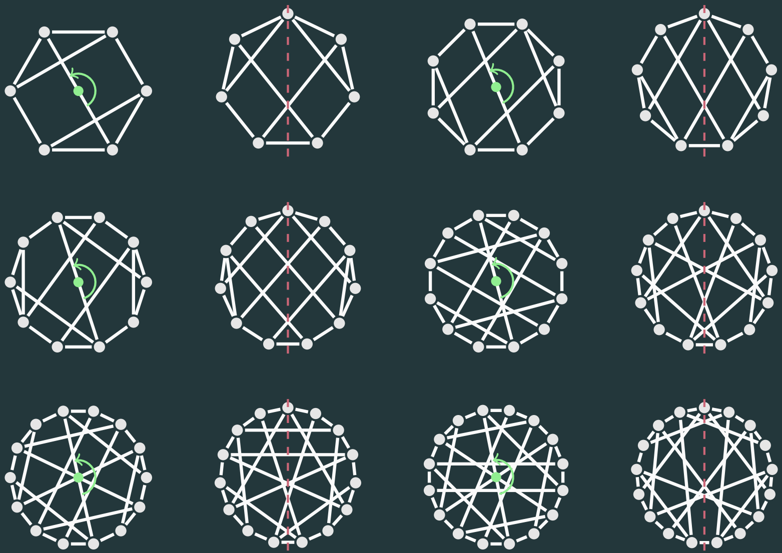
Common Properties



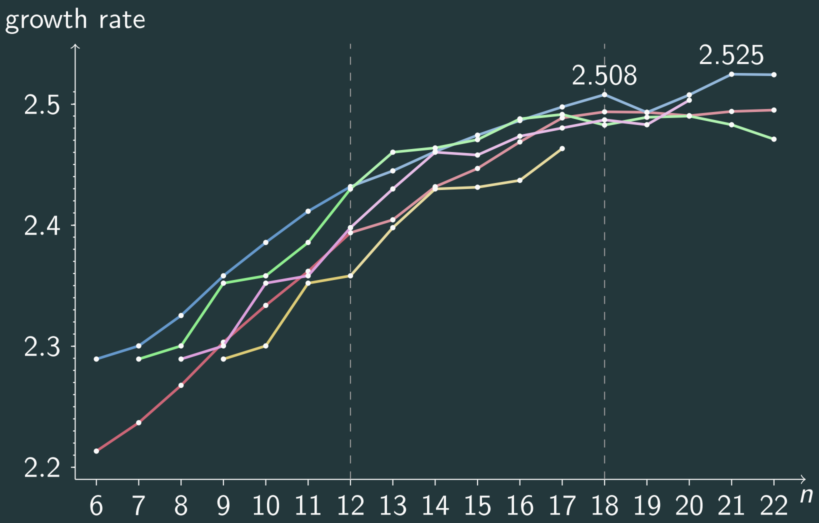
Common Properties



Common Properties

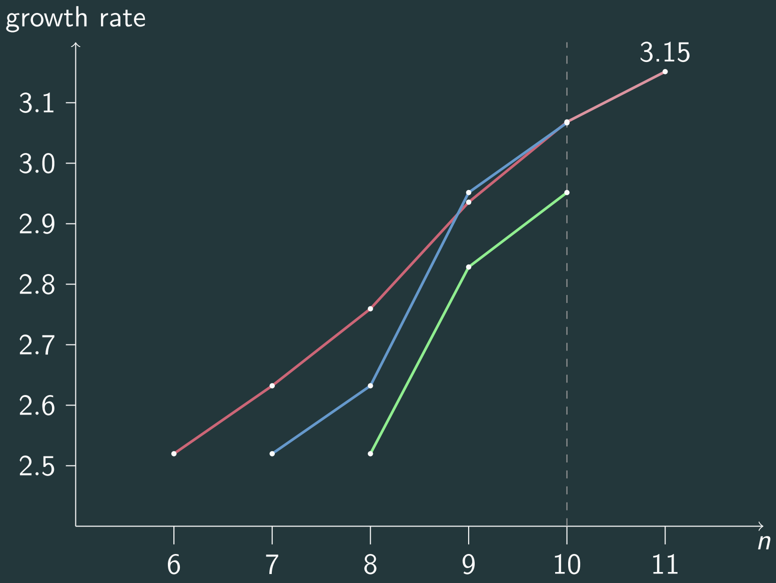


Lower Bounds



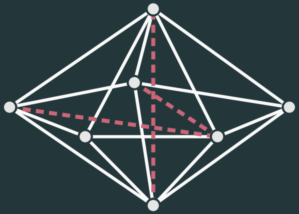
Space

Computations



Distance geometry subsystems

$$\begin{pmatrix}
0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 0 & d_{12}^2 & d_{13}^2 & d_{14}^2 & d_{15}^2 & d_{16}^2 & x_1 \\
1 & d_{21}^2 & 0 & d_{23}^2 & x_2 & x_3 & d_{26}^2 & d_{27}^2 \\
1 & d_{31}^2 & d_{32}^2 & 0 & d_{34}^2 & x_4 & x_5 & d_{37}^2 \\
1 & d_{41}^2 & x_2 & d_{43}^2 & 0 & d_{45}^2 & x_6 & d_{47}^2 \\
1 & d_{51}^2 & x_3 & x_4 & d_{54}^2 & 0 & d_{56}^2 & d_{57}^2 \\
1 & d_{61}^2 & d_{62}^2 & x_5 & x_6 & d_{65}^2 & 0 & d_{67}^2 \\
1 & x_1 & d_{72}^2 & d_{73}^2 & d_{74}^2 & d_{75}^2 & d_{76}^2 & 0
\end{pmatrix}$$



- Square algebraic subsystem
- Less inequalities

Coupler Curves

First attempts

- Local methods
    - Stochastic, gradient descent
- Global methods
    - Huge size of parameter space

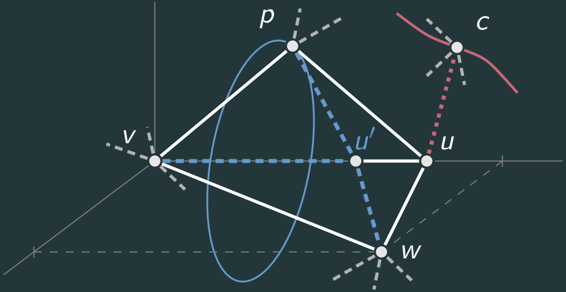
Coupler Curves

Coupler curve approach

- Visualization
- Development of a method that combines global and local searching
- Reduce the sampling space

Coupler Curves

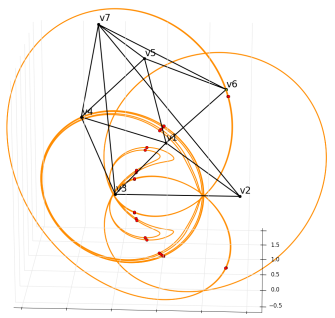
Invariance of coupler curve



- The coupler curve of c is invariant to the position of u
- 2−parameter family changing 4 edge lengths
- Increase of the number of real embeddings

Coupler Curves

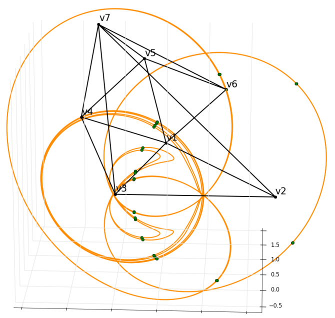
An example: G_{48}



- Moving the center of the sphere and adjusting the radius we were able to find the maximal number of embeddings.

Coupler Curves

An example: G_{48}



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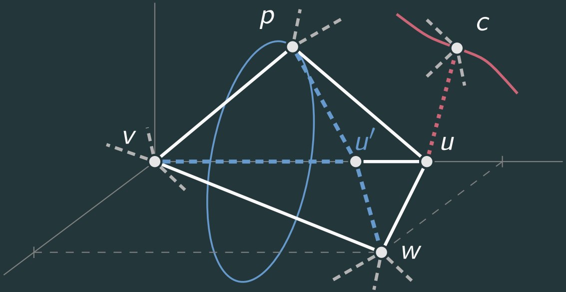
Coupler Curves

Sampling

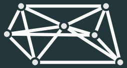


Results

Full list of real embeddings for 7-vertex graphs

G_{48}

G_{32a}



G_{32b}

G_{24}

G_{16a}

G_{16b}

Results

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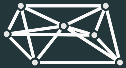


G_{32b}

G_{24}

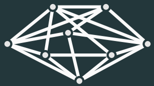
G_{16a}

G_{16b}

8-vertex graphs

G_{128}

G_{160}



$r_3(G_{128}) = 128$ $\quad r_3(G_{160}) \geq 132$

Results

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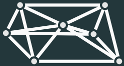

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8-vertex graphs

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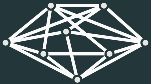

$r_3(G_{128}) = 128 \quad r_3(G_{160}) \geq 132$

Lower bound for real embeddings

2.6553^n (previous: 2.51984^n)

Further Research

- Find minimal k such that for all G with n vertices $c_d(G) \in \mathcal{O}(k^n)$
- Conjecture: $k \leq 3$ in 2d
- Computational limits