Rigidity percolation

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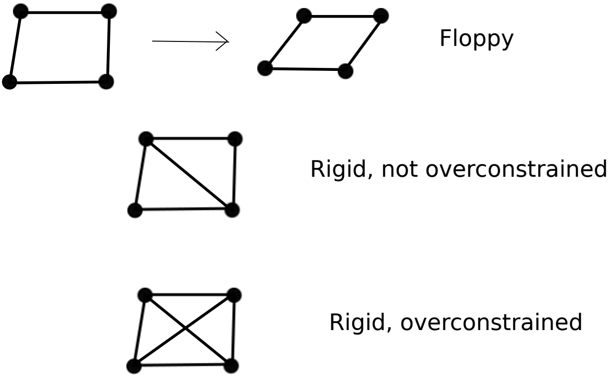
Rigidity

- Consider bars, which have a fixed length, linked together by "joints". Is the system rigid or floppy ?

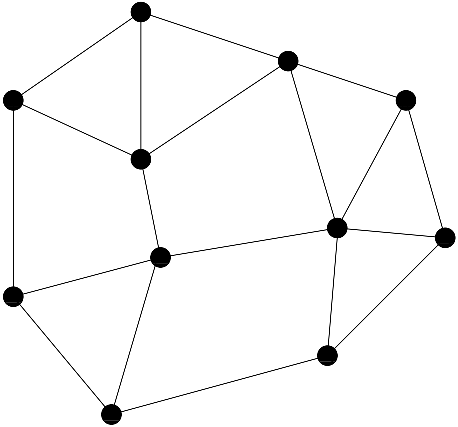
Example in 2 dimensions; bar lengths are fixed, not the angles:



Rigidity

- When there are only a few joints and bars, it is easy...

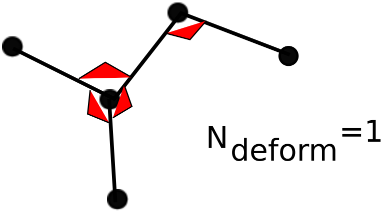
What about this network, with 11 sites?



- Is it floppy? Rigid? How many floppy modes? Where?

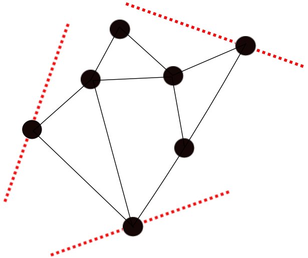
Related problems

• Bond bending constraints: angles between two adjacent bonds have to be kept fixed ($D = 3$)



Related problems

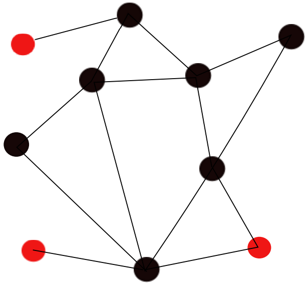
• Bond bending constraints: angles between two adjacent bonds have to be kept fixed ($D = 3$)
• Rigidity with "sliders": some joints constrained to move on a line



Related problems

- Bond bending constraints: angles between two adjacent bonds have to be kept fixed ($D = 3$)
- Rigidity with "sliders": some joints constrained to move on a line

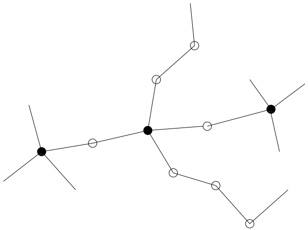
- Rigidity with "pinned" joints, which cannot move at all



An application : "covalent glasses"

• Example: a disordered network with Germanium and Selenium atoms. Ge = 4 bonds; Se = 2 bonds.

• Bond lengths and angles between two adjacent bonds can be considered as constraints ($\sim$ the energy needed to modify them is larger than the temperature).

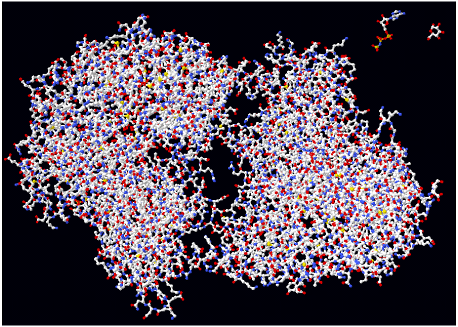


Each bond: 1 length constraint; each *Se* atom: 1 angular constraint; each *Ge* atom: 5 angular constraints.

$\rightarrow$ Go from "floppy" to "rigid" by increasing the *Ge* fraction.

Another application: protein rigidity (MF Thorpe and coworkers)

- Proteins are large biological molecules. An example (hexokinase):



Let's simplify:

Atoms $\rightarrow$ balls; chemical (or other strong) bonds $\rightarrow$ bonds; weak interactions $\rightarrow$ forgotten!

$\rightarrow$ is the simplified structure floppy or rigid?

$\rightarrow$ if floppy, what are the possible deformations?

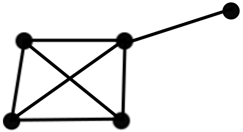
Constraint counting

Maxwell's idea: constraint counting
• each joint starts with 2 degrees of freedom
• each bar removes one degree of freedom
→ First try: formula for the number of remaining degrees of freedom, $N_{d.o.f.}$; N joints, M bars:

$$N_{d.o.f.} = 2N - M \text{ if } M < 2N - 3 \; ; \; N_{d.o.f.} = 3 \text{ if } M \geq 2N - 3$$

• Cannot be correct... Need to count redundant constraints:

$$N_{d.o.f.} = 2N - M + N_{redundant}$$



N=5; M=7
$N_{redundant} = 1$
$N_{d.o.f.} = 4$

From geometry to graph theory: Laman theorem

• Power of constraint counting: replace a geometrical problem by a discrete, graph theoretical one.

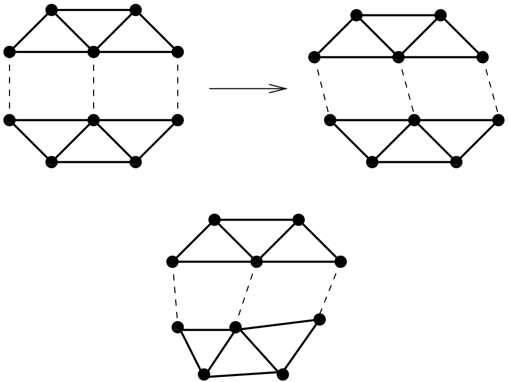
Question: is it possible to keep this desirable feature, correcting the approximations of constraint counting?

• Generic rigidity in 2D can be characterized in a purely graph theoretical way (Laman 1970):

G has a redundant constraint $\iff$ there is a subgraph with n vertices, m edges and $m > 2n - 3$.

$\rightarrow \sim$ constraint counting on each subgraph to detect redundant constraints

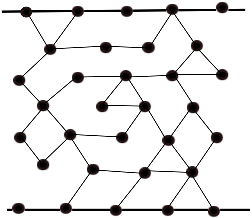
Generic rigidity



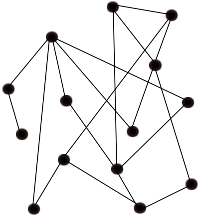
Top: a non generic realization; Laman theorem does not apply.
Bottom: a generic realization of the same graph.

Second ingredient: probabilities

In many cases, the structure is too large to be known exactly (think of covalent glasses for instance) → one would like to use a probabilistic description



Each link between a pair of neighboring vertices is present with proba. p<1

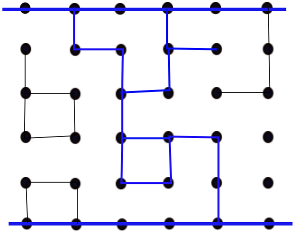


Links put "randomly", no geometry.

It is a percolation problem.

"Standard" percolation

- "connectivity" percolation = well studied since the 60's



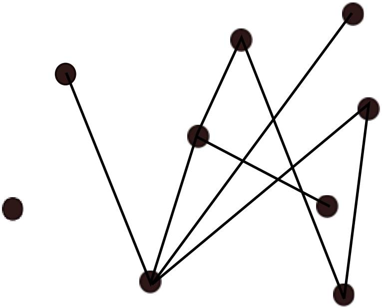
- Each link is present with proba. p, and absent with proba. 1-p

- Question: is there a path from top to bottom?

NB1: standard percolation is analog to "rigidity" percolation with one "degree of freedom" per vertex
NB2: standard percolation on a random graph = appearance of a "giant connected component"

Erdos-Renyi random graphs

Definition of $\mathcal{G}(n, c/n)$: n vertices; any pair of vertices connected with proba. c/n. There is no notion of space.



Some properties: approximately $nc/2$ edges; Poisson $\mathcal{P}(c)$ degree distribution; few small loops$\cdots$

Questions for rigidity percolation

• Is there a well defined threshold p_c for the appearance of a "macroscopic rigid cluster"?

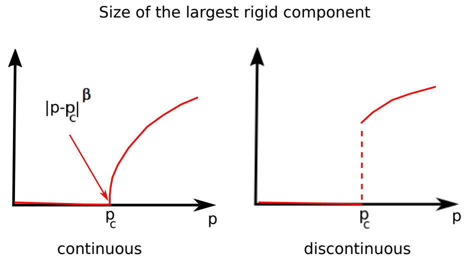
$$p < p_c \Rightarrow \text{percolation probability} = 0$$

$$p > p_c \Rightarrow \text{percolation probability} = 1$$

Answer: yes for random graphs and lattices (Numerics in the 90's; Holroyd $\sim$2000); threshold computed by Kasiwisvanathan, Moore and Theran (KMT 2011) for $\mathcal{G}(n, c/n)$ random graphs, unknown for lattices.

Questions for rigidity percolation

- Size of the largest rigid component? Continuous/discontinuous at p_c?



Questions for rigidity percolation

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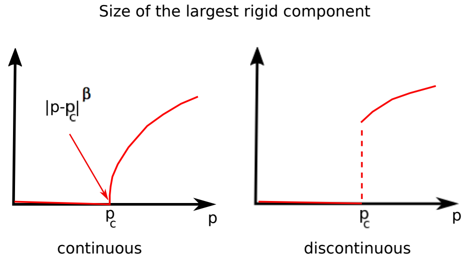
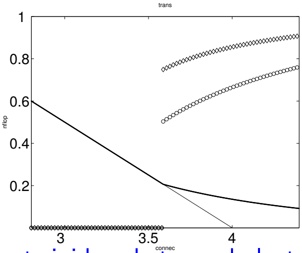


Answer:
-Discontinuous for $\mathcal{G}(n, c/n)$ random graphs (Theran)
-seems to be continuous for lattices (Jacobs-Thorpe, Duxbury-Moukarzel 90's, numerics).

Questions for rigidity percolation

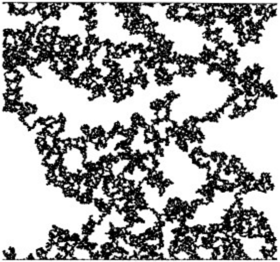
• Size of the largest rigid component? Continuous/discontinuous at p_c?
Example: Erdös-Rényi random graph $\mathcal{G}(n, c/n)$. Vary c



Size of the biggest rigid and stressed clusters, and number of "floppy modes" vs mean connectivity

Questions for rigidity percolation

• For lattices, what happens close to threshold? = "Critical" behavior? $\beta = ?$ (critical exponent, exciting for statistical physicists); fractal dimension?



Overconstrained regions (Simulation by P. Duxbury et al.)

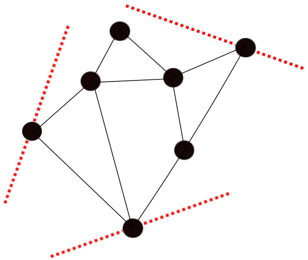
Answer: unknown. Critical exponents seem to be different from standard percolation.

Goals

Fully understand the 2D lattice case: difficult... More modest goals:

1. Find models that can be solved;
2. Explore similarities/differences standard percolation/rigidity percolation: study models that interpolate between both.

→ Study rigidity percolation with sliders on random graphs



→ Study other kind of "simple" lattices (eg. hierarchical).

Rigidity with sliders

• Consider a structure with n_1 sites with sliders, n_2 free sites and m bars. One slider = one constraint
→ modify constraint counting

Difficulty: sliders "pin" the rigid components to the plane
→ Distinguish between free, partly pinned, and pinned rigid clusters

A Laman-type theorem (I. Streinu, L. Theran, 2010).
Redundant constraint $\iff$ subgraph with

$$n'_1 + 2n'_2 - m' - \max(3 - n'_1, 0) < 0$$

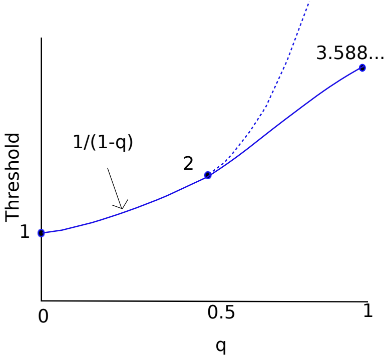
→ A graph theoretical approach possible (under a genericity condition, as usual)

Rigidity percolation with sliders

- Erdös-Renyi random graph $\mathcal{G}(n, c/n)$, with $n = n_1 + n_2$
$n_1 = (1 - q)n$, $n_2 = qn$.
$1 - q =$ proportion of sites with sliders
- $q = 0$: ordinary percolation = well known; continuous
- $q = 1$: rigidity percolation, discontinuous; threshold $c = 3.588\ldots$
- **What happens in between?**

Threshold

- percolation threshold vs proportion of sliders



- $c^* = 1/(1-q)$ for $q \leq 1/2$
- For $q > 1/2$, implicit expression for $c^*(q)$:

$$c^* = \frac{\xi^*}{1 - e^{-\xi^*} - q\xi^* e^{-\xi^*}}, \; \frac{\xi^*(1 - e^{-\xi^*} - q\xi^* e^{-\xi^*})}{(1+q)(1 - e^{-\xi^*} - q\xi^* e^{-\xi^*}) - q(\xi^*)^2 e^{-\xi^*}} = 2\,.$$

Rigidity percolation with sliders, 2

Theorem: (JB, M. Lelarge, D. Mitsche)
Let $G \sim \mathcal{G}(n, c/n)$ an Erdos-Renyi random graph, with a fraction $1 - q$ of sliders. Then, we can compute $c^*(q)$, such that with high probability (proba $\to 1$ when $n \to \infty$):

- If $c < c^*(q)$, there is no giant rigid component
- If $c > c^*(q)$, there is a giant rigid component

Furthermore, for $q < 1/2$ the transition is continuous, and for $q > 1/2$ it is discontinuous.

NB: $c^*(q = 0) = 1$ and $c^*(q = 1) = 3.588\ldots$

Size of the largest rigid component

- Size of the largest component at threshold: jump for $q > 1/2$:

$\sim$ rigidity without sliders.

- Continuous transition for $q < 1/2$: $\sim$ connectivity percolation.
- Discontinuous transition for $q > 1/2$.

$\rightarrow$ *tricritical point* at $q = 1/2$ (statistical mechanics jargon)

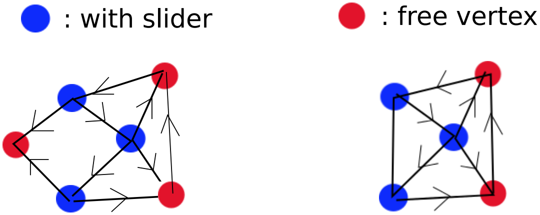
Strategy of proof

- **Step 1:** Link with *orientability* (generalizes the case without sliders)

-Intuition: one bond removes one degree of freedom to one of the two vertices it links

-Vertices with or without slider: 1 or 2 degree of freedom

→ Link with "orientability"



orientable

not orientable

Strategy of proof, 2

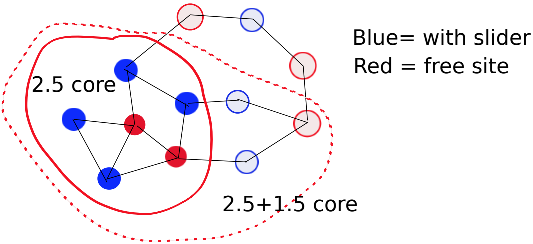
- **Step 2:** Thresholds for orientability and percolation are equal
"Rigid" $\Rightarrow$ "Non orientable" $=$ easy
"Non orientable" $\Rightarrow$ "Rigid" $=$ more laborious

- **Step 3:** Compute the threshold for orientability $\rightarrow$ method introduced by M. Lelarge
$\sim$ rigorous "cavity method", a heuristic introduced by physicists.

Step 4: type of transition

- For $q > 1/2$ ("rigidity-like" transition), a density argument applies: rigid components must be dense enough, and dense subgraphs must have a minimal size of order n (uses again the generalization of L. Theran's lemma).
$\rightarrow$ discontinuous transition

- For $q < 1/2$ ("connectivity-like" transition), we need "cores"



Remove recursively blue sites with less than 2 links and red sites with less than 3. What remains is the "2.5-core". Then add recursively blue sites with one link to the core, and red sites with 2. One gets the "$2.5 + 1.5$-core".

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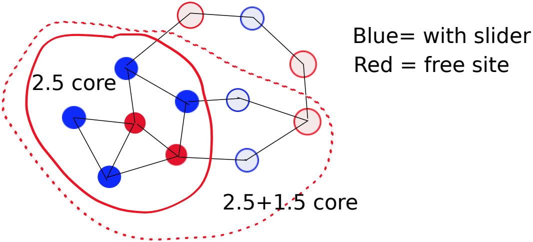


Then show: largest rigid component $\subset 2.5 + 1.5$-core

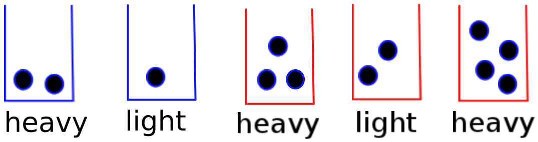
- Compute the size of the $2.5 + 1.5$-core and show it is small.

Step 5: Size of cores

- Size of the $3 + 2$ core $=$ conjecture in Kasivisvanathan-Moore-Theran 2011.

- Strategy: use Janson-Luczak technique

Bins = vertices, with sliders (blue) or without (red)
Balls = half edges



$\rightarrow$ good knowledge of degree distributions after the core construction
$\rightarrow$ possible to control the process growing the 3+2 core.

Conclusions on random graphs

- Complete phase diagram with a tricritical point
- Proof combines many "old" ideas: strategy Theran et al. relating to orientability; M. Lelarge's technique to compute orientability threshold; Janson-Luczak technique to compute the size of cores
- What about rigidity with some pinned sites? Conjecture by physicists (Moukarzel '03): the discontinuous transition may disappear, but there is no continuous transition... *A proof seems accessible -joint work with Dieter Mitsche and Louis Theran*
- Physics literature: tree-like heuristics give access to much more detailed results (Large Deviation Cavity Method); could these be transformed into theorems? A general question, beyond rigidity.

Beyond random graphs?

- Random graphs: much easier than percolation problems on lattices . . .
- whereas problems on lattices, or at least on graphs with some geometric content, are a priori more interesting for physics.
- Understand the phase transition on regular lattices (beyond existence proof by Holroyd)? Precise numerical simulations would be useful; I don't even have heuristic theoretical ideas... $\rightarrow$ a lot to do here!