

A Decidability Problem on Planar Protein 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 [3]

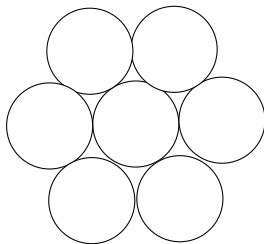


Figure 1: A locked 7 ball configuration

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 said to be a disjunction of distinct terms:

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

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

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

[7]

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.[5]

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 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. [1]

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 .* [8]

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

Definition 2.6 (Polygonal Chain). A polygonal chain $P = (v_0, v_1, \dots, v_{n-1})$ is a sequence of consecutively joined segments (or edges) $e_i = v_i v_{i+1}$ of fixed lengths $l_i = |e_i|$, in a plane. [2]

A chain is said to be closed if $v_{n-1} = v_1$, otherwise it is said to be open. Hinged polygons have been researched for decades and related to linkage problems [2, 4].

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)

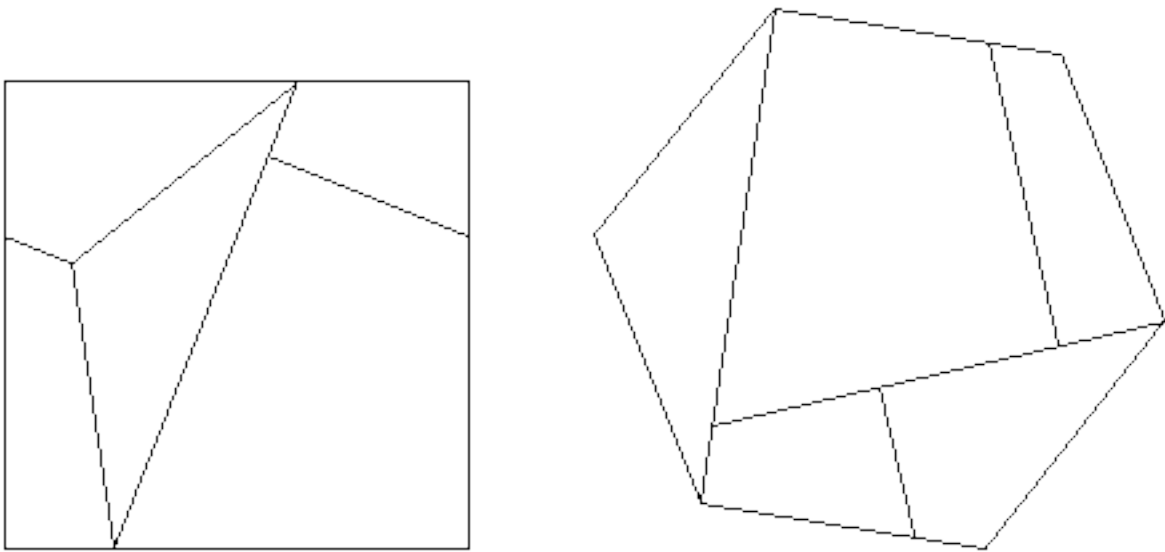


Figure 2: An axample of two polygons of equal area that can be rearranged into the other by the given partition.[6]

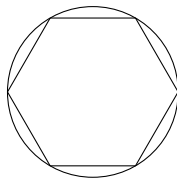


Figure 3: A circumscribed hexagon

- (ii)
- (iii)
- (iv)
- (v)
- (vi)
- (vii)
- (viii)
- (ix)
- (x)

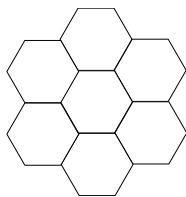


Figure 4: A locked 7 hexagonal configuration. (needs to modify picture by placing red points for hing points.)

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

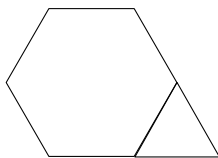


Figure 5: This is the shape that resides in boundary of the lattice.

a hinge point at one vertex where the locking shape and boundary meet.

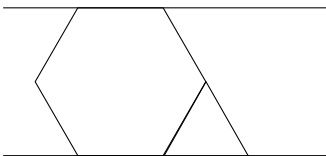


Figure 6: A locking shape in the lattice boundary's channel.

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

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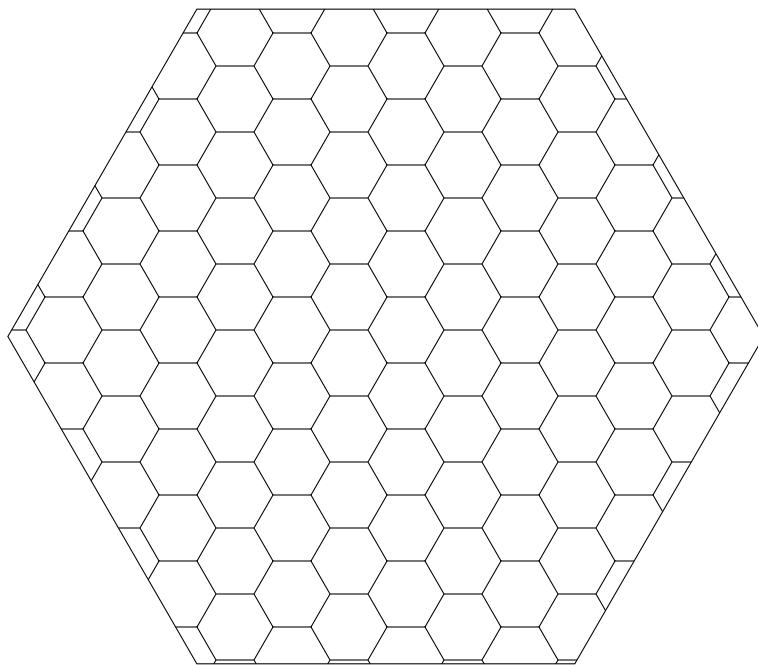


Figure 7: A portion of a hexagonal lattice.

3.2 Decidability of Problem

test

3.3 Hexagonal Locked Configuration

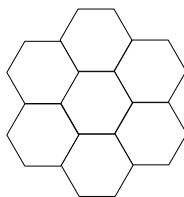


Figure 8: 7 hexagonal configuration

4 Conclusion

We conclude..

References

- [1] Omer Angel, Martin T. Barlow, Ori Gurel-Gurevich, and Asaf Nachmias. Boundaries of planar graphs, via circle packings. November 2013.
- [2] T. Biedl, E. Demaine, M. Demaine, S. Lazard, A. Lubiw, J. O'Rourke, M. Overmars, S. Robbins, I. Streinu, G. Toussaint, and S. Whitesides. Locked and unlocked polygonal chains in 3d, 1999.
- [3] Heinz Breu and David G. Kirkpatrick. Unit disk graph recognition is NP-hard. *Computational Geometry*, 9(1-2):3-24, 1998. Special Issue on Geometric Representations of Graphs.
- [4] J. Canny. *The Complexity of Robot Motion Planning*. ACM doctoral dissertation award. MIT Press, 1988.
- [5] E.D. Demaine and J. O'Rourke. *Geometric Folding Algorithms: Linkages, Origami, Polyhedra*. Cambridge University Press, 2008.
- [6] David Eppstien. The Geometry Junkyard, November 2013.
- [7] S.S. Skiena. *The Algorithm Design Manual*. Springer, 2009.
- [8] K. Stephenson. *Introduction to Circle Packing: The Theory of Discrete Analytic Functions*. Cambridge University Press, 2005.