Combinatorial Rigidity and the Molecular Conjecture

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1. Introduction

Generic rigidity in the plane is a graph theoretic property:

Theorem 1 *(Laman - 1970)[7] A graph is generically rigid in the plane if and only if it has a subset $|E|$ of edges with*

$$|E| = 2|V(E)| - 3$$

and, for every subset $F \subseteq E$,

$$|F| \leq 2|V(F)| - 3.$$

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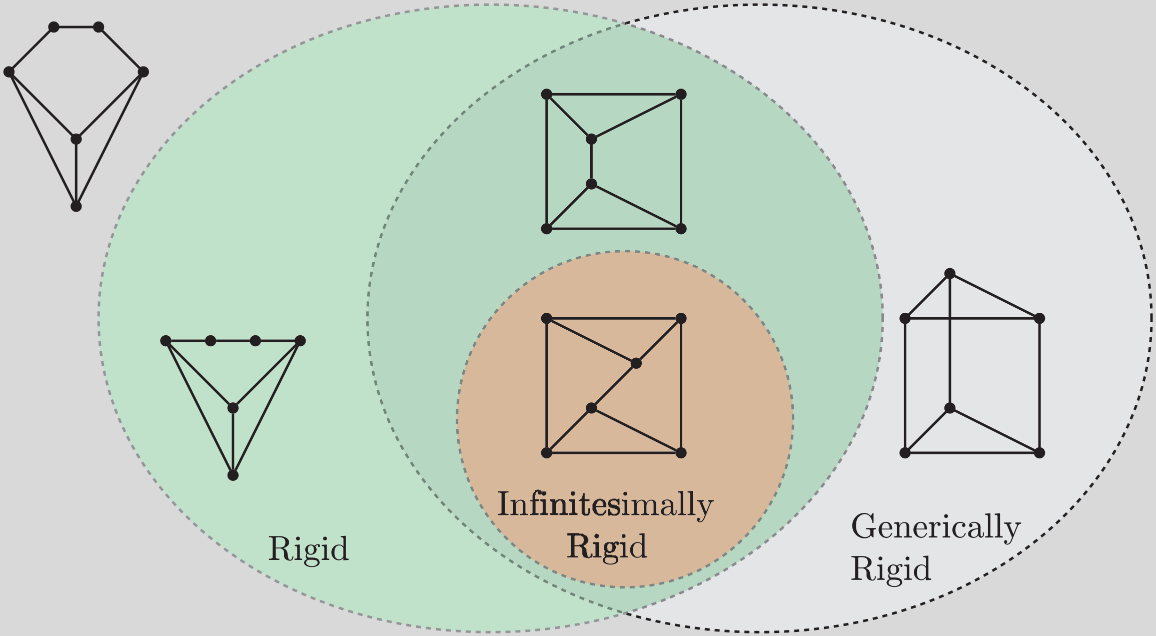
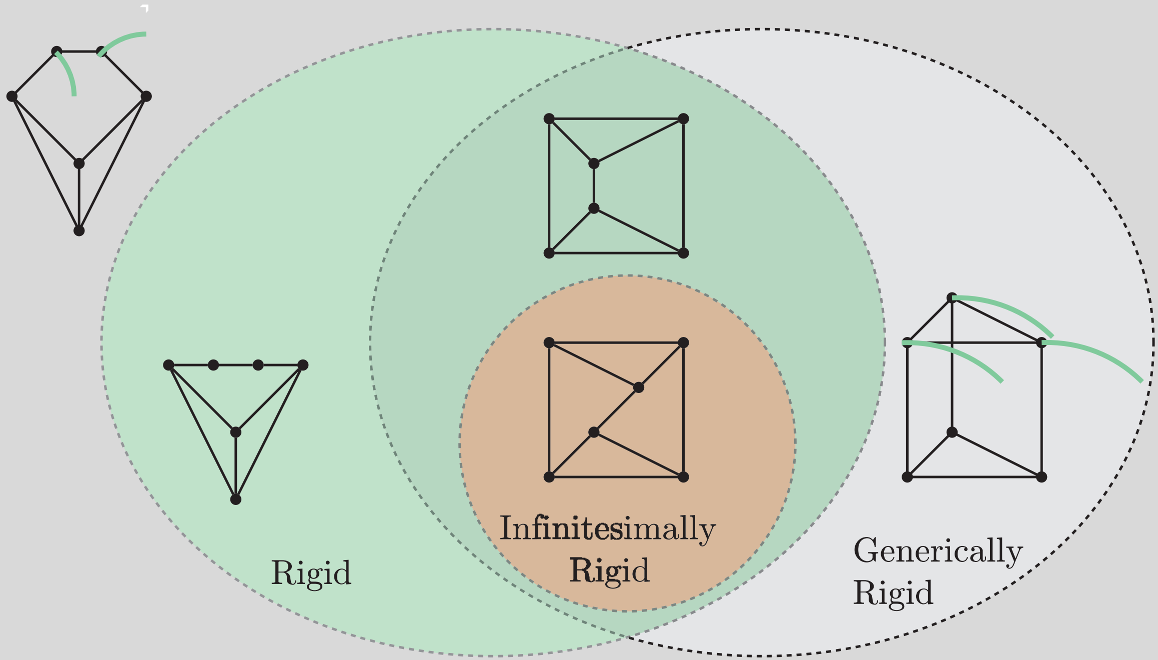
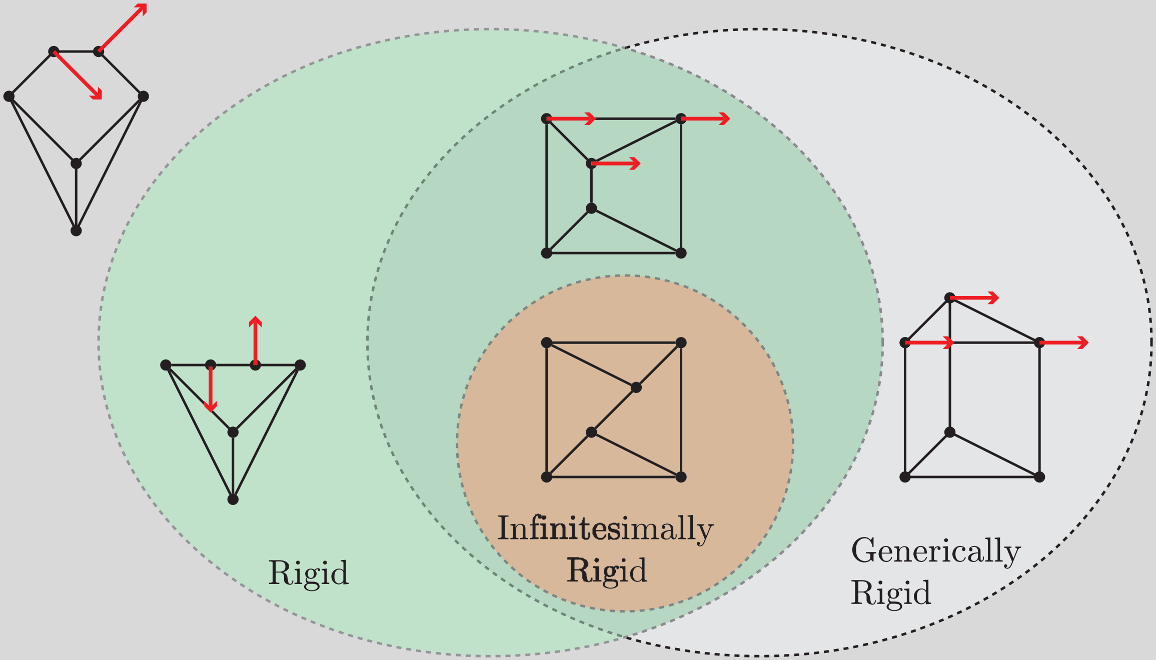


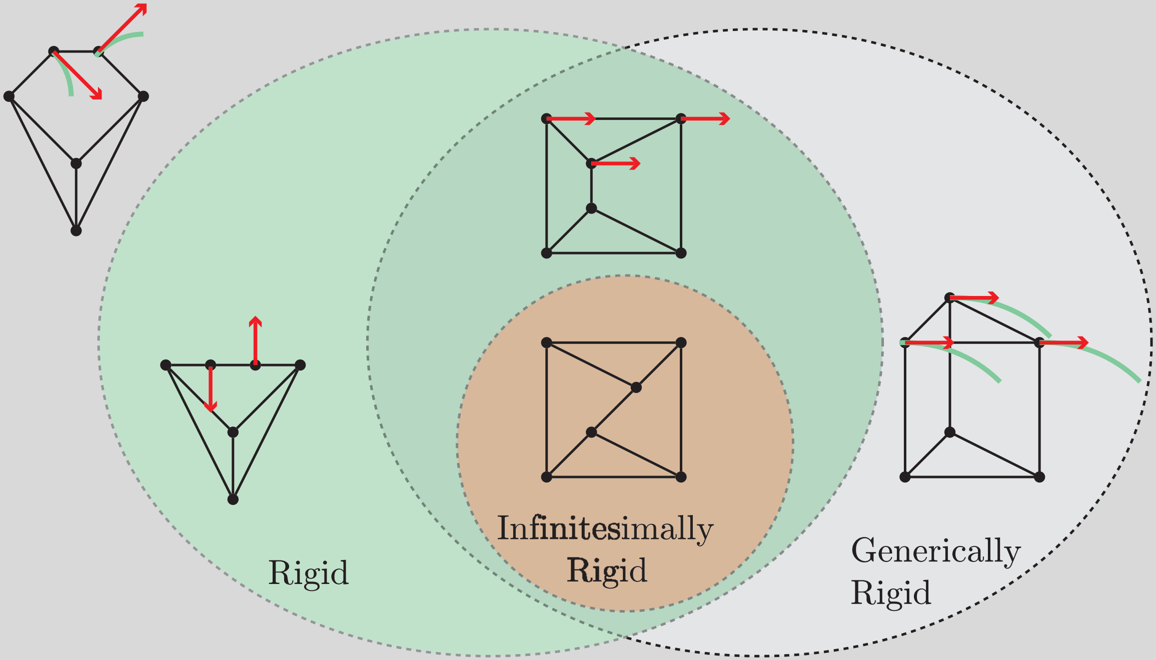
Rigidity
Different notions of rigidity.



Rigidity
Non rigid graphs have a motion.



Non-infinitesimally rigid graphs have initial velocity candidates.



Generic rigidity is a property of the graph, *not* the embedding.

2. Type of Rigidity

We will use the term *framework* (in m-space) to denote a triple $(V, E, \overrightarrow{p})$, where (V, E) is a graph and $\overrightarrow{p}$ is an embedding (injection) of V into real m-space.

We say that a framework is *globally rigid* (in m-space) if all solutions to the system of quadratic equations obtained from requiring all edge lengths to be fixed, with the coordinates of the vertices as variables, correspond to congruent frameworks; we say that a framework is *rigid* (in m-space) if all solutions to the corresponding system in some neighborhood of the original solution (as a point in mn-space) come from congruent frameworks.

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We say that a given framework $(V, E, \overrightarrow{p})$ is *generic* if all frameworks corresponding to points in a neighborhood of $P = \overrightarrow{p}(V)$ in $\mathbb{R}^{nm}$ are rigid or not rigid as is $(V, E, \overrightarrow{p})$. A set of points P in m-space is said to be *generic* if each framework $(V, E, \overrightarrow{p})$ with $\overrightarrow{p}(V) = P$ is generic.

If $G(V, E)$ is not rigid, we call the maximal rigid subgraphs of G the *rigid components* and note that rigid components partition E. Then $\mathcal{M}(G)$ is the direct sum over its restrictions on the rigid components.
The following theorem is equivalent to Laman's Theorem 1, it uses the rank function of $\mathcal{M}$ rather than independence to characterize rigidity.

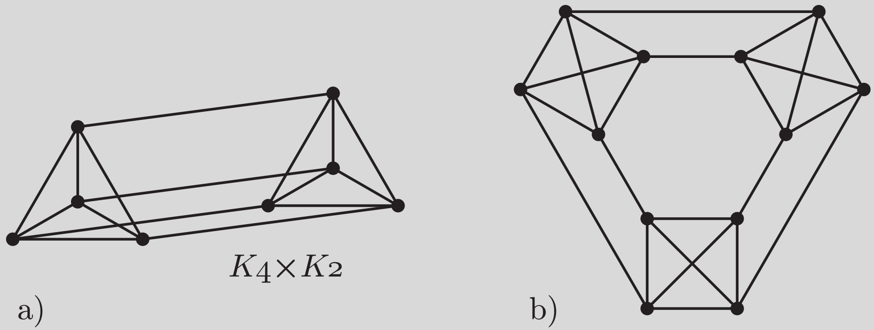
Theorem 2 *[9] Let $G = (V, E)$ be a graph. Then G is rigid if and only if for all families of induced subgraphs $\{G_i = (V_i, E_i)\}_{i=1}^m$ such that $E = \cup_{i=1}^m E_i$ we have $\sum_{i=1}^m (2|V_i| - 3) \geq 2|V| - 3$.*

$G(V, E)$ is called *redundantly rigid* if $G(V, E - e)$ is rigid for all $e \in E$, i.e. the removal of a single edge e from the rigid graph G does not destroy rigidity. Redundant rigidity is a key to characterize global rigidity.

Theorem 3 *[5] Let G be a graph. Then G is globally rigid if and only if G is a complete graph on at most three vertices, or G is both 3-connected and redundantly rigid.*

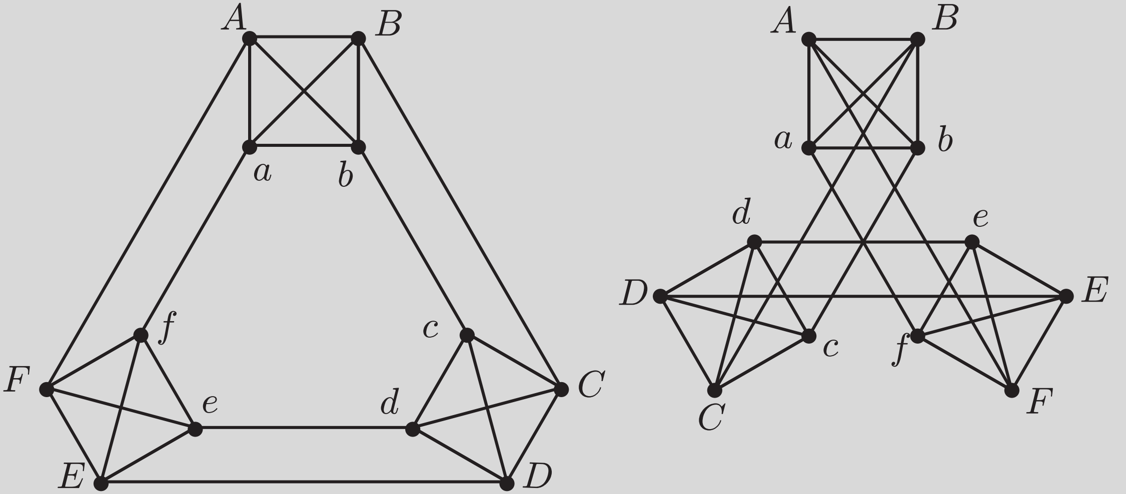
3. Vertex transitive graphs

Theorem 4 *A four-regular vertex transitive graph is generically rigid in the plane if and only if it contains no subgraph isomorphic to* K_4*, or is* K_5 *or one of the graphs in the following figure.*

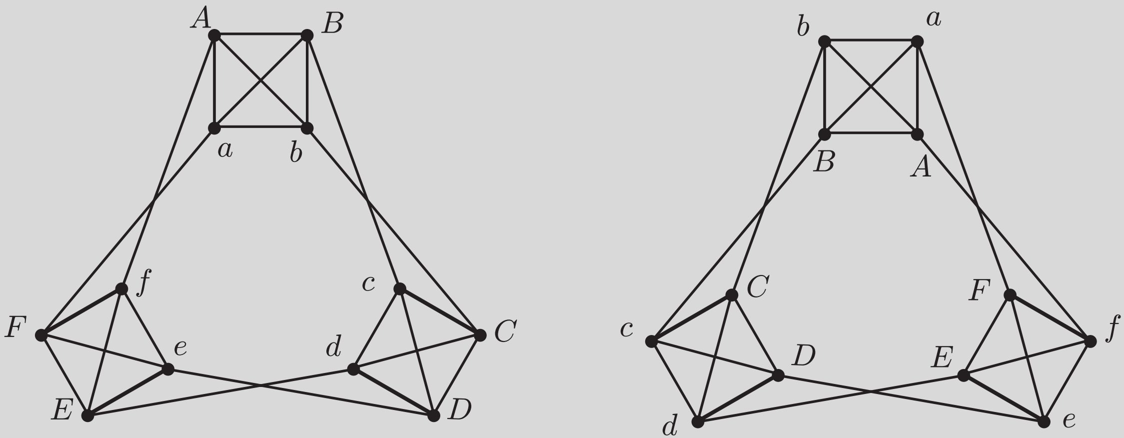


Vertex transitive rigid graphs containing K_4.

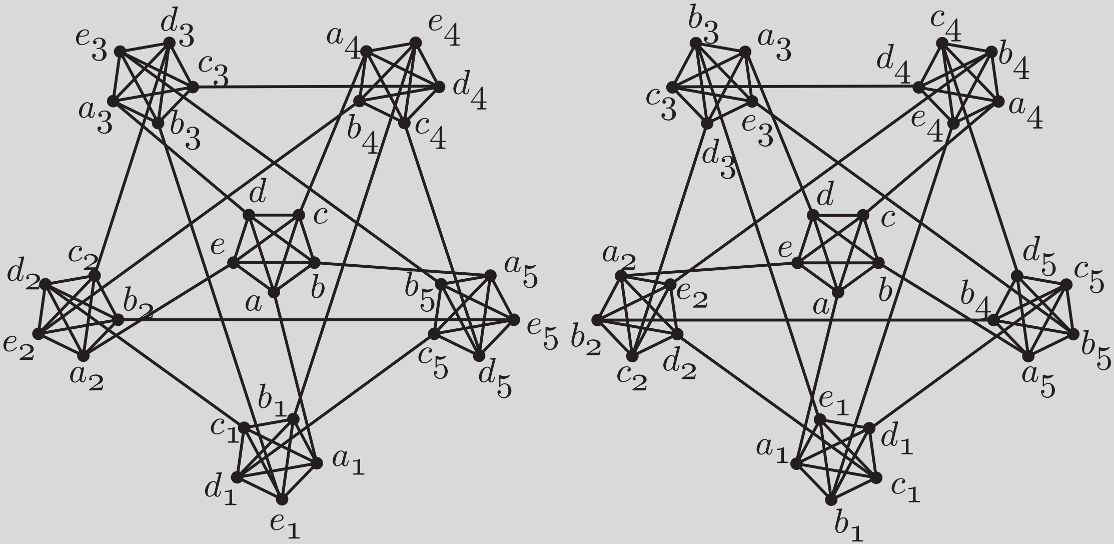
Theorem 5 *Let G be a connected k-regular vertex transitive graph on n vertices. Then G is not rigid if and only if either:*
(a) $k = 2$ and $n \geq 4$.
(b) $k = 3$ and $n \geq 8$.
(c) $k = 4$ and G has a factor consisting of s disjoint copies of K_4 where $s \geq 4$
(d) $k = 5$ and G has a factor consisting of t disjoint copies of K_5 where $t \geq 8$.



Two embeddings which are rigid, but neither infinitesimally rigid nor globally rigid.

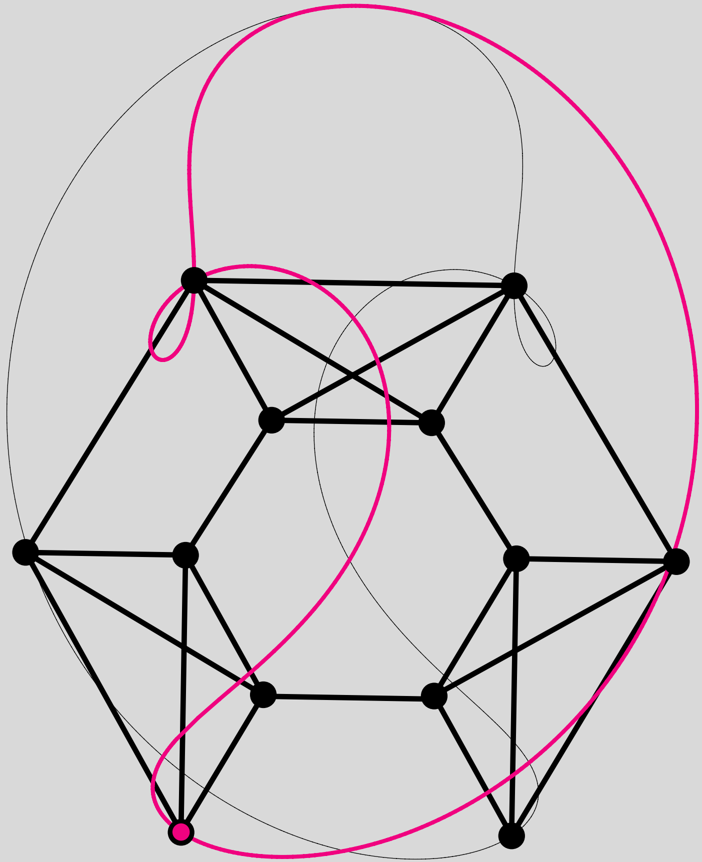


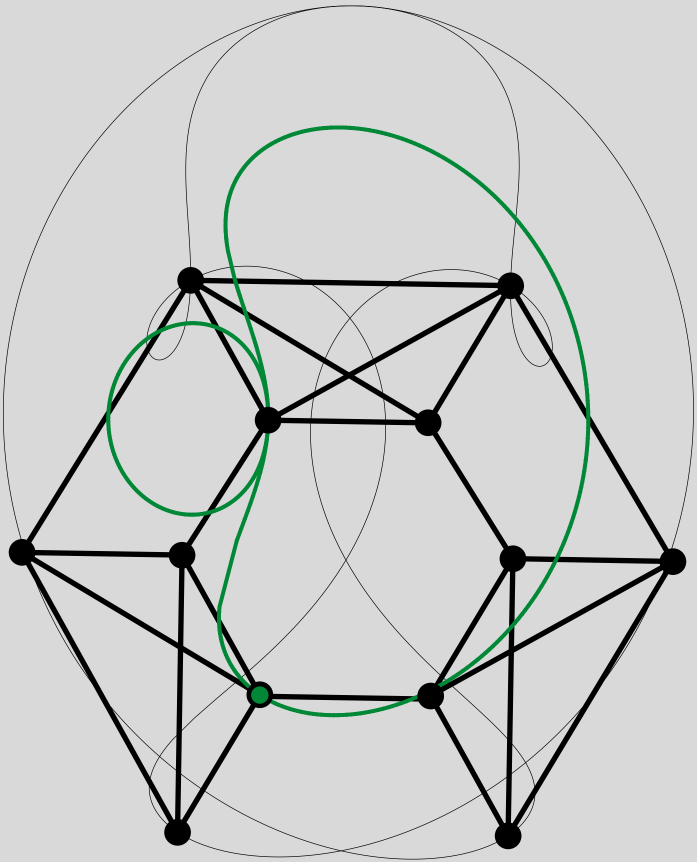
Two embeddings which are rigid and infinitesimally rigid but not globally rigid.

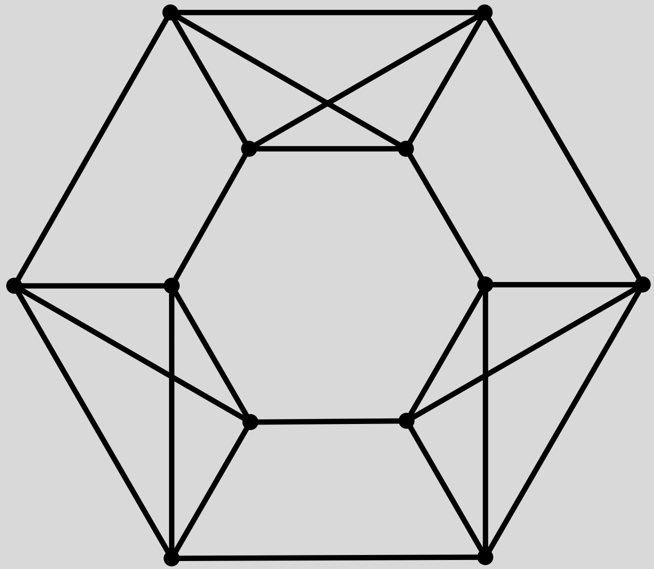


Two embeddings which are rigid, but not globally rigid.

4. Example







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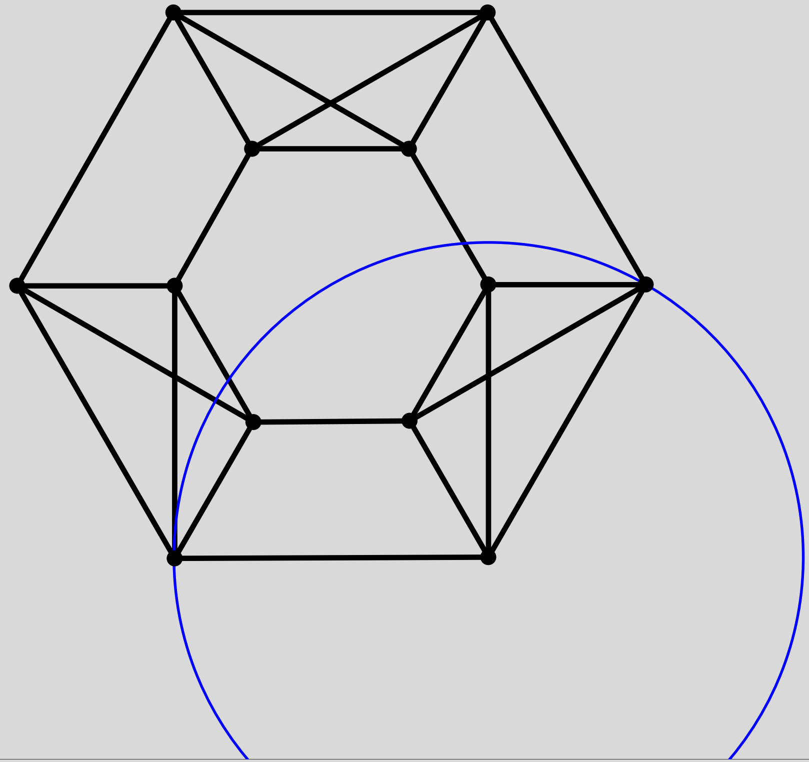
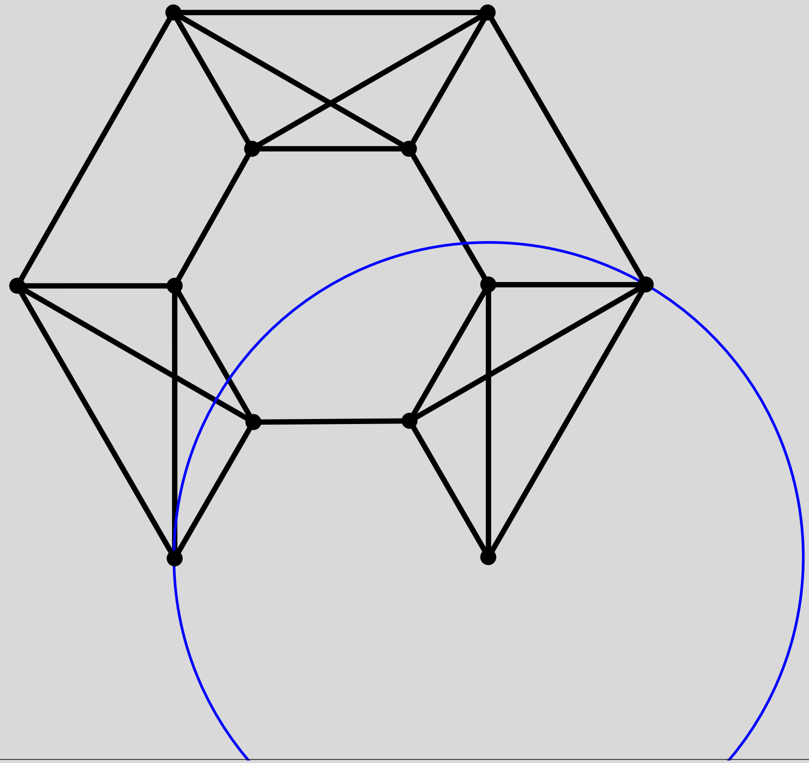
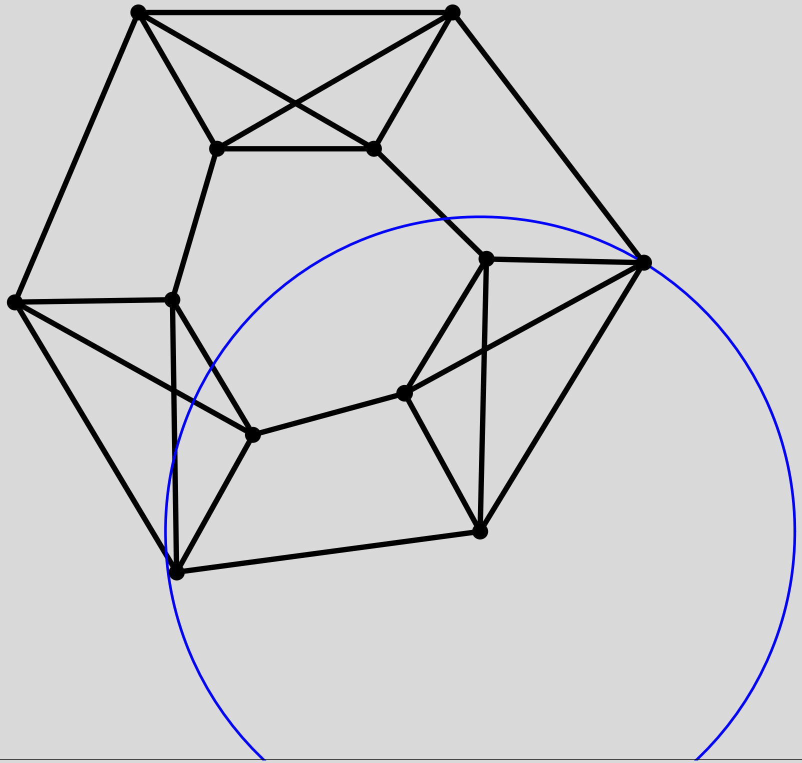
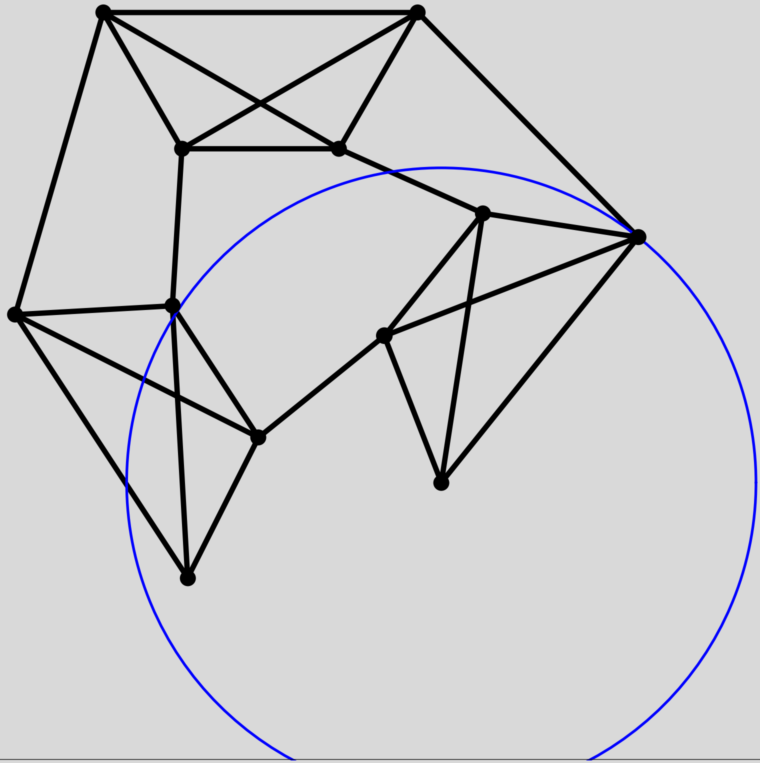
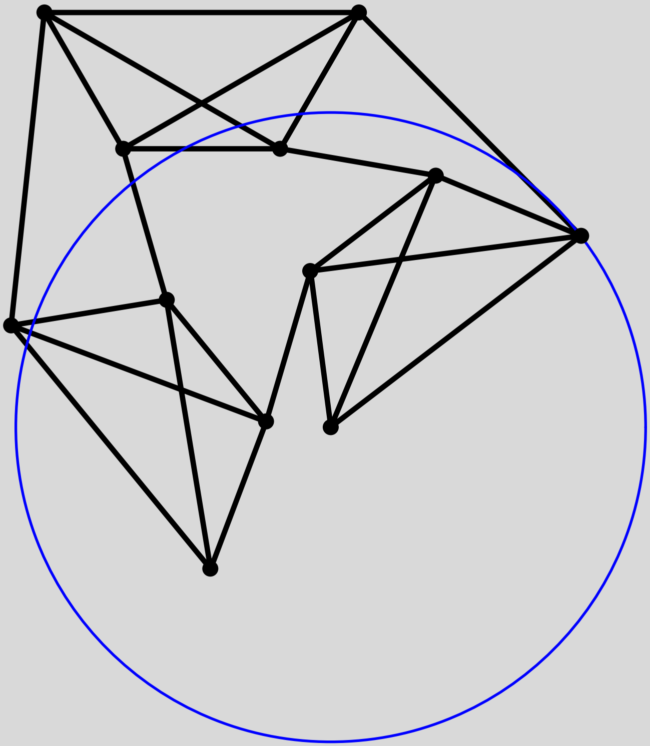
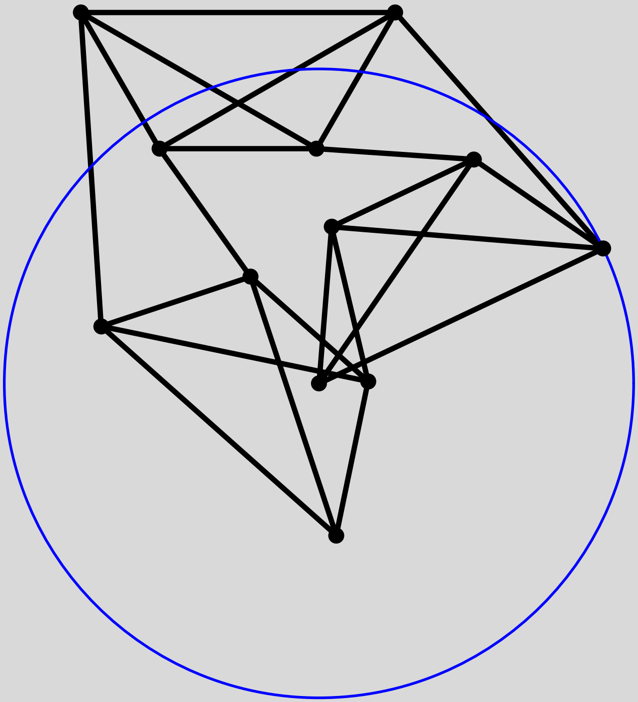


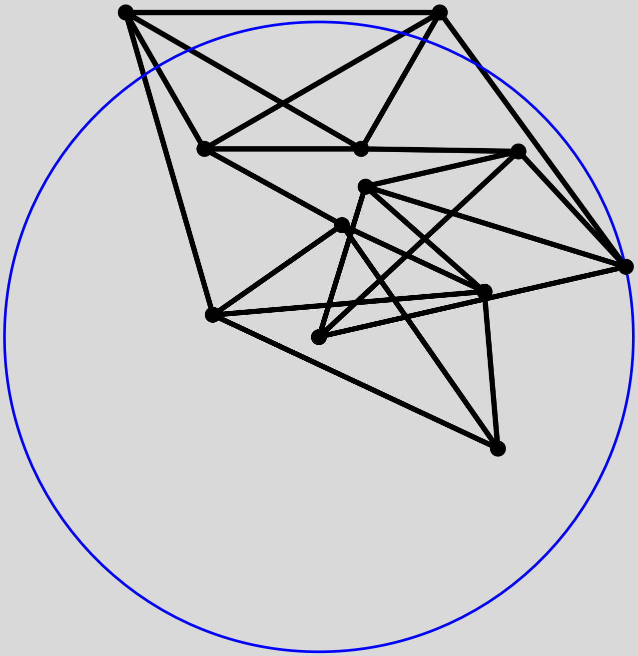


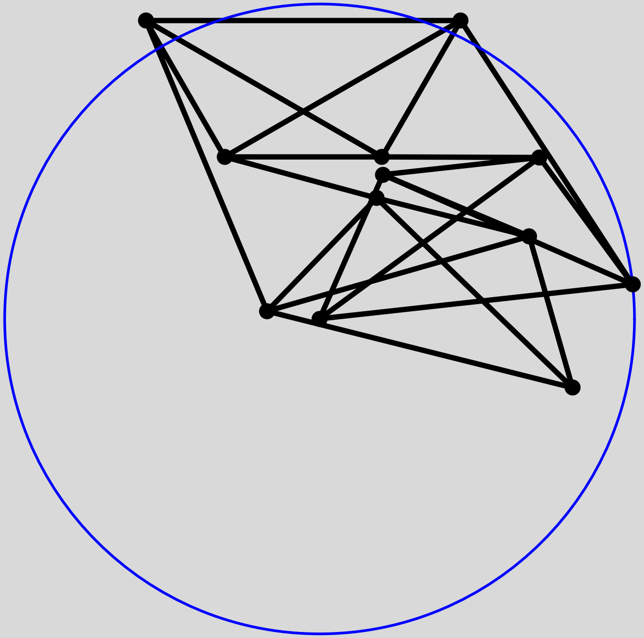


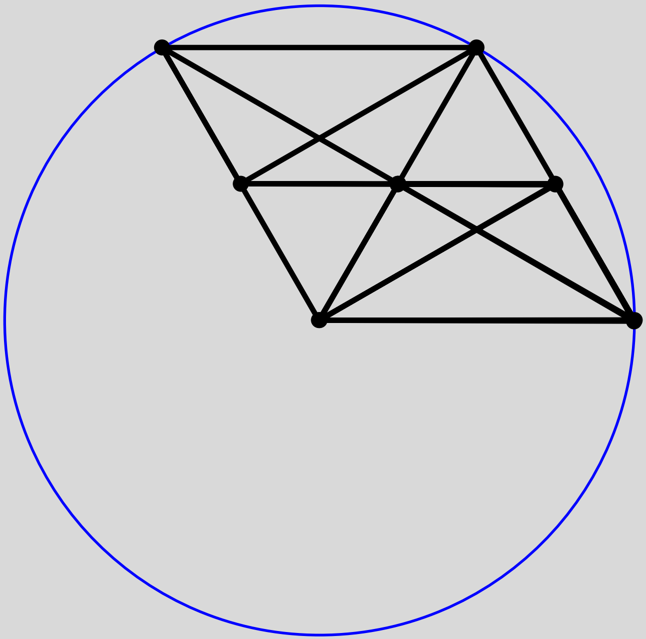












However,Lovász and Yemini [9] note that their proof technique will show that $G - \{e_1, e_2, e_3\}$ is rigid for all $e_1, e_2, e_3 \in E$, and hence that G is redundantly rigid. This result was combined with Theorem 3 in [5] to deduce

Theorem 6 *Every* 6*-connected graph is globally rigid.*

5. Random graphs

Let $G_{n,d}$ denote the probability space of all d-regular graphs on n vertices with the uniform probability distribution. A sequence of graph properties A_n holds asymptotically almost surely, or a.a.s. for short, in $G_{n,d}$ if $\lim_{n\to\infty} \Pr_{G_{n,d}}(A_n) = 1$. Graphs in $G_{n,d}$ are known to be a.a.s. highly connected. It was shown by Bollobás [1] and Wormald [12] that if $G \in G_{n,d}$ for any fixed $d \geq 3$, then G is a.a.s. d-connected. This result was extended to all $3 \leq d \leq n-4$ by Cooper et al. [3] and Krivelevich et al. [6]. Stronger results hold if we discount 'trivial' cutsets. In [13], Wormald shows that if $G \in G_{n,d}$ for any fixed $d \geq 3$, then G is a.a.s. cyclically $(3d-6)$-edge-connected.

Theorem 7 *If $G \in G_{n,4}$ then G is a.a.s. globally rigid.*

In fact this result holds for all $d \geq 4$.

Theorem 8 *If $G \in G_{n,d}$ and $d \geq 4$ then G is a.a.s. globally rigid.*

Let $G(n,p)$ denote the probability space of all graphs on n vertices in which each edge is chosen independently with probability p. In the following we will assume that all logarithms are natural. We will need the following results on $G(n,p)$.

Lemma 1 *Let $G \in G(n,p)$, where $p = (\log n + k \log\log n + w(n))/n$, $k \geq 2$ is an integer and $\lim_{n\to\infty} w(n) = \infty$. For each fixed integer t, let S_t be the set of vertices of G of degree at most t. Then, a.a.s.*
(a) S_{k-1} is empty,
(b) no two vertices of S_t are joined by a path of length at most two in G,
(c) $G - S_{t-1}$ is non-empty and t-connected.

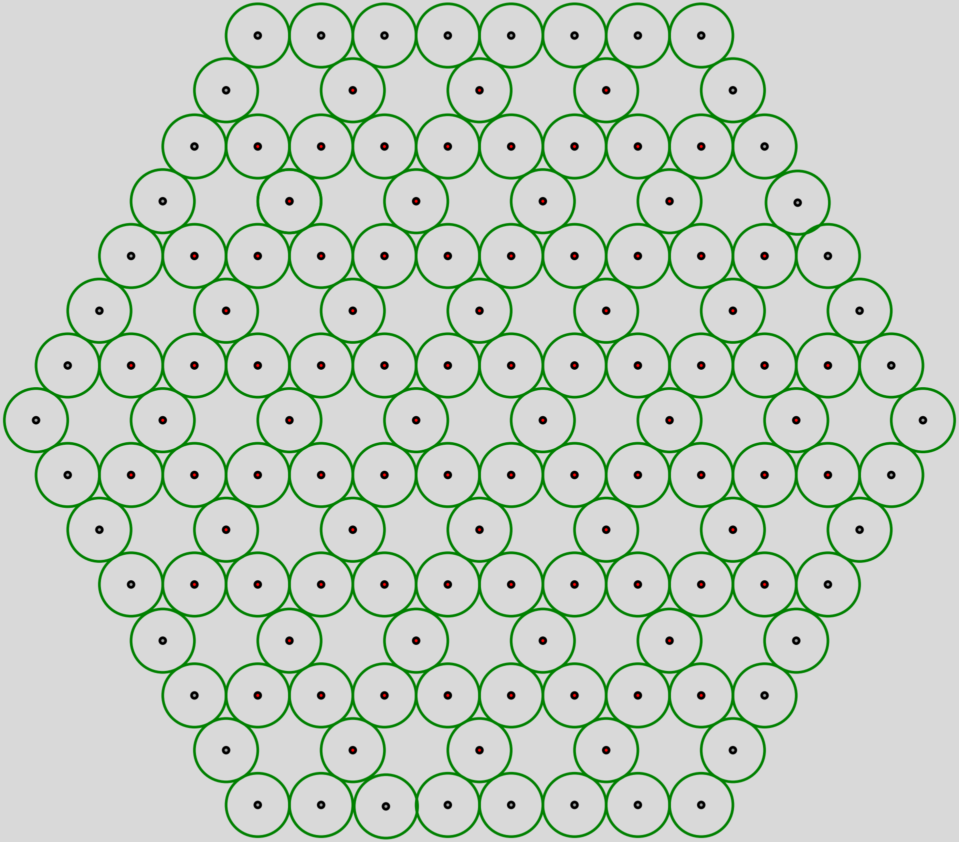
Proof: Facts (a) and (b) are well known, see for example [2]. Fact (c) follows from (a), (b) and [10, Theorem 4] $\square$

Theorem 9 *Let $G \in G(n,p)$, where $p = (\log n + k \log\log n + w(n))/n$, and $\lim_{n\to\infty} w(n) = \infty$.*
(a) If $k = 2$ then G is a.a.s. rigid.
(b) If $k = 3$ then G is a.a.s. globally rigid.

PROOF: (a) We adopt the notation of Lemma 1. It follows from Lemma 1 that a.a.s. $S_1 = \emptyset$ and $G - S_5$ is a.a.s. 6-connected. Hence $G - S_5$ is a.a.s. (globally) rigid by Theorem 6. Since adding a new vertex joined by at least two new edges to a rigid graph preserves rigidity, it follows that G is a.a.s. rigid.
(b) This follows in similar way to (a), using the facts that $S_2 = \emptyset$ and that adding a new vertex joined by at least three new edges to a globally rigid graph preserves global rigidity. $\square$

The bounds on p given in Theorem 9 are best possible since if $G \in G(n,p)$ and $p = (\log n + k \log\log n + c)/n$ for any constant c, then G does not a.a.s. have minimum degree at least k, see [2].

The Kagome Lattice



Let $Geom(n, r)$ denote the probability space of all graphs on n vertices in which the vertices are distributed uniformly at random in the unit square and each pair of vertices of distance at most r are joined by an edge. Suppose $G \in Geom(n, r)$. Li, Wan and Wang [8] have shown that if $n\pi r^2 = \log n + (2k - 3)\log\log n + w(n)$ for $k \geq 2$ a fixed integer and $\lim_{n\to\infty} w(n) = \infty$, then G is a.a.s. k-connected. As noted by Eren et al. [4], this result can be combined with Theorem 6 to deduce that if $n\pi r^2 = \log n + 9\log\log n + w(n)$ then G is a.a.s. globally rigid. On the other hand, it is also shown in [8] that if $n\pi r^2 = \log n + (k-1)\log\log n + c$ for any constant c, then G is not a.a.s. k-connected. It is still conceivable, however, that if $n\pi r^2 = \log n + \log\log n + w(n)$ then G is a.a.s. rigid, and that if $n\pi r^2 = \log n + 2\log\log n + w(n)$ then G is a.a.s. globally rigid.

6. More general structures

Bar and joint frameworks

rigid bars (edges), universal joints (vertices)

Body and hinge frameworks

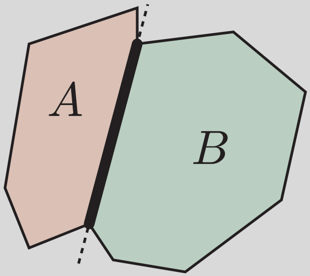
rigid bodies (vertices), hinges (edges)

n-space: Generic Body and Hinge Frameworks

Solved

Body and Hinge Frameworks in 3-space:

Each rigid body has 6 degrees of freedom.
If two bodies are joined along a linear hinge the resulting structure has one internal degree of freedom.
Each hinge removes 5 degrees of freedom.



Graph $G = (B, H)$
B: vertices for abstract bodies,
H: for pairs of bodies sharing a hinge.
Necessary condition for independence:

$$5|H'| \leq 6|B'| - 6$$

Theorem 10 (Tay and Whiteley – 1984) *The necessary condition is also sufficient for generic independence.*

Algorithms:

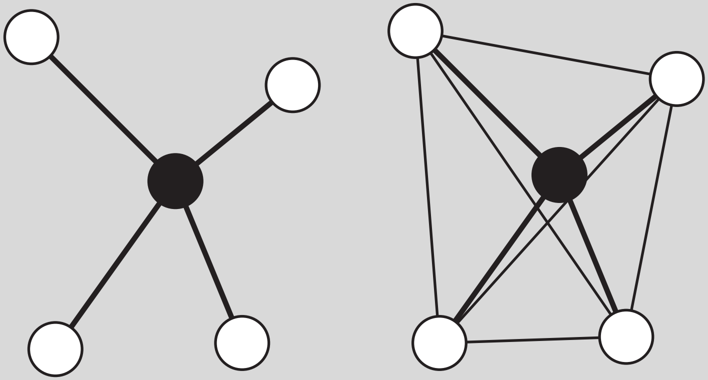
$$6|B'| - 6 = 6(|B'| - 1)$$

or
6 spanning trees in $5G(B, H)$, which is the multi-graph obtained from $G(B, H)$, by replacing each edge by a set of 5 parallel edges.

7. Modeling molecules

(special graphs) - can we predict rigidity?

Single atom and associated bonds

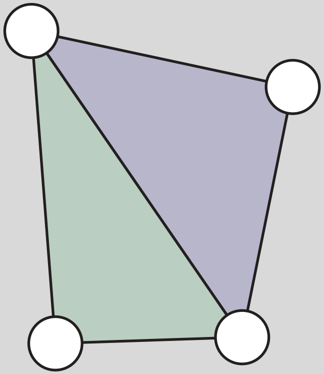


$$|V| = 5 \qquad |E| = 10$$

$$|E| = 3|V| - 5 \qquad \text{overbraced}$$

Adjacent atom clusters

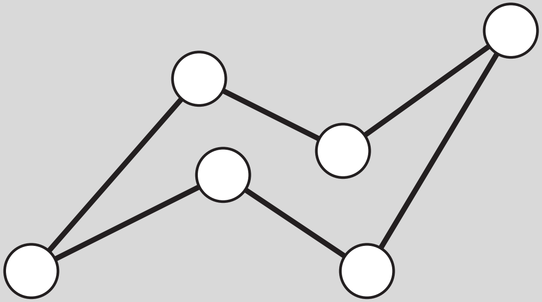
Flexible

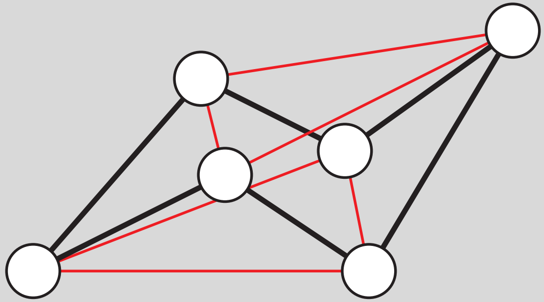


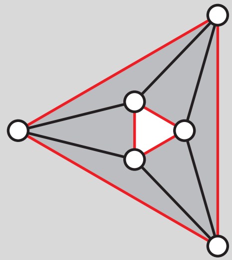
$$|B| = 2, |H| = 1, \qquad 5|H| = 6|B| - 7,$$
$$|V| = 4, |E| = 5, \qquad |E| = 3|V| - 7$$

Rings of atoms:

Ring of 6 atoms and bonds







Bar and Joint: $|V| = 6,\ |E| = 12,\quad |E| = 3|V| - 6$

Body and hinge: $|B| = 6,\ |H| = \ 6,\ 5|H| = 6|B| - 6$

Just the right number to be rigid - generically.

Graph G of atoms and covalent bonds
Can we use the body and hinge model to predict rigidity?
Problem: Some hinges are concurrent
Special geometry may lower rank!

Graph G of atoms and covalent bonds
To utilize the bar and joint model, form G^2:
The new edges model second neighbor bond bending pairs.
Count as

$$3|V| - 6$$

priority system on bond edges.
Problem: for general graphs G the rank may be lower. (May work for G^2?)

Lots of experimental evidence
Proofs of correctness for special classes of graphs
Plausibility arguments related to other conjectures on 3-space rigidity
Sketched proof of equivalence of the two conjectures.
Conjectures embedded in implemented algorithms: FIRST on the web (Arizona State University)

8. Molecular Conjecture in the Plane

Given: Simple graph $G = (V, E)$.

- Regard G as a body and pin graph of a structure in the plane:

  Vertices are bodies.

  Edges denote pins.

- Note: Each pin connects just two bodies. Otherwise we would need a hyper-graph.

- Realizations:
  - Amorphous bodies. Embedding specifies the location of the pins.
  - Line bodies. Embedding may specify either lines or pins.
  - Question: Does the line realization always exist?

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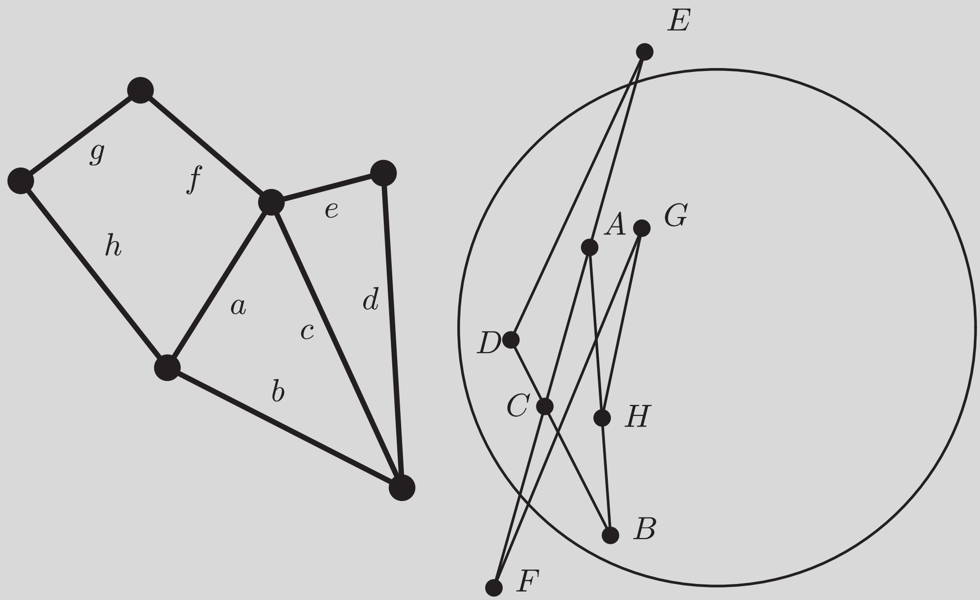
9. Realization in the Plane.

Theorem 11 *If $G = (V, E)$ is simple, then a pin collinear structure exists.*

Take any generic embedding of the structure graph $G = (V, E)$ in $\mathbb{R}^2$. Form the polar of that embedding.

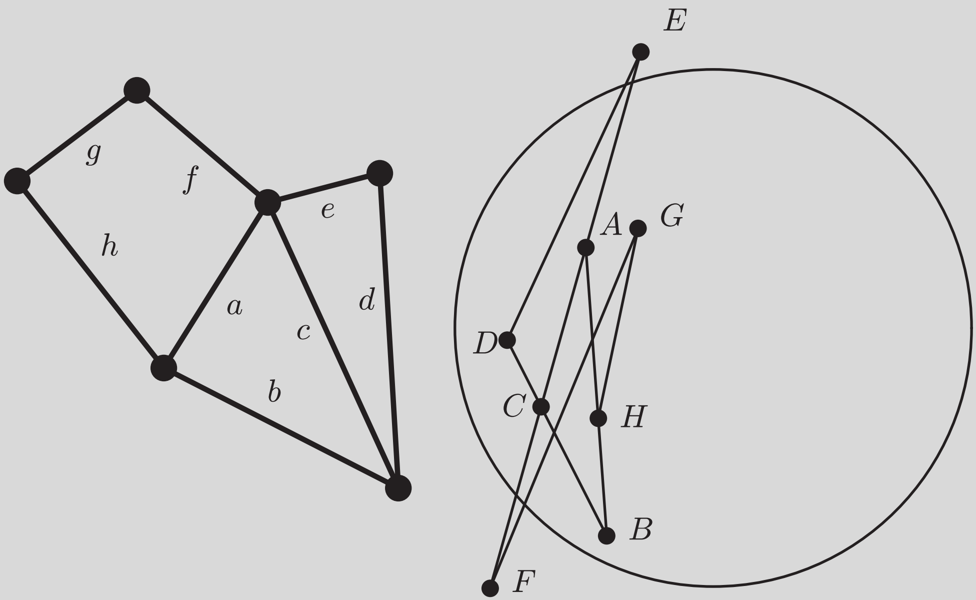


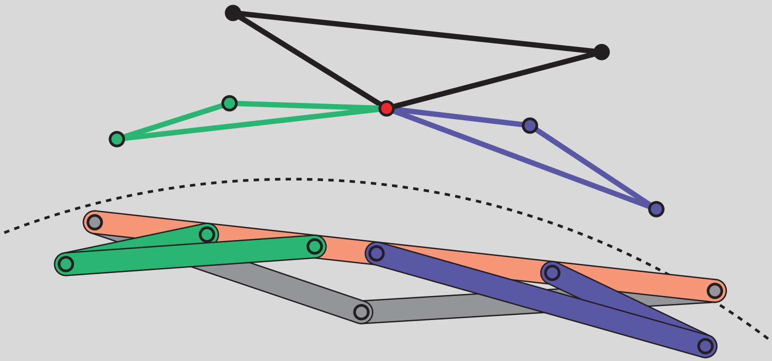
Question:

Is the polar generic as a line-pin structure?

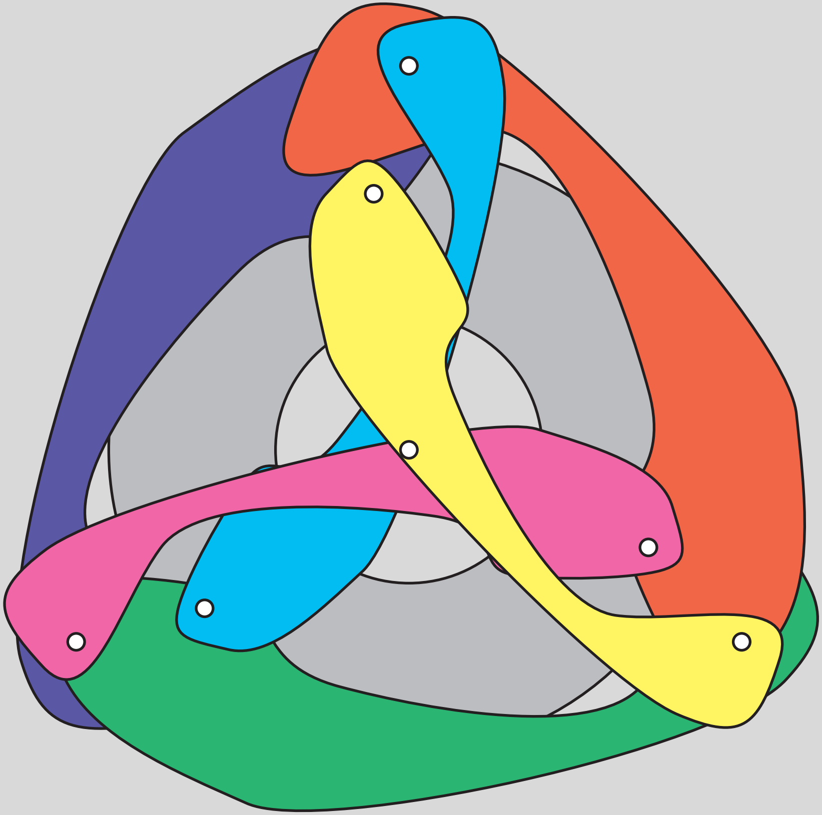
Question:

Does it have the same rank as a generic body-pin structure?

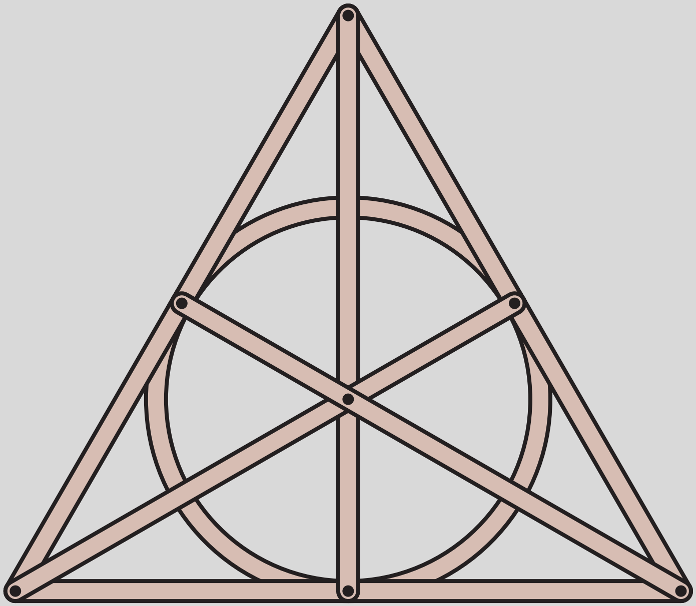




A general body-pin structure:



The incidence structure is a hyper-graph. Does it have a pin collinear realization?



Theorem 12 *A multigraph G can be realized as an infinitesimally rigid body and hinge framework in $\mathbb{R}^d$ if and only if $\left(\binom{d+1}{2}-1\right)G$ has $\binom{d+1}{2}$ edge-disjoint spanning trees. (Tay and Whiteley, 1984)*

Recent Advances in the Generic Rigidity of Structures, Tiong-Seng Tay and Walter Whiteley Structural Topology # 9, 1984
Many body and hinge structures are built under additional constraints. For example in architecture flat panels may be used in which all hinges are coplanar. In molecular chemistry, we can model molecules by rigid atoms hinged along the bond lines so that all hinges to an atom are concurrent. This is the natural projective dual for the architectural condition.
Conjecture: A multigraph is generically rigid for hinged structures in n-space iff it is generically rigid for hinged structures in n-space with all hinges of body v_i in a hyperplane H_i of the space.

Jackson and Jordan show that the body-and-pin and rod-and-pin 2-polymatroids of a graph are identical. As a solution to the molecular conjecture they formulate

Theorem 13 *Let $G(V, E)$ be a multigraph. Then the following statements are equivalent:*
(a) G has a realization as an infinitesimally rigid body and hinge framework in $\mathbb{R}^2$.
(b) G has a realization as an infinitesimally rigid body-and-hinge framework (G, q) in $\mathbb{R}^2$ with each of the sets of points $\{q(e) : e \in E_G(v)\}, v \in V$, collinear.
(c)$2G$ contains 3 edge disjoint spanning trees.

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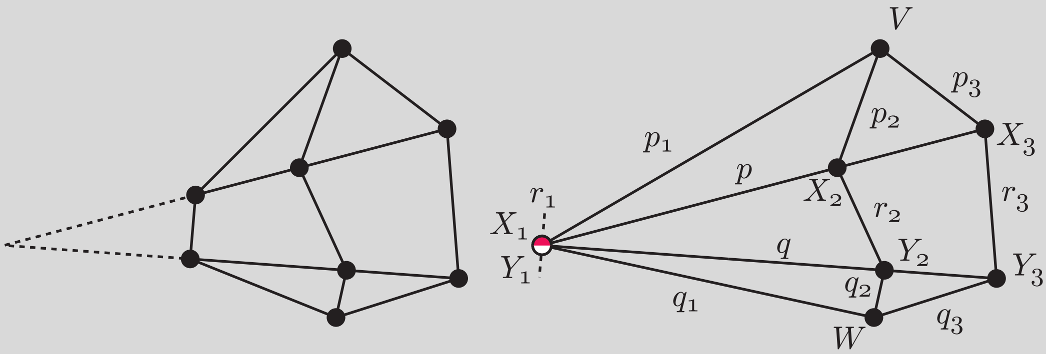

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$$\begin{array}{c}
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 & r_3 & & & & & -r_3 & \\
 & -x & x & & & & & \\
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 & & & & -y & y & & \\
 & & & & & -y & y & \\
-p_1 & & & p_1 & & & & \\
-p_2 & & p_2 & & & & & \\
-p_3 & p_3 & & & & & & \\
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 & & & & & q_2 & & -q_2 \\
 & & & & & & q_3 & -q_3
\end{bmatrix}
\end{array}$$

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-p_3 & p_3 & & & & & & \\
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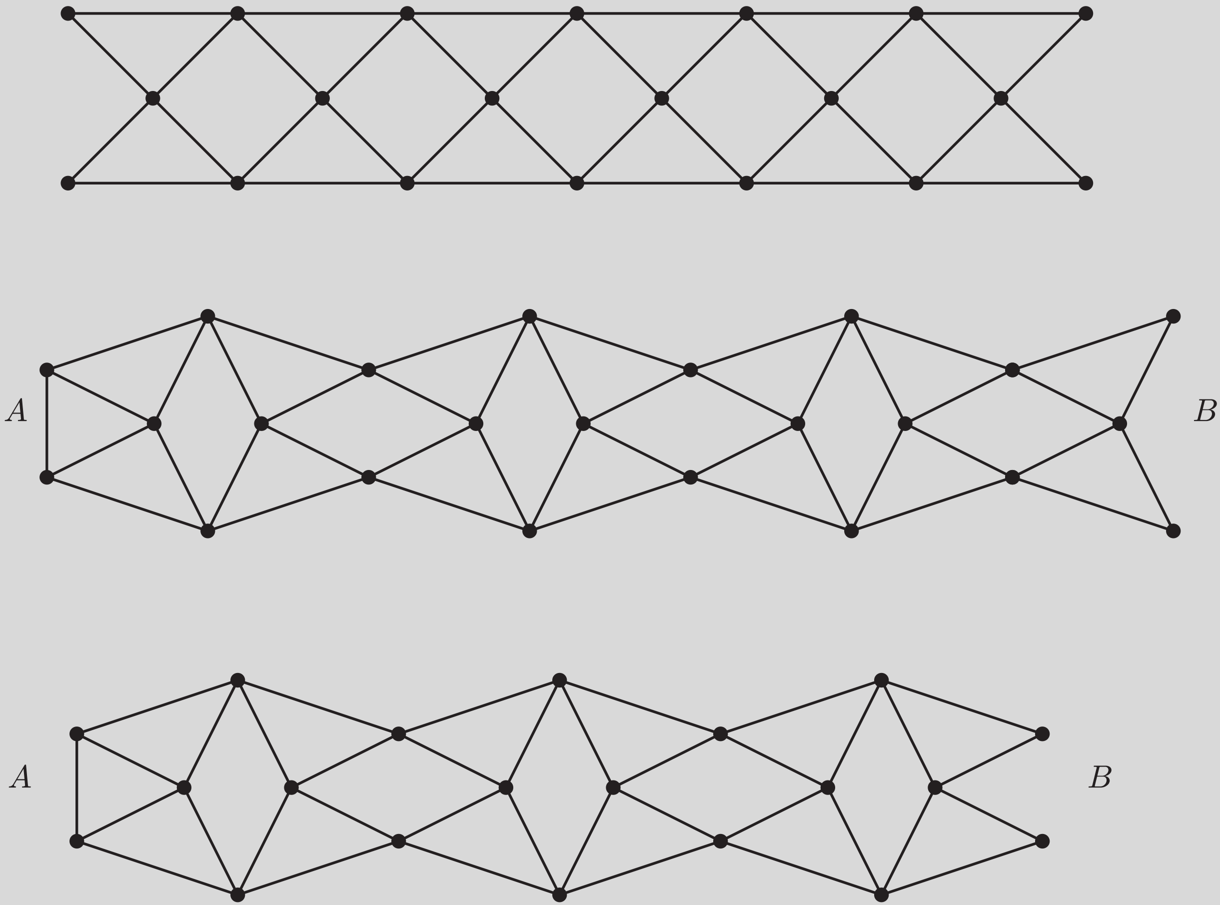
\end{array} \\
\begin{bmatrix}
 & & & r_1^{\perp} & & & & \\
 & & & r_1 & & & & \\
 & & r_2 & & & -r_2 & & \\
 & r_3 & & & & & -r_3 & \\
 & -x & x & & & & & \\
 & & -x & & x & & & \\
 & & & & -y & y & & \\
 & & & & & -y & y & \\
-p_1 & & & & p_1 & & & \\
-p_2 & & p_2 & & & & & \\
-p_3 & p_3 & & & & & & \\
 & & & & q_1 & & & -q_1 \\
 & & & & & q_2 & & -q_2 \\
 & & & & & & q_3 & -q_3
\end{bmatrix}
\end{array}
$$

10. Combinatorial Allostery



11. Open problems

- Is the solution of the molecular conjecture useful for computational biology?
- Translate combinatorial allostery to molecules.
- Are random 6-regular graphs rigid in 3-space?
- Generalizations to tensegrities?
- Can sparse random graphs be realized as unit distance graphs?

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