A Decidability Problem on Planar Protien Folding

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Abstract

We look into the decidability of whether a hinged configuration locks.

1 Introduction

We look into the decidability of continuity on planar configuration space using regular, unitary hexagonal polygons. These polygons can also represent unit disk configurations [1]

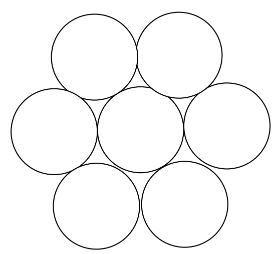

Figure 1: A locked 7 ball configuration

Motivation Protein folding, graphite, crystalline structures in metallurgy.

Outline Section 2 covers the necessary mathematical concepts to understanding the problem. Section 3 explains the problem, Section 4 covers the results and findings about the problem. Section 5, the conclusion, offers final remarks on the problem.

2 Background

Here we review some of the necessary mathematics behind the problem.

2.1 SAT Problems

Problem 2.1 (Satisfiability Problem). Let $\{x_i\}_{i=1}^n$ be boolean variables, and $t_i \in \{x_i\}_{i=1}^n \cup \{\bar{x}_i\}_{i=1}^n$. A *clause* is is said to be a disjuction of distinct terms:

$$t_1 \vee \cdots \vee t_{j_k} = C_k$$

Then the *satisfiability problem* is the decidability of a conjuction of a set of clauses, i.e.:

$$\wedge_{i=1}^{m} C_i$$

[**?**]

2.1.1 3-SAT Problems

A 3-SAT problem is a SAT problem with all clauses having only three boolean variables.

2.2 Linkages

Definition 2.1 (Linkage)**.** A collection of fixed-length 1D segments joined at their endpoints to form a graph.

Definition 2.2 (Graph)**.** An ordered pair $G = (V, E)$ comprising a set V of vertices or nodes together with a set E of edges or lines

Definition 2.3 (Cycle)**.** A closed walk with no repetitions of vertices or edges allowed, other than the repetition of the starting and ending vertex

Definition 2.4 (Configuration)**.** A specification of the location of all the link endpoints, link orientations and joint angles.[2]

2.3 Dissections

Problem 2.2 (Polygonal Dissection). Given two polygons of equal area, P_1 and P_2, partition P_1 into smaller pieces,$\{P_{1,i}\}_{i=1}^{n}$, rearrange the pieces to form P_2. /citefrederickson1997dissections

2.4 Circle Packing

Definition 2.5 (Circle Packing)**.** P of a planar graph G is a set of of circles with disjoint interiors $\{C_v\}_{v \in G}$ such that two circles are tangent if and only if the corresponding vertices form an edge. [**?**]

Theorem 2.1 (Circle Packing Theorem)**.** *For every connected simple planar graph G there is a circle packing in the plane whose intersection graph is (isomorphic to) G. [4]*

2.4.1 Circle Packings and Polygonal Linkages

Given a circle of radius r, we establish the isomorphism to a hexagon by circumscribing the vertices of the regular hexagon.

2.4.2 Hinged Polygons

Hinged polygons have been researched for decades and related to linkage problems [**?**, **?**] Consider the locked configuration of figure 4. We can configure the hexagons to be locked by placing hing points as follows: To prove that it is a locked configuration:

(i)

(ii)

(iii)

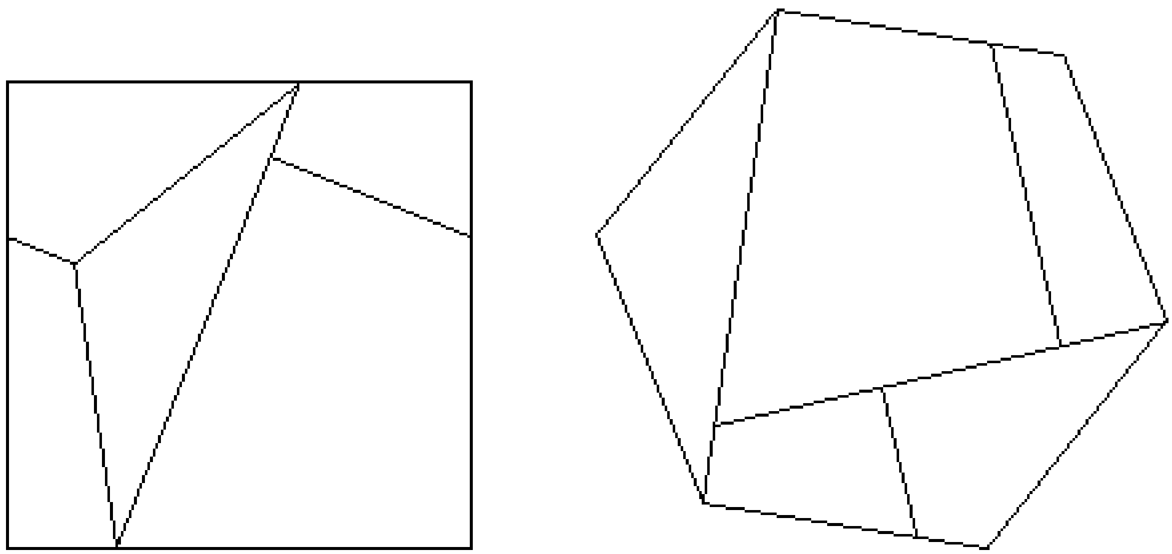

Figure 2: An axample of two polygons of equal area that can be rearranged into the other by the given partition.[**?**]

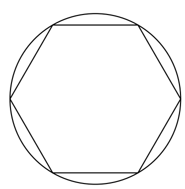

Figure 3: A circumbscribed hexagon

(iv)

(v)

(vi)

(vii)

(viii)

(ix)

(x)

2.4.3 Hinged Hexagons

The Shapes Figure 5 is a locking shape: Figure 5 shall reside in the boundary of a lattice and have a hinge point at one vertex where the locking shape and boundary meet.

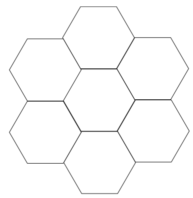

Figure 4: A locked 7 hexagonal configuration. (needs to modify picture by placing red points for hing points.)

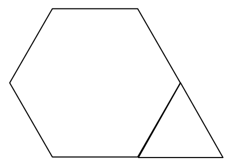

Figure 5: This is the shapte that resides in boundary of the lattice.

Junctions We define junctions to be the point three hexagons meet in a hexagonal lattice, e.g. Figure 7.

Central Scaling

Junctions in Conjunctive Normal Form Explain the configurations we're interested in.

2.4.4 Configurations and Locked Configurations

3 Problem

3.1 Problem Statement

text

3.2 Decidability of Problem

test

3.3 Hexagonal Locked Configuration

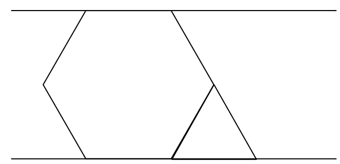

Figure 6: A locking shape in the lattice boundary's channel

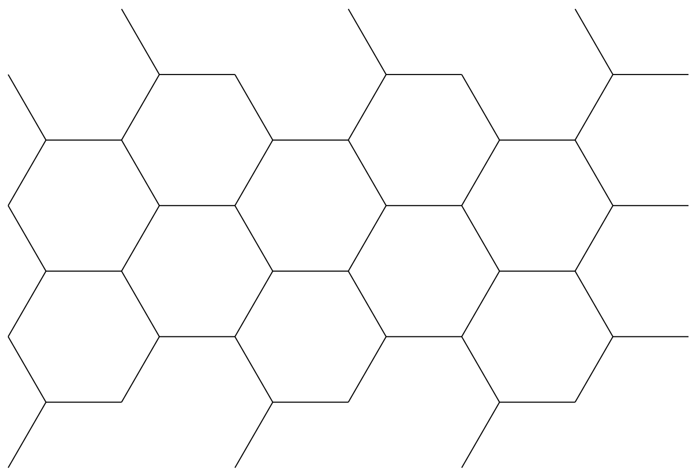

Figure 7: A portion of a hexagonal lattice.

4 Conclusion

We conclude..

References

[1] Heinz Breu and David G. Kirkpatrick. Unit disk graph recognition is np-hard. *Computational Geometry*, 9(12):3 – 24, 1998. Special Issue on Geometric Representations of Graphs.

[2] E.D. Demaine and J. O'Rourke. *Geometric Folding Algorithms: Linkages, Origami, Polyhedra*. Cambridge University Press, 2008.

[3] G.N. Frederickson. *Dissections: Plane and Fancy*. Cambridge University Press, 1997.

[4] K. Stephenson. *Introduction to Circle Packing: The Theory of Discrete Analytic Functions*. Cambridge University Press, 2005.

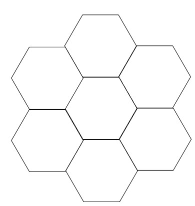

Figure 8: 7 hexagonal configuration