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Generically globally rigid zeolites in the plane

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Abstract

A d-dimensional zeolite is a d-dimensional body-and-pin framework with a (d+1)-regular underlying graph G. That is, each body of the zeolite is incident with d+1 pins and each pin belongs to exactly two bodies. The corresponding d-dimensional combinatorial zeolite is a bar-and-joint framework whose graph is the line graph of G.

We show that a two-dimensional combinatorial zeolite is generically globally rigid if and only if its underlying 3-regular graph G is 3-edge-connected. The proof is based on a new rank formula for the two-dimensional rigidity matroid of line graphs.

1 Introduction

A *d*-dimensional zeolite is a *d*-dimensional body-and-pin framework in which each body is incident with d + 1 pins and each pin belongs to exactly two bodies. In the underlying graph G of the zeolite vertices correspond to bodies and two vertices are adjacent if and only if the corresponding bodies share a pin. Thus the underlying graph of the zeolite is (d + 1)-regular.

By replacing the bodies by complete bar frameworks one obtains a *d*-dimensional combinatorial zeolite. It is a bar-and-joint framework whose graph is the line graph of the underlying graph G of the zeolite. (The line graph L(G) of a graph G = (V, E) is the simple graph with vertex set $\{v_e : e \in E\}$, where two vertices v_e, v_f are adjacent if and only if e, f have a common end-vertex in G.) See Figure 1 for a two-dimensional example.

The investigation of these structures is motivated in part by the existence (and flexibility properties) of real zeolites, which are molecules formed by corner-sharing tetrahedra, see e.g. [3]. Planar plate frameworks (which contain planar zeolites as a special case), in which each body is a regular polygon, have also been studied in the combinatorial rigidity literature [2]. In this paper we shall consider the (global) rigidity properties of planar combinatorial zeolites in generic position.

Roughly speaking, a combinatorial zeolite is globally rigid if its bar lengths uniquely determine the whole framework, up to congruence. Brigitte Servatius and Herman

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Figure 1: A 3-regular graph G and its line graph L(G). The shaded triangles of the bar-and-joint framework on L(G) correspond to the bodies in the two-dimensional zeolite whose underlying graph is G.

Servatius [9] asked whether there is a simple necessary and sufficient condition, in terms of its underlying graph, for the global rigidity of a planar zeolite whose vertices are in generic position. We shall give an affirmative answer in Section 3 by showing that a planar combinatorial zeolite is generically globally rigid if and only if its 3-regular underlying graph is 3-edge-connected. The proof is based on a new rank formula for the two-dimensional rigidity matroid of line graphs. This formula, along with the necessary definitions, is given in Section 2. The last section is devoted to some concluding remarks.

2 Rigidity of line graphs

We shall need the following basic notions of combinatorial rigidity. For a detailed survey of the area we refer the reader to [1, 10]. A *d*-dimensional (bar-and-joint) framework is a pair (G, p), where G = (V, E) is a graph and p is a map from V to \mathbb{R}^d . We also say that (G, p) is a realization of G in \mathbb{R}^d . We can think of the edges and vertices of G in the framework as rigid (fixed length) bars and universal joints, respectively. Two frameworks (G, p) and (G, q) are equivalent if corresponding edges have the same lengths, that is, if ||p(u) - p(v)|| = ||q(u) - q(v)|| holds for all pairs u, vwith $uv \in E$, where ||.|| denotes the Euclidean norm in \mathbb{R}^d . Frameworks (G, p), (G, q)are congruent if ||p(u) - p(v)|| = ||q(u) - q(v)|| holds for all pairs u, v with $u, v \in V$. We shall say that (G, p) is globally rigid if every framework which is equivalent to (G, p) is congruent to (G, p).

Rigidity is a weaker property of frameworks than global rigidity. Intuitively, a framework is rigid if it has no continuous deformations. Equivalently, and more formally, a framework (G, p) is *rigid* if there exists an $\epsilon > 0$ such that, if (G, q) is equivalent to (G, p) and $||p(u) - q(u)|| < \epsilon$ for all $v \in V$, then (G, q) is congruent to (G, p).

A framework (G, p) is said to be *generic* if the set containing the coordinates of all its points is algebraically independent over the rationals. It is known that rigidity as well as global rigidity are generic properties of *d*-dimensional frameworks for all *d*, that is, the (global) rigidity of a generic realization of a graph *G* depends only on the graph *G* and not the particular realization. We say that the graph *G* is *rigid*, respectively *globally rigid*, in \mathbb{R}^d if every (or equivalently, if some) generic realization of *G* in \mathbb{R}^d is rigid, respectively globally rigid. Many of the (global) rigidity properties of a generic framework (*G*, *p*) are determined by an associated matroid, the *d*-dimensional rigidity matroid $\mathcal{R}_d(G)$, defined on the edge set of *G*. We denote the rank of $\mathcal{R}_d(G)$ by $r_d(G)$.

In what follows we shall focus on the case d = 2. In this case rigidity and the rank function of the rigidity matroid are well characterized. It is known that a graph G = (V, E) is rigid in \mathbb{R}^2 if and only if $r_2(G) = 2|V| - 3$. It is also known that the edge set of G is independent in $\mathcal{R}_2(G)$ if and only if each subset $X \subseteq V$ with $|X| \ge 2$ induces at most 2|X| - 3 edges [7]. Lovász and Yemini [8] characterized rigid graphs in \mathbb{R}^2 by providing a formula for $r_2(G)$, in terms of 'thin covers' of G. We shall use the following refinement of their result, which uses rigid components, see [1, Section 4.4]. We define a *rigid component* of a graph G = (V, E) to be a maximal rigid subgraph of G. By the *glueing lemma* (see [10, Lemma 3.1.4]), which says that the union of two rigid graphs with at least two vertices in common is rigid, it follows that any two rigid components of G.

Theorem 2.1. [1, 8] Let H = (V, E) be a graph with rigid components $H_1, H_2, ..., H_t$. Then

$$r_2(H) = \sum_{i=1}^{l} (2|C_i| - 3)$$

where $C_i = V(H_i), 1 \leq i \leq t$.

Let G = (V, E) be a graph. For a family \mathcal{F} of pairwise disjoint subsets of V let $E_G(\mathcal{F})$ denote the set, and $e_G(\mathcal{F})$ the number, of edges of G connecting distinct members of \mathcal{F} . For a partition \mathcal{P} of V let

$$def_G(\mathcal{P}) = 3(|\mathcal{P}| - 1) - 2e_G(\mathcal{P})$$

denote the *deficiency* of \mathcal{P} in G and let

$$def(G) = max\{def_G(\mathcal{P}) : \mathcal{P} \text{ is a partition of } V\}.$$

We say that a partition \mathcal{P} of V is *tight* if $\operatorname{def}_G(\mathcal{P}) = \operatorname{def}(G)$ holds. Note that $\operatorname{def}(G) \geq 0$, since $\operatorname{def}_G(\{V\}) = 0$. For example, the graph G on Figure 1 has $\operatorname{def}(G) = 1$. The vertex sets of the four disjoint copies of ' K_4 minus an edge' in G form a tight partition of G.

The following rank formula (which is implicit in [6]) shows that the 'degree of freedom' of L(G) is equal to the deficiency of G.

Theorem 2.2. Let G = (V, E) be a graph with minimum degree at least two. Then

$$r_2(L(G)) = 2|E| - 3 - def(G).$$
(1)

Proof: First we prove that the right hand side is an upper bound on $r_2(L(G))$. Since |V(L(G))| = |E|, we have $r_2(L(G)) \le 2|E| - 3$. Thus we may assume that $def(G) \ge 1$. Let $\mathcal{Q} = \{Q_1, Q_2, ..., Q_t\}$ be a tight partition of V. Since $def(G) \ge 1$, we must have $t \ge 2$.

For $v \in V$ let B(v) denote the set of vertices in L(G) corresponding to the edges incident with v in G. Since G has minimum degree at least two, we have $|B(v)| \ge 2$ for all $v \in V$. Let $X_i = \bigcup_{v \in Q_i} B(v)$, for $1 \le i \le t$. Since each set B(v) contains at least two vertices, we have $|X_i| \ge 2$ for $1 \le i \le t$. Furthermore, $|\{X_i : v_e \in X_i\}| \le 2$ for each vertex v_e of L(G) with equality if and only if $e \in E_G(Q)$. Thus $\sum_{i=1}^t |X_i| = |E| + e_G(Q)$. Since every edge of L(G) is induced by some X_i and each set $X \subseteq V(L(G))$ with $|X| \ge 2$ induces at most 2|X| - 3 independent edges in $\mathcal{R}_2(L(G))$, we can deduce that

$$r_2(L(G)) \leq \sum_{i=1}^t (2|X_i| - 3) = 2|E| + 2e_G(\mathcal{Q}) - 3t$$

= 2|E| - 3 - def(G).

To prove that equality holds consider the rigid components $H_1, H_2, ..., H_t$ of L(G)and let $C_i = V(H_i)$ for $1 \le i \le t$. Since each set $B(v), v \in V$, induces a complete (and hence rigid) subgraph in L(G), we must have $B(v) \subseteq C_i$ for some $1 \le i \le t$. Furthermore, since $|B(v)| \ge 2$ for all $v \in V$, the maximality of the C_i 's and the glueing lemma imply that each B(v) is contained in exactly one set C_i . Let $Q_i = \{v \in V : B(v) \subseteq C_i\}, 1 \le i \le t$. Observe that $Q_i \ne \emptyset$ for all $1 \le i \le t$, since each rigid component H_i has at least one edge, say $v_e v_f$. Hence there is a vertex $x \in V$ which is a common end-vertex of edges e, f in G. Thus $|B(x) \cap C_i| \ge 2$ and hence, by the glueing lemma, $B(x) \subseteq C_i$ and $x \in Q_i$ must hold. It follows that $Q = \{Q_1, Q_2, ..., Q_t\}$ is a partition of V.

Claim 2.3. $v_e \in C_i \cap C_j$ for some $v_e \in V(L(G))$ and $1 \leq i < j \leq t$ if and only if $e \in E_G(Q_i, Q_j)$.

Proof: First suppose $v_e \in C_i \cap C_j$. Consider an edge $v_e v_f \in E(H_i)$. As above, we may deduce that there is a vertex $x \in V$, incident with e, f, with $x \in Q_i$. Similarly, by considering an edge $v_e v_h \in E(H_j)$ we obtain that there is a vertex $y \in V$, incident with e, h, with $y \in Q_j$. This implies that e = xy and $e \in E_G(Q_i, Q_j)$.

Conversely, suppose that $e = xy \in E_G(Q_i, Q_j)$. Then $B(x) \subseteq C_i$, $B(y) \subseteq C_j$. Since $v_e \in (B(x) \cap B(y))$, we have $v_e \in C_i \cap C_j$, as required.

By using Theorem 2.1 and Claim 2.3 we obtain

$$r_2(L(G)) = \sum_{i=1}^t (2|C_i| - 3) = 2|E| + 2e_G(\mathcal{Q}) - 3t$$

= $2|E| - 3 - \operatorname{def}(\mathcal{Q}) \ge 2|E| - 3 - \operatorname{def}(G),$

which completes the proof.

The lower bound on the minimum degree of G in Theorem 2.2 cannot be weakened. This follows by observing that if G is a star then L(G) is rigid but G is highly deficient.

3 Globally rigid zeolites

Globally rigid graphs in \mathbb{R}^2 have been characterized by Jackson and Jordán [5]. We say that a graph G is *redundantly rigid* in \mathbb{R}^2 if G - e is rigid in \mathbb{R}^2 for all $e \in E(G)$.

Theorem 3.1. [5] Let H be a graph. Then H is globally rigid in \mathbb{R}^2 if and only if H is a complete graph on at most three vertices or H is 3-vertex-connected and redundantly rigid in \mathbb{R}^2 .

If H is a line graph of a 3-regular graph then a simpler characterization follows from the next theorem.

Theorem 3.2. Let G = (V, E) be a 3-regular graph. Then L(G) is 3-vertex-connected and redundantly rigid in \mathbb{R}^2 if and only if G is 3-edge-connected.

Proof: First suppose that G - F has two connected components D_1, D_2 for some $F \subseteq E$ with $|F| \leq 2$. Since G is 3-regular, there must be an edge in D_i for i = 1, 2. This implies that the vertex set in L(G) corresponding to F is a separating vertex set in L(G). Thus L(G) is not 3-vertex-connected. This proves the 'only if' direction.

To see the 'if' part, suppose that G is 3-edge-connected. This implies that L(G) is 3-vertex-connected, since each separating vertex set in L(G) gives rise to a separating edge set of G of the same size.

Next we show that L(G) is redundantly rigid. We need the following claim.

Claim 3.3. Let H be a graph with minimum degree at least two and suppose that H can be made 3-edge-connected by adding at most one edge. Then L(H) is rigid.

Proof: By Theorem 2.2 it suffices to show that def(H) = 0. Consider a partition $\mathcal{P} = \{X_1, X_2, ..., X_t\}$ of V(H) with $t \ge 2$. Since H can be made 3-edge-connected by adding at most one edge, all but at most two members X_i of \mathcal{P} satisfy $e_H(X_i, V(H) - X_i) \ge 3$, and all members satisfy $e_H(X_i, V(H) - X_i) \ge 2$. Hence

$$2e_H(\mathcal{P}) \ge 3t - 2 > 3(|\mathcal{P}| - 1).$$

Thus def(H) = 0.

Now consider and edge $p = v_e v_f$ of L(G). This edge corresponds to a pair of edges e = xy, f = xz in G with a common end-vertex. Since G is 3-edge-connected, we can apply Claim 3.3 to H = G - e to deduce that L(H) is rigid.

It is easy to check that L(G) - p can be obtained from L(H) by adding a new vertex and connecting it to three distinct vertices of L(H). This operation is known to preserve rigidity (in fact, connecting the new vertex to two vertices of L(H) would already preserve rigidity, see e.g. [10, Lemma 2.1.3]). Thus L(G) - p is rigid. This proves that L(G) is redundantly rigid, as required.

By Theorems 3.1 and 3.2 we obtain:

Corollary 3.4. A two-dimensional combinatorial zeolite is globally rigid if and only if its underlying graph is 3-edge-connected.

4 Concluding remarks

The charaterization of global rigidity provided by Corollary 3.4 has algorithmic implications, too. Given a 3-regular graph G on n vertices, the best known running time bound for testing whether L(G) satisfies both conditions of Theorem 3.1 is $O(n^2)$. However, testing whether G is 3-edge-connected can be done in linear time. Since Gis 3-regular, this gives rise to an improved O(n) time bound for testing global rigidity of two-dimensional combinatorial zeolites.

The characterization of rigid (or globally rigid) graphs in \mathbb{R}^d , for $d \geq 3$, is not known. Even the special case of three-dimensional combinatorial zeolites appears to be difficult. Nevertheless, one might conjecture that for all positive integers da d-dimensional combinatorial zeolite is globally rigid if and only if its underlying (d+1)-regular graph is (d+1)-edge-connected (or possibly (d+1)-vertex-connected). This natural extension of Corollary 3.4, which is correct for $d \leq 2$, fails in \mathbb{R}^3 : a counterexample, due to Bill Jackson [4], is shown in Figure 2.



Figure 2: A 4-vertex-connected 4-regular graph G for which L(G) is not rigid (and hence not globally rigid) in \mathbb{R}^3 . The line graph of G behaves like a body-and-hinge framework whose underlying graph is a cycle of length 8, and hence it is easily shown to be flexible. (Thus a cycle of length 7 would also be a counterexample.)

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