Rigidity of Molecular Frameworks

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Abstract

A d-dimensional framework (G, p) is a graph G = (V, E) together with a map $p: V \to \mathbb{R}^d$. The framework is generic if the co-ordinates of all the points $p(v), v \in V$, are algebraically independent over \mathbb{Q} . Let (G, p) and (G, q) be frameworks. Then:

- (G, p) and (G, q) are equivalent if |p(u) p(v)| = |q(u) q(v)| for all $uv \in E$.
- (G, p) and (G, q) are congruent if |p(u) p(v)| = |q(u) q(v)| for all $u, v \in V$.
- (G, p) is *rigid* if there exists an $\epsilon > 0$ such that every framework (G, q) which is equivalent to (G, p) and satisfies $|p(v) q(v)| < \epsilon$ for all $v \in V$, is congruent to (G, p). (This is equivalent to saying that there is no 'continuous deformation' of (G, p) which preserves the lengths of all its edges.)

It is known that the rigidity of a generic framework (G, p) depends only on the graph G and not the particular map p. Hence we say a graph G is rigid in \mathbb{R}^d if some, or equivalently all, generic frameworks (G, p)are rigid. The problem of characterizing which graphs are rigid in \mathbb{R}^d has been solved when d = 1, 2 but it is a difficult open problem for $d \geq 3$. There is some evidence, however, that the problem may become tractable for squares of graphs in \mathbb{R}^3 . Indeed, Tay and Whiteley have conjectured a combinatorial characterisation for when such graphs are rigid. Their conjecture is known as the 'Molecular Conjecture' since molecules can be modelled as squares of graphs in \mathbb{R}^3 . I will describe the conjecture and give some partial results. This work is joint with Tibor Jordán.