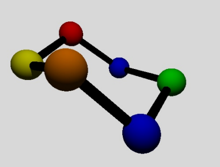
Euclidean Embedding of Rigid Graphs

Ioannis Z. Emiris

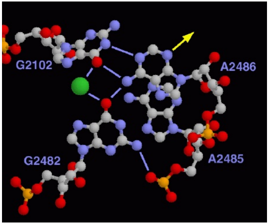
University of Athens



ACAC-2010

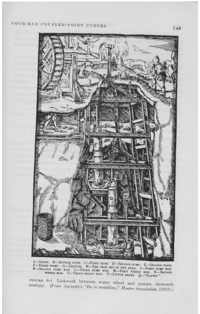
Outline

Bioinformatics



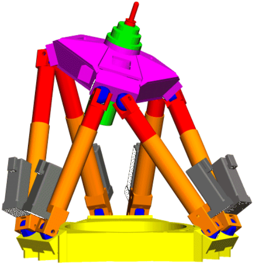
- NMR spectroscopy yields (approximate) distances, hence 3d structure, in solution [K.Wüthrich, ETHZ, Chemistry Nobel'02]
- X-ray crystallography: more accurate distances but in crystal state, which takes ~ 1 year.
- Software for ≥ 100 atoms:
  Dyana [Güntert,Mumenthaler,Wüthrich'97],
  Embed [Crippen,Havel'88], Disgeo [Havel,Wuthrich'98],
  Dgsol [Moré,Wu], Abbie [Hendrickson], etc

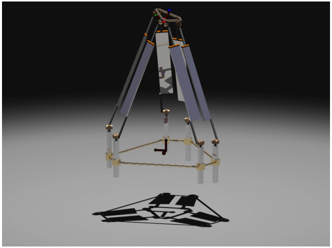
Robotics


FOUR-BAR COUPLER-POINT CURVES 149

A—Shaft. B—Bottom pump. C—First tank. D—Second pump. E—Second tank. F—Third pump. G—Trough. H—The iron set in the axle. I—First pump rod. K—Second pump rod. L—Third pump rod. M—First piston rod. N—Second piston rod. O—Third piston rod. P—Little axles. Q—"Claws."

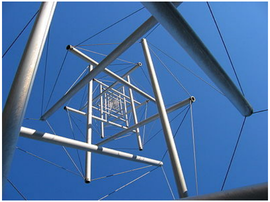
Figure 6-1 Linkwork between water wheel and pumps, sixteenth century. [*From Agricola's "De re metallica," Hoover translation* (1912).]

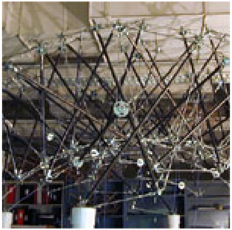




Engineering

- Architecture, tensegrity





- Topography (Surveyors)

Problem definition

Embed-$\mathbb{R}^d$: Find a function which maps vertices to points $\in \mathbb{R}^d$ so as to preserve the given (Euclidean) distances, $d \geq 1$.

Counting: Given a rigid graph, determine max #embeddings in $\mathbb{R}^d$ (modulo rigid motions), assuming generic edge lengths.
Rigid motions: translation, rotation.

Generic / Minimal Rigidity

- Graph G is generically rigid in $\mathbb{R}^d$ iff for generic edge lengths it has a finite number of embeddings in $\mathbb{R}^d$, modulo rigid motions.
- Graph G is minimally rigid iff it becomes non-rigid (flexible) once an edge is removed.

We call generically minimally rigid graphs simply rigid.

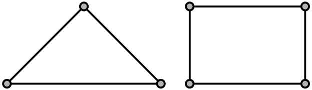


Figure: A rigid vs a non-rigid (flexible) graph in $\mathbb{R}^2$.

Rigidity Condition

Theorem (Maxwell:1864,Laman'70)

Graph $G = (V, E)$ is rigid in $\mathbb{R}^2$ iff:

- $|E| = 2|V| - 3$, *and*
- $|E'| \leq 2|V'| - 3, \;\forall$ *vertex-induced subgraph* (V', E').

This is the (combinatorial) "Laman condition" for rigidity in $\mathbb{R}^2$.

Henneberg steps

Adding a vertex while preserving rigidity:

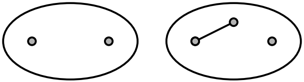


Figure: H_1 and H_2 steps

Henneberg steps

Adding a vertex while preserving rigidity:

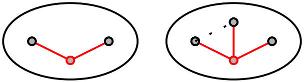


Figure: H_1 and H_2 steps

Henneberg steps

Adding a vertex while preserving rigidity:

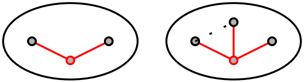


Figure: H_1 and H_2 steps

Figure: Examples for $n = 6$

Planar construction

Definition

A H_1 (resp. H_2) construction is a succession of H_1 (resp. H_1 and H_2) steps, which begins with a triangle.

Theorem (Henneberg,Whiteley-Tay)

Graph G is Laman iff it has a H_2 construction.

Rigidity in $\mathbb{R}^3$

Generalized condition: $|E| = 3|V| - 6$, $|E'| \leq 3|V'| - 6$.
Counterexample: Double Banana.

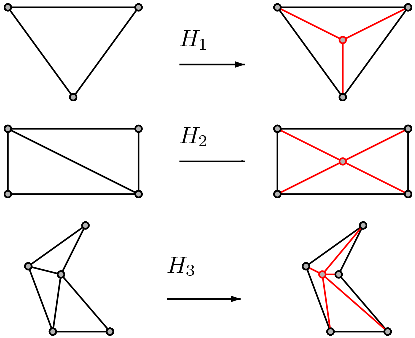
Theorem (Gluck,Aleksandrov)

The 1-skeleta of simplicial (convex) polyhedra are rigid in $\mathbb{R}^3$.
Notice they satisfy $|E| = 3|V| - 6$, $|E'| \leq 3|V'| - 6$.

Open: Complete characterization; other classes.

3 Henneberg steps in $\mathbb{R}^3$

H_1, H_2, H_3 steps replace $k-1$ diagonals in $(k+2)$-cycle, by new vertex and $k+2$ edges, for $k = 1, 2, 3$:



Henneberg construction in $\mathbb{R}^3$

A H_3 construction is a succession of H_1, H_2, H_3 steps, starting at the 3-simplex (tetrahedron), or K_4 graph.

Theorem (Bowen-Fisk'67)

A graph is the 1-skeleton of a simplicial polyhedron in $\mathbb{R}^3$ *iff it admits a* H_3 *construction.*

Embedding complete graphs

- Consider (unknown) points $p_0, \dots, p_n \in \mathbb{R}^d$, and given distances

$$d_{ij}^2 = |p_i - p_j|^2,\ d_{i0}^2 = |p_i|^2,\ \text{ by setting } p_0 = 0.$$

- Now define (Gram) matrix G as follows:

$$d_{ij}^2 = |p_i|^2 - 2p_i^T p_j + |p_j|^2 \ \Leftrightarrow\ p_i^T p_j = \frac{d_{i0}^2 - d_{ij}^2 + d_{j0}^2}{2} =: G_{ij},$$

hence $G = [p_1, \dots, p_n]^T \cdot [p_1, \dots, p_n]$.

- The Singular Value Decomposition yields

$$G = V \Sigma V^T \Rightarrow P = \sqrt{\Sigma} \cdot V^T.$$

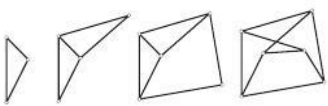
Decision problem

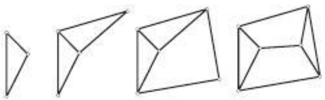
- Given complete set of exact distances: Embed-$\mathbb{R}^d \in$ P.
- Given incomplete set of exact distances [Saxe'79].
  Embed-$\mathbb{R} \in$ NP-hard. Reduction of set-partition.
  Embed-$\mathbb{R}^k \in$ NP-hard, for $k \geq 2$, even if weights $\in \{1, 2\}$.
- (Approximate) Embed-$\mathbb{R}^2 \in$ NP-hard for planar rigid graphs with all weights $= 1$ [Cabello,Demaine,Rote'03]
- Given distances $\pm\epsilon$, approximate-Embed$-\mathbb{R}^d \in$ NP-hard [Moré,Wu'96].
- Every graph with *n* vertices can be embedded in *some* Euclidean space *(of any dimension)* with distortion in $O(\log n)$ [Bourgain'93].

Counting Planar Embeddings

Construct all non-isomorphic graphs:

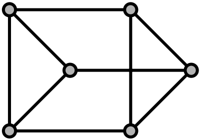
$n =$	3	4	5	6
#graphs	1	1	3	
upper bound	2	4	8	24
lower bound	2	4	8	24
H_1 sequence	Δ	$\Delta 1$	$\Delta 11$	$\Delta 111$
H_2 sequence				$\Delta 112$



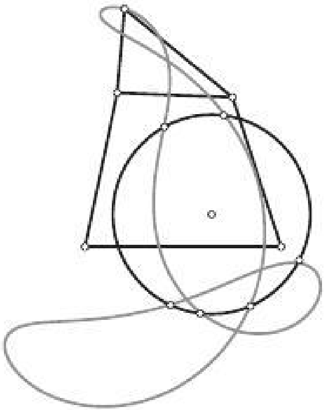


Small cases

- The triangle (Δ) has exactly 2 embeddings (reflections).
- H_1 exactly doubles the generic #embeddings (2 circles).
  Open: Does H_2 at most quadruple #embeddings?
- $n = 6$: H_2 graphs:
  $K_{3,3}$ has 16 embeddings [Walter-Husty'07]
  Desargues' graph has 24 [Hunt'83] [Gosselin,Sefrioui,Richard'91]
  (aka 3-prism, planar parallel robot)



Desargues graph: lower bound

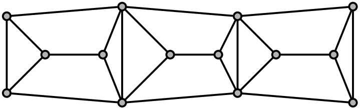


[Borcea,Streinu'04]

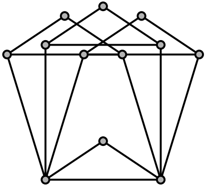
Lower Bounds in $\mathbb{R}^2$

[Borcea,Streinu'04]

- Caterpillar Desargues has $24^{n/4} \simeq 2.21^n$ embeddings.



- Desargues fan has $2 \cdot 12^{n/3-1} \simeq 2.29^n/6$ embeddings.



Smallest case is $n = 9$, yields 288.

Algebraic upper bounds

#embeddings = #solutions $\in \mathbb{R}^{nd}$ of a polynomial system, corresponding to edges E and $\binom{d+1}{2}$ "pin-down" equations:

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

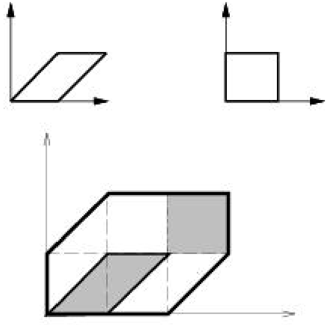
$$\text{in } \mathbb{R}^3 : \begin{cases} x_1 = y_1 = z_1 = 0, \\ y_2 = z_2 = 0, \\ z_3 = 0, \\ (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2 = l_{ij}^2, \quad (i,j) \in E. \end{cases}$$

Use bounds in $\mathbb{C}^{nd}$:

- classical, Bézout ($= \prod$ degrees),
- sparse, mixed volume (of exponents of nonzero terms).

Example

System $c_{11} + c_{12}xy + c_{13}x^2y + c_{14}x$, $c_{31} + c_{32}y + c_{33}xy + c_{34}x$, with Newton polytopes:



has Mixed Volume $= 3 \;= V(P_1 + P_2) - V(P_1) - V(P_2)$.

General Upper Bound

- Bézout: $\Theta(2^{nd})$.
- [Borcea-Streinu'04] by distance matrices:

$$\prod_{k=0}^{n-d-2} \frac{\binom{n-1+k}{n-d-1-k}}{\binom{2k+1}{k}} \approx 2^{nd},$$

$$\binom{2n-4}{n-2} \approx \frac{4^{n-2}}{\sqrt{\pi(n-2)}}, \qquad d = 2,$$

Planar Upper Bound

- Mixed volume $= 4^n$ [Steffens-Theobald'08]
- Sparseness A Laman graph, $n \geq 8$, with k degree-2 vertices has [E-Tsigaridas-Varvitsiotis'09]

$$\leq 2^{k+1}\, 4^{n-k-5} \text{ embeddings.}$$

Desargues graph: upper bound

[Collins'02]: Planar quaternion $q = q(d, \theta) \in \mathbb{R}^4$,

$$\text{transformation } M = \begin{bmatrix} q_4^2 - {q_3}^2 & -2q_3q_4 & 2q_1q_4 - 2q_2q_3 \\ 2q_3q_4 & {q_4}^2 - {q_3}^2 & 2q_1q_3 + 2q_2q_4 \\ 0 & 0 & 1 \end{bmatrix}$$

- $q_3^2 + q_4^2 = 1, \;\; |(Mv_i)^T v_j| - d_{ij}^2 = \text{hom}(q_i) - c = 0 :$ MV $= 12$.
- Equivalent: $\text{hom}(q_i) = c(q_3^2 + q_4^2)$, dehomogenize $z_i = q_i/q_4$.
- First equation is $z_3^2 + 1 = z_0$, system has MV=6.

Small cases

$n =$	3	4	5	6	7	8	9	10
upper	2	4	8	24	56	128	512	2048
lower	2	4	8	24	48	96	288	576
H_1	Δ	$\Delta 1$	$\Delta 11$	$\Delta 111$	$\Delta 1111$	$\Delta 11111$	$\Delta 1^6$	
H_2				$\Delta 112$	$\Delta 1112$	$\Delta 11112$	$\Delta 1^5 2$ $\Delta 1^4 21$ $\Delta 1^4 22$	

- Classified all isomorphic graphs by SAGE, applied Mixed volume on distance equations [E-Tsigaridas-Varvitsiotis:GD'09].
- For $n = 7$: upper bound by distance matrices (was 64).
  $\exists$ graph with 56 complex roots; others with upper bound < 56

Distance matrix

A distance matrix M is square, $M_{ii} = 0$, $M_{ij} = M_{ji} \geq 0$.

It is embeddable in (Euclidean) $\mathbb{R}^d$ iff

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

Distance geometry

Theorem (Cayley'41,Menger'28,Schoenberg'35)

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

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

and, for any minor D indexed by rows/columns $0, i_1, \ldots, i_k$,

$$(-1)^k \, D(i_1, \ldots, i_k) \geq 0, \quad k = 2, \ldots, d + 1.$$

Corollary

- *For* $k = 2$, $D(i,j) = 2M_{ij} \geq 0$,
- *for* $k = 3, 4$, *we get the triangular/tetrangular inequalities.*

Corollary

Points p_i *embed in* $\mathbb{R}^d$, *for min* d, *iff corresponding Gram matrix* $P^T P$ *has rank* d *and is positive semidefinite (all eigenvalues* ≥ 0*).*

Cyclohexane

$$\begin{array}{c} \\ p_1 \\ p_2 \\ p_3 \\ p_4 \\ p_5 \\ p_6 \end{array} \begin{array}{c} \begin{array}{cccccc} p_1 & p_2 & p_3 & p_4 & p_5 & p_6 \end{array} \\ \begin{bmatrix} 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & u & c & x_{14} & c & u \\ 1 & u & 0 & u & c & x_{25} & c \\ 1 & c & u & 0 & u & c & x_{36} \\ 1 & x_{14} & c & u & 0 & u & c \\ 1 & c & x_{25} & c & u & 0 & u \\ 1 & u & c & x_{36} & c & u & 0 \end{bmatrix} \end{array}$$

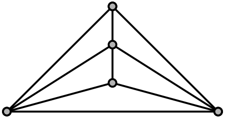
Known $u = 1.526\AA$ (adjacent), $\phi \simeq 110.4^{o} \Rightarrow c \simeq 2.29\AA$ (triangle)
Rank $= 5 \Leftrightarrow$ vanishing of all 6×6 minors:
Yields a 3×3 system with Mixed volume $= 16$.

Embeddings in $\mathbb{R}^3$

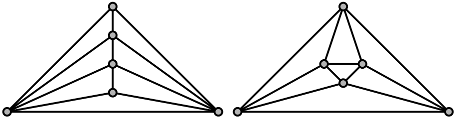
- The 3-simplex (tetrahedron, K_4) has exactly 2 embeddings: reflections about the plane.
- H_1 exactly doubles the generic #embeddings: 3 spheres intersect generically at 2 points.
  Open: do H_2, H_3 multiply #embeddings by at most $4, 8$?
- Sparseness: Consider $n \geq 6$, k degree-3 vertices. Then, there exist at most $2^{k+1}8^{n-k-5}$ embeddings [ETV'09].

Small Cases

$n = 5$: Unique graph, 4 embeddings (tight):



$n = 6$: 2 non-isomorphic graphs; RHS with 16 embeddings (tight):



Better mixed volumes

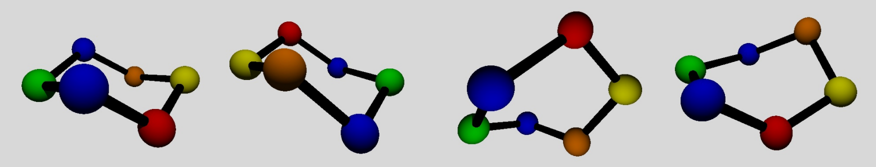
Mixed volume of distance equations in $\mathbb{R}^3$ is loose in $\mathbb{C}^*$.
Pf. Bernstein's 2nd Thm [1975]

Remove spurious solutions with new variables s_i:

$$\begin{aligned}
x_i &= 0, & i &= 1,2,3\\
y_i &= 0, & i &= 1,2\\
z_i &= 0, & i &= 1\\
s_i &= x_i^2 + y_i^2 + z_i^2, & i &= 1,\dots,n\\
s_i + s_j - 2x_ix_j - 2y_iy_j - 2z_iz_j &= l_{ij}^2, & (i,j) &\in E
\end{aligned}$$

The case $n = 6$

- Mixed Volume (of new system) $= 16$.
- The cyclohexane has 16 real embeddings [E-Mourrain'99]
- The "jigsaw" parallel robot has 16 real configurations.

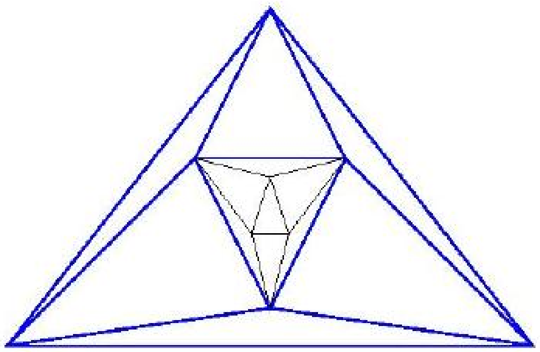


4 cyclohexanes (chairs, and boats/crowns) given 6 fixed distances and angles, or 12 distances.

Lower bound in $\mathbb{R}^3$

The Cyclohexane caterpillar has $\approx 16^{n/3} \simeq (2.52)^n$ embeddings.

Proof. Copies of Cyclohexanes with common triangle. For $n \geq 9$.



Small cases

$n =$	4	5	6	7	8	9	10
upper	2	4	16	32	160	640	2560
lower	2	4	16	32	64	256	512
H_1	Δ	$\Delta 1$	$\Delta 11$	$\Delta 111$	$\Delta 1^4$	$\Delta 1^5$	$\Delta 1^6$
H_2	—	—	$\Delta 12$	$\Delta 1^2 2$	$\Delta 1^3 2$ $\Delta 1^2 2^2$ $\Delta 1^2 21$	$\Delta 1^4 2$ $\Delta 1^3 2^2$ $\Delta 1^3 21$ $\Delta 1^2 2^3$	$\Delta 1^5 2$ $\Delta 1^4 2^2$ $\Delta 1^4 21$ $\Delta 1^3 2^3$ $\Delta 1^3 21^2$ $\Delta 1^3 212$ $\Delta 1^3 2^2 1$ $\Delta 1^2 2^4$

Using SAGE, and Mixed volumes [E-Tsigaridas-Varvitsiotis:GD'09].

Matrix completion

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

Complexity:

- Solving PSD programs with arbitrary precision $\in P_{\mathbb{R}}$ (interior-point or ellipsoid algorithms).
- Unknown whether PSD-program $\in \mathrm{NP}_{bit}$.
- Unknown whether PSD-feasibility $\in \mathrm{P}_{bit}$ (weak poly-time).
- Recall: interior-point, ellipsoid algorithms for LP are in P_{bit}.

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 M with graph G has a distance-matrix completion iff G is chordal.
  Proof: all principal submatrices embed $\Rightarrow$ matrix embeds.
  [$\Leftarrow$] algorithm in P [Laurent'98].
- Thm [Laurent] If #edges added to make G chordal is $O(1)$, then distance-matrix completion $\in$ P_{bit}.
- Generally, minimizing #edges to make G chordal is NP-hard.

Complete subgraphs

- Thm [Laurent]. Suppose G contains no clique K_4. Then, PSD-completion is in $P_{\mathbb{R}}$.
- Consider a clique missing edges incident to vertex v. Then, in poly-time, M is PSD-completed and its min embedding dimension (MED) computed [E-Fragoudakis-Markou], e.g:

$$\mathrm{MED}(v - G_1 \equiv G_2) = \max\{\mathrm{MED}(v - G_1), \mathrm{MED}(G_1 \equiv G_2)\}.$$

- Same for star of cliques K_i: $\mathrm{MED}(\mathrm{star}) = \max_i\{\mathrm{MED}(K_i)\}$.

Generalizations

Body-and-bar structures

Define graph by mapping bodies to vertices, bars to edges.
Structure is rigid in $\mathbb{R}^d$ iff graph = edge-disjoint union of $\binom{d+1}{2}$ spanning trees [Tay'84]

Body-and-hinge and body-and-bar/hinge structures

Replace Hinge by $\binom{d+1}{2} - 1$ edges.
Same characterization of rigidity [Whiteley'88] [Tay'89]

Molecular Conjecture proven [Katoh-Tanigawa'09]

A graph corresponds to a rigid Body-and-hinge structure in $\mathbb{R}^d$ iff it corresponds to a rigid Panel-and-hinge structure.

Open

- Specific embedding numbers, better lower bounds.
- Combinatorial characterization in $\mathbb{R}^3$.
- Count embeddings of body-and-bar, body-and-hinges structures.
- How about other distance norms?
- Tensegrity

Thank you!