Algebraic and combinatorial bounds on the embedding number of distance graphs

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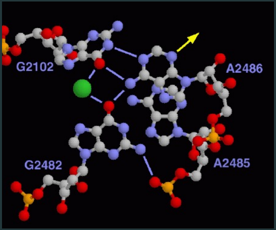

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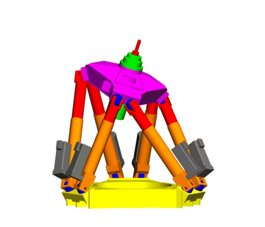
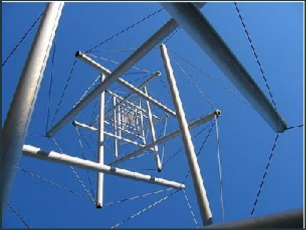
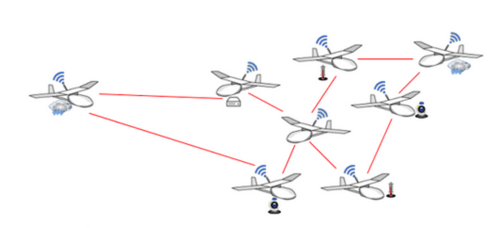
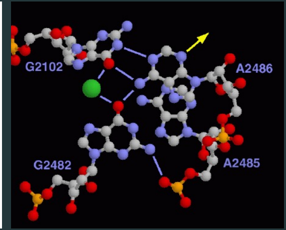








NMR yields distances, hence 3D structure, in solution
[Wüthrich, Chemistry Nobel'02]

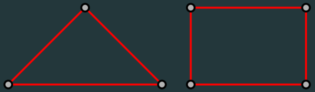
Definitions

Minimally generically rigid graphs

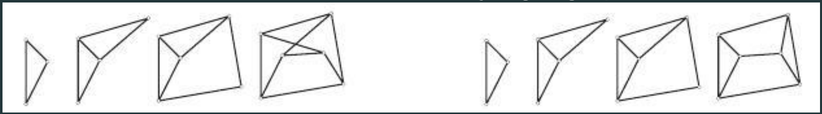
Study simple undirected weighted graphs G: weights are distances.

- A Euclidean embedding $\rho \colon V \to \mathbb{R}^d$ of graph $G = (V, E, \lambda)$ respects edge lengths $\lambda_{u,v} = \|\rho(u) - \rho(v)\|$, $(u, v) \in E$.
- Complex embedding $\rho \colon V \to \mathbb{C}^d$: $\lambda_{u,v} = \|\rho(u) - \rho(v)\|$, $(u, v) \in E$.
- G is (generically) rigid if the number of embeddings (for generic lengths) is finite modulo rigid transforms.
- G is *minimally* rigid if $G \setminus \{e\}$, $\forall e \in E$, is not rigid (flexible).

Rigid vs flexible graphs

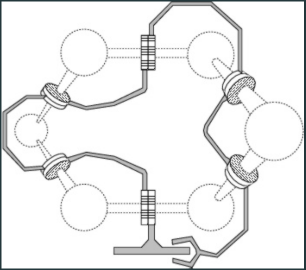


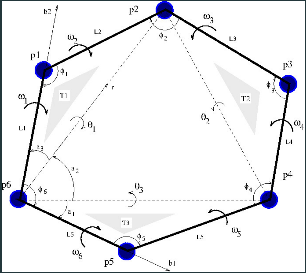
Construction of minimally rigid graphs

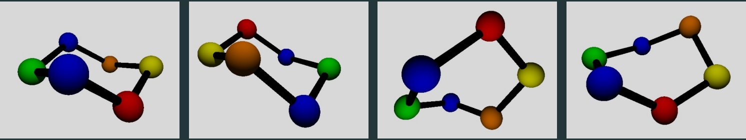


$K_{3,3}$ Desargues

Cyclohexane







Given 6 distances and angles, or 12 distances (Laman count).

Algebraic bound = 16: tight in $\mathbb{R}^3$.

4 conformations in nature [E,Mourrain'99:Algorithmica]

Edge count

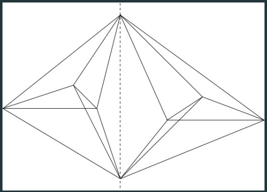
Theorem (Maxwell:1864)

If $G = (V, E)$ is generically minimally rigid, and $|V| = n$, then

- $|E| = d \cdot n - \binom{d+1}{2}$, *and*
- $|E'| \leq d \cdot |V'| - \binom{d+1}{2}$, $\forall$*vertex-induced subgraph* (V', E').

[Pollaczek-Geiringer] [Laman'70]
Equivalence in $d = 2$, and
$d = 3$ for simplicial polytopes [Gluck'75]

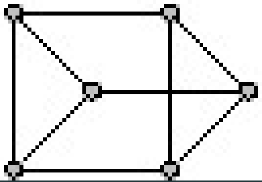
No equivalence generally in $d = 3$:
Double banana, $n = 8, |E| = 18$.



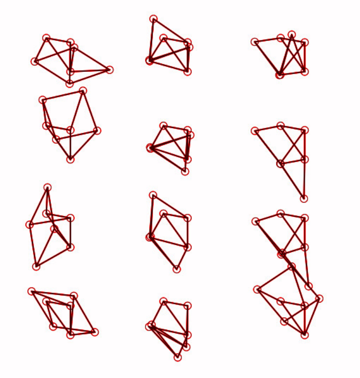
Further question: count / enumerate the embeddings.

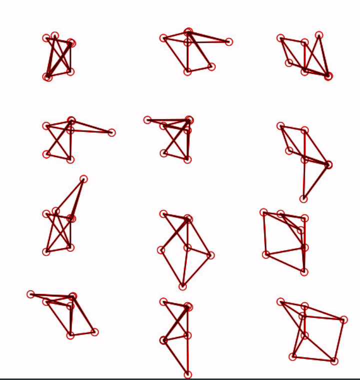
Small cases in $\mathbb{R}^2$

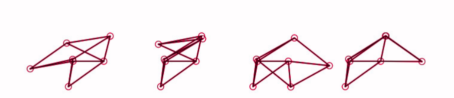
- The triangle has 2 embeddings (reflections).
- $n = 6$: two "nontrivial" (H_2) graphs:
  – $K_{3,3}$ has 16 embeddings [Walter-Husty'07]
  – Desargues' graph has 24 (3-prism, planar parallel robot) [Hunt'83] [Gosselin,Sefrioui,Richard'91] [Borcea,Streinu'04]



$n = 7$: 56 conformations in $\mathbb{R}^2$ [E,Moroz'11]







Algebraic formulation

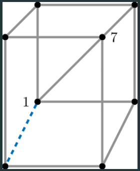
#embeddings = #solutions of a polynomial system expressing edge lengths, and $\binom{d+1}{2}+1$ constraints to fix the graph, remove scaling

$$\text{in } \mathbb{R}^2 : \begin{cases} x_1 = y_1 = 0, \\ x_2 = 1, y_2 = 0, \\ (x_i - x_j)^2 + (y_i - y_j)^2 = \lambda_{ij}^2, \quad (i,j) \in E. \end{cases}$$

$$\text{in } \mathbb{R}^3 : \begin{cases} x_1 = y_1 = z_1 = 0, \\ x_2 = 1, y_2 = z_2 = 0, \\ z_3 = 0, \\ (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2 = \lambda_{ij}^2, \quad (i,j) \in E. \end{cases}$$

Enumeration problem

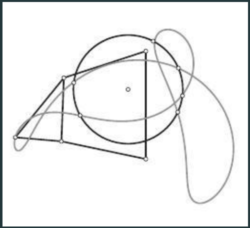
- #complex embeddings bounds #Euclidean embeddings. Usually equal, exception is the Jackoson-Owen graph

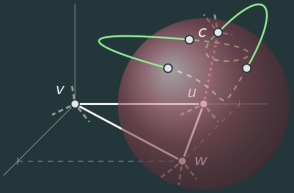


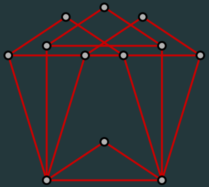
- Bézout's (trivial) bound on quadratic system implies $O(2^{dn})$.

Enumeration: lower bounds

- …on real embedding numbers: $\Omega(2.381^n)$ for $\mathbb{R}^2$, $\Omega(2.639^n)$ for $\mathbb{R}^3$ [Bartzos,E,Legersky,Tsigaridas'21]
- …on complex embedding numbers: $\Omega(2.507^n)$ for $\mathbb{C}^2$, $\Omega(3.067^n)$ for $\mathbb{C}^3$ [Grasegger et al.'20].







Enumeration: upper bounds

- Determinantal varieties [Harris,Tu'84]
- Determinantal variety on distance matrices [Borcea,Streinu'04]
- Mixed volume of Newton polytopes
  [Steffens,Theopald'10] ignores roots at (toric) infinity:
  $X_{i1}^2 + X_{i2}^2 = s_i, \; s_i + s_j - 2X_{i1}X_{j1} - 2X_{i2}X_{j2} = \lambda_{ij}^2.$

  No asymptotic improvement on Bézout's.
- First improvement for $d \geq 5$ [Bartzos,E,Schicho'20] using multi-homogeneous Bézout and permanents.
- State of art: First improvement for all d by graph orientations [Bartzos,E,Vidunas'21-22]; namely $O(3.77^n)$ for $d = 2$.

Decision problem

- Given *complete* set of exact distances: Embed-$\mathbb{R}^d \in$ P.
- Given incomplete set of exact distances [Saxe'79]:
  Embed-$\mathbb{R} \in$ NP-hard. Reduction of set-partition.
  Embed-$\mathbb{R}^d \in$ NP-hard, for $d \geq 2$, even if lengths $\in \{1, 2\}$.
- Embed-$\mathbb{R}^2 \in$ NP-hard for planar graphs with all lengths $= 1$ [Cabello,Demaine,Rote'03]
- Given distances $\pm\epsilon$, approximate-Embed-$\mathbb{R}^d \in$ NP-hard [Moré,Wu'96]

Algebraic interlude

Multihomogeneous Bézout bound

Given a square system of m polynomials let $A_1, \dots, A_n$ be a partition of the variables, $m_j = |A_j|$, $m = m_1 + \cdots + m_n$.

The i-th polynomial is homogeneous of degree d_{ij} in A_j.

Let $y_1, \dots, y_n$ be symbolic parameters.

Then, the number of isolated roots in $\mathbb{P}^{m_1} \times \cdots \times \mathbb{P}^{m_n}$ is bounded by the coefficient of $y_1^{m_1} \cdots y_n^{m_n}$ in

$$\prod_{i=1}^{m} (d_{i1} \cdot y_1 + \cdots + d_{in} \cdot y_n).$$

$a_1^2 - a_2 + 1$, $a_1 a_2 - 2$: $(2y_1 + y_2) \cdot (y_1 + y_2) = 2y_1^2 + 3y_1 y_2 + y_2^2$.

Multihomogeneous system

Embedding coordinates $X_v \in \mathbb{C}^d$, $v \in V$:

$$\sum_{i=1}^{d} X_{vi}^2 = s_v,\ v \in V; \quad s_u + s_v - 2\langle X_u, X_v \rangle = \lambda_{uv}^2,\ (u,v) \in E.$$

n variable subsets $\{X_v, s_v\}$, symbolic parameter y_v.

Fix K_d (d vertices) thus defining (V', E').

Then:

$$\prod_{i=1}^{n-d} 2y_i \cdot \prod_{k=1}^{|E'|} (y_{k_1} + y_{k_2}) = 2^{n-d} \prod_{i=1}^{n-d} y_i \cdot \prod_{k=1}^{|E'|} (y_{k_1} + y_{k_2}),$$

m-Bézout = coefficient of $y_1^d \cdots y_{n-d}^d$ in product of sums $\times 2^{n-d}$.

Permanent method

Given $m \times m$ matrix A, per $(A) = \sum_{\sigma \in S_m} \prod_{i=1}^{m} A_{i,\sigma(i)}$.

Theorem

Let A contain degrees d_{ij}. The m-Bézout bound equals

$$per\,(A)\,/\,(m_1! \cdots m_n!).$$

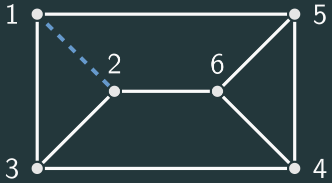
For rigid graphs this becomes $2^{n-d} \cdot \text{per}\,(A)\,/\,d!^{n-d}$.

Using permanent bounds [Brègman-Minc'63,'73], m-Bézout improves Bézout's bound for $d \geq 5$ [Bartzos,E,Schicho]

Desargues

per $(A) = 32$, actual embeddings $c_2(G) = 24$, $c_{S^2}(G) = 32$

	$(1,3)$	$(2,3)$	$(1,5)$	$(2,6)$	$(3,4)$	$(4,5)$	$(4,6)$	$(5,6)$
x_3	1	1	0	0	1	0	0	0
y_3	1	1	0	0	1	0	0	0
x_4	0	0	0	0	1	1	1	0
y_4	0	0	0	0	1	1	1	0
x_5	0	0	1	0	0	1	0	1
y_5	0	0	1	0	0	1	0	1
x_6	0	0	0	1	0	0	1	1
y_6	0	0	0	1	0	0	1	1



Graph orientations

Orientations and m-Bézout

Observation [Bartzos,E,Schicho'20]
For rigid $G(V, E)$, fixed $K_d = (v_1, \ldots v_d)$, let $G' = (V, E \setminus E(K_d))$.
Set $B = \#$orientations of G', constrained so that:

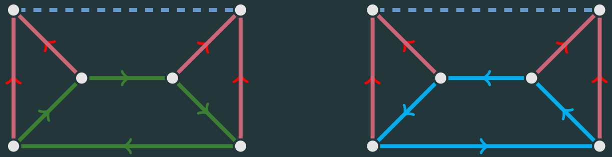
- the outdegree of $v_1, \ldots, v_d$ is 0,
- the outdegree of every $v_i \in V \setminus V(K_d)$ is d.

Then, B equals the coefficient of $y_1^d \cdots y_{n-d}^d$ in

$$\prod_{k=1}^{|E'|} (y_{k_1} + y_{k_2}).$$

Corollary. The embedding number of G in $\mathbb{C}^d$ is bounded by $2^{n-d}B$

Desargues



$d = 2$, fixed K_2 is the dashed edge,

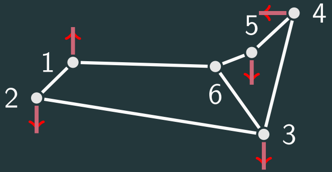
$B = 2$ orientations $\Rightarrow 2 \cdot 2^{6-2} = 32$ bound,

actually 24 real/complex embeddings [Hunt'83].

Pseudographs

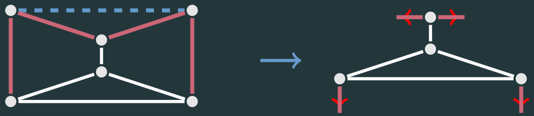
A pseudograph $L(U, F, H)$ is a collection s.t.

- U is the set of vertices
- F is a set of (normal) edges (u, v)
- H is a set of *hanging (half) edges* (u)



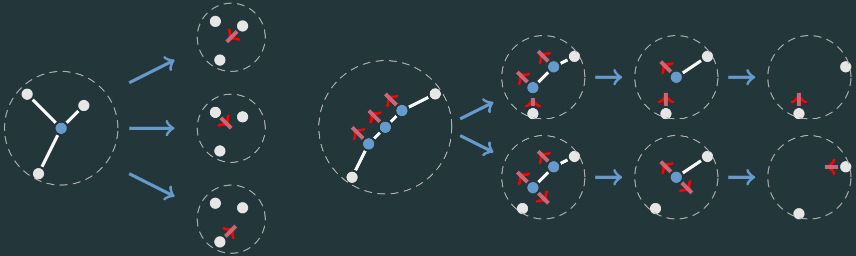
The normal subgraph $G'(U, F)$ is connected.

Example: Fixed $e^* = (v_1, v_2) \in E$. $U = V \setminus \{v_1, v_2\}$,
$F = \{e \in E : v_1, v_2 \notin e^*\}$, $H = \{e \in E : v_1 \text{ xor } v_2 \in e^*\}$



Count constrained orientations

- Elimination step removes $\ell \geq 1$ vertices, and 2ℓ adjacent edges, keeping the pseudograph connected.
- Deleted/Hanging edges directed towards removed vertex.
- Cost = #pseudographs generated per step
- The product of costs bounds B = #constrained orientations.
- Vertex and Path elimination steps:



Bound on orientations

Theorem (Bartzos,E,Vidunas'20)

For pseudographs of n vertices, k hanging edges, $B \le \alpha_d^n \cdot \beta_d^{k-1}$*:*

$$\alpha_d = \max_{p \ge d} \left(2^{p-d} \binom{p}{d}^{2d-3} \right)^{1/(2p-3)}, \; \beta_d = \left(2 / \binom{p}{d}^2 \right)^{1/(2p-3)}$$

for p maximizing α_d*; note* $\beta_d < 1$*.*

Corollary For Laman graphs, #complex embeddings $\le \left(4 \cdot (3/4)^{1/5}\right)^{n-2} = O\left(3.776^n\right)$.

Asymptotic bounds

Complex embedding number $= O(b^n)$, where b is as follows:

$d =$	2	3	4	5	6
[Bartzos,E,Vidunas'21]	3.776	6.840	12.69	23.90	45.53
[Bartzos,E,Schicho'20]	4.899	8.944	16.73	31.75	60.79
Bézout	4	8	16	32	64

Same results for spherical embeddings.

Extensions

Distance matrix

Square matrix M, with real entries, $M_{ii} = 0$, $M_{ij} = M_{ji} \geq 0$.

M is embeddable in $\mathbb{R}^d$ iff $\exists$ points $p_i \in \mathbb{R}^d \ : \ M_{ij} = \frac{1}{2}\,\mathrm{dist}(p_i, p_j)^2$.

Theorem (Cayley'41,Menger'28)

M embeds in $\mathbb{R}^d$ for min d, iff Cayley-Menger (border) matrix has

$$rank \begin{bmatrix} 0 & 1 \\ 1 & M \end{bmatrix} = d + 2,$$

and, for any $(k+1) \times (k+1)$ border minor D:

$$(-1)^k D \geq 0, \quad k = 2, \ldots, d+1\,.$$

The latter are strict inequalities iff d is minimum.

Approximate input

Model noisy distances by intervals.

Improve upper/lower bounds by triangular/tetrangular inequalities.

Use graph algorithms (e.g. All-min-paths) [Havel]

Structure-preserving matrix perturbations.

Theorem. [Wicks,Decarlo'95] Given matrix and specific entries allowed to change, we can compute a continuous, locally differentiable function minimizing σ_n.

Method applied for $\sigma_n, \sigma_{n-1}, \ldots, \sigma_{n-5}$ [Nikitopoulos,E'02]

Incomplete data

Embedding is equivalent to completing an incomplete matrix so as to get a PSD Gram (or distance) matrix: expressed as feasibility of a PSD program.

Complexity:

- Solving PSD programs with arbitrary precision $\in P_{\mathbb{R}}$ (interior-point or ellipsoid algorithms).
- Recall: interior-point, ellipsoid algorithms for LP are in P_{bit}.
- Open whether LP in $\mathrm{P}_{\mathbb{R}}$ (strong polytime).

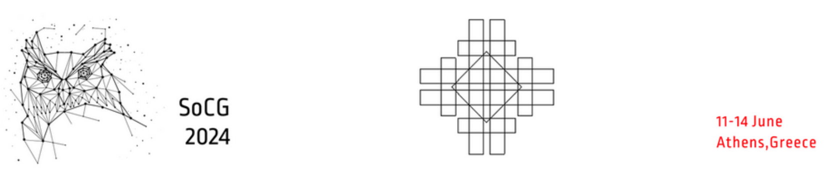
Chordal Graphs

- A graph is chordal if it contains NO empty cycle of length ≥ 4.
- Thm [Grone,Sa,Johnson,Wolkowitz'84] [Bakonyi,Johnson'95] Every partial distance matrix with graph G has valid completion iff G is chordal.
  [$\Leftarrow$] poly-time algorithm [Laurent'98]
- Thm [Laurent] If #edges needed to make G chordal is $O(1)$, then distance-matrix completion $\in \mathrm{P}_{bit}$.
- Generally, minimizing #edges to make G chordal is NP-hard.

Contributions / Further questions

- First nontrivial upper bounds on embedding number.
- Closed formula of upper bound on graph orientations.
- m-Bézout bound better than by permanent
- Tensegrity: edge weight correspond to intervals
- Specific counts, Global rigidity (unique embedding)
- Polynomial-time cases of permanent

Thank you!



See you in Athens for SoCG / CG-Week 2024