CALIFORNIA STATE UNIVERSITY, NORTHRIDGE

PROTEIN FOLDING: PLANAR CONFIGURATION SPACES OF DISC ARRANGEMENTS AND HINGED POLYGONS: PROTEIN FOLDING IN FLATLAND

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For the degree of Master of Science in Mathematics

By

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ABSTRACT

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Insert Abstract here

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 [4]

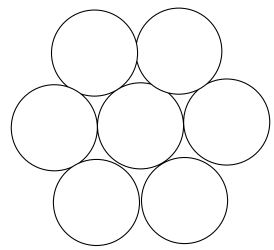

Figure 1: A locked 7 ball configuration

Motivation Protein folding, graphite, crystalline structures in metallurgy; disc packing; hexagonal configurations; Determine whether chemical structures are realizable.

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. The definitions found in this chapter are those found in [9, 11, 8].

2.1 Linkages

Definition 2.1 (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 2.2 (Linkage)**.** A collection of fixed-length 1D segments joined at their endpoints to form a graph.

A linkage can be thought of as a type of path-connected graph, i.e. the segments of a linkage are the edges of a graph, and the endpoints of the segments are the vertices. For this paper, we restrict our self to linkages that are simple planar graphs, i.e. a linkage that:

(i) does not have multiple edges between any pair of vertices,

(ii) does not have edges that cross, or

(iii) have loops (i.e. $(v,v) \in E$).

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.[6]

Definition 2.5 (Configuration Space)**.** The space of all configurations of a linkage.

A configurations space is said to be continuous if for any two configurations, $\mathscr{A}$ and $\mathscr{B}$ of a linkage L, $\mathscr{A}$ can be continuously reconfigured to $\mathscr{B}$ such that, the reconfigurations reside in the configuration domain, L remains rigid throughout reconfiguration (i.e. all links' lengths are preserved), and no violations of linkage intersection conditions.

Definition 2.6 (Pinned Joint)**.** A vertex of a graph (or linkage) that is fixed to a position in a plane.

Definition 2.7 (Free Joint)**.** A vertex of a graph (or linkage) that is not fixed to a position in a plane.

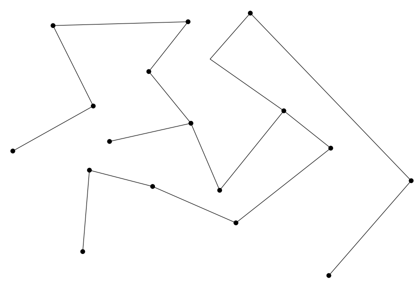

Figure 2: A linkage with joints.

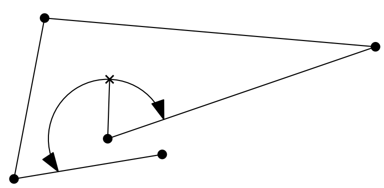

Figure 3: The cross represents a free joint; the pinned joints are denoted as disks. The range of motion shown by the arc describes the continous configuration space of the linkage.

For illustrations in the remainder of this paper, free joints will be represented as crosses and pinned joints will be represented as disks.

2.1.1 Polygonal Linkages

2.2 Circle Packing

Definition 2.8 (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. [2]

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.*

A proof of Theorem 2.1 is found in [11].

2.2.1 Circle Packings and Polygonal Linkages

Given a circle of radius r and its center point, (x, y), we establish the isomorphism to a hexagon by circumscribing the vertices of the regular hexagon.

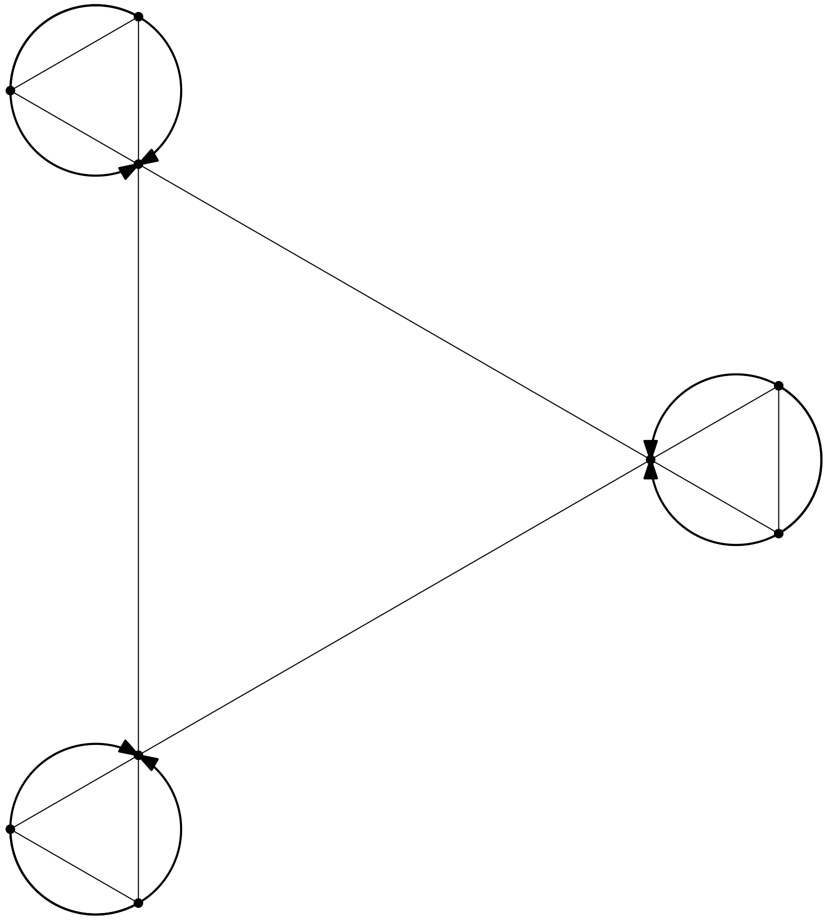

Figure 4: **Not sure how to describe this graph with free joints, pinned joints. Do I need to define another joint(i.e. axis of rotation joint)?**

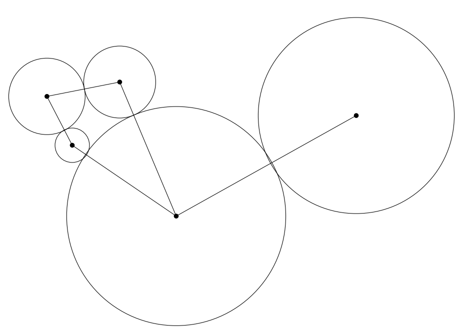

Figure 5: This figure is an example of a circle packing for the given simple planar graph.

2.2.2 Hinged Polygons

Definition 2.9 (Polygonal Chain)**.** A polygonal chain $P = (v_0, v_1, \ldots, v_{n-1})$ 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. [3]

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 [3, 5].

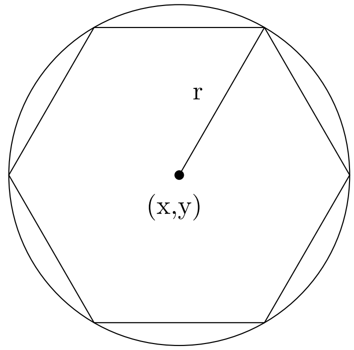

Figure 6: A circumbscribed hexagon

Consider the locked configuration of figure 7. We can configure the hexagons to be locked by placing hinged points as follows:

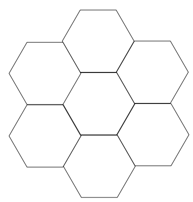

Figure 7: A locked 7 hexagonal configuration. (needs to modify picture by placing red points for hing points.)

2.2.3 Hinged Hexagons

Theorem 2.2. *Any finite collection of polygons of equal area has a common hinged dissection. [1]*

The Shapes Figure 8 is a locking shape: Figure 8 shall reside in the boundary of a lattice and have a hinge

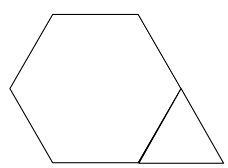

Figure 8: This is the shape that resides in boundary of the lattice.

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

Junctions We define junctions to be the point three hexagons meet in a hexagonal lattice, e.g. Figure 10.

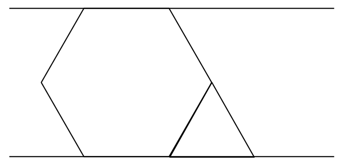

Figure 9: A locking shape in the lattice boundary's channel.

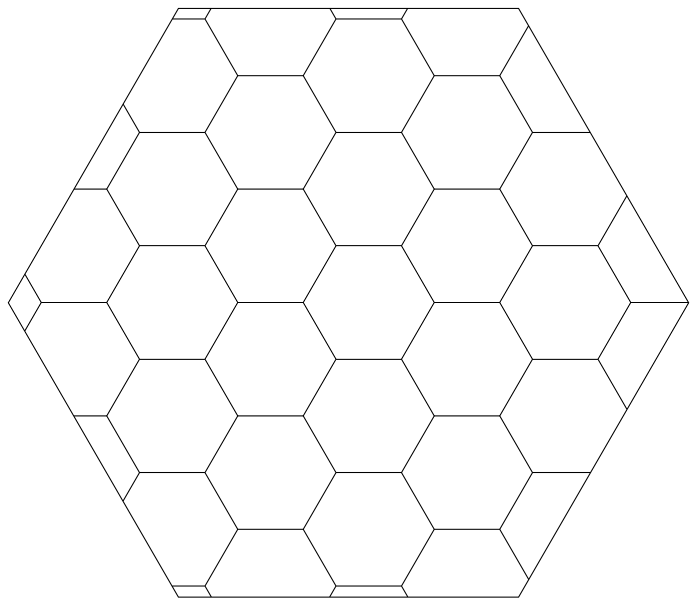

Figure 10: A portion of a hexagonal lattice.

Central Scaling

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

3 Configuration Spaces of Polygonal Chains

3.0.4 Configurations and Locked Configurations

3.1 Dissections

Problem 3.1 (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. [8]

3.2 SAT Problems

Problem 3.2 (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:

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

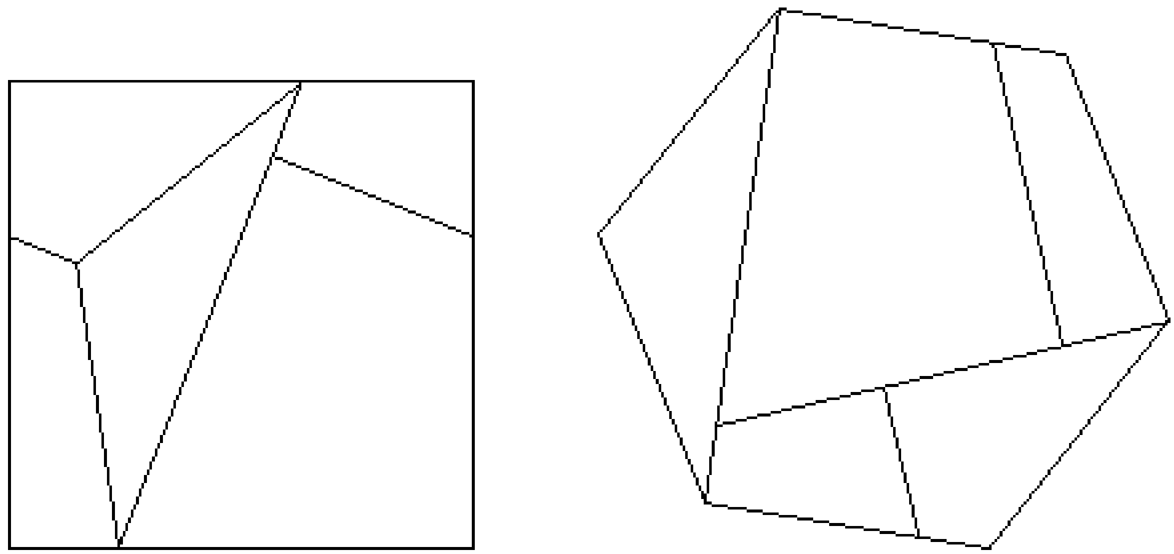

Figure 11: An axample of two polygons of equal area that can be rearranged into the other by the given partition.[7]

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

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

[10]

3.2.1 3-SAT Problems

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

4 Problem

4.1 Problem Statement

text

4.2 Decidability of Problem

test

4.3 Hexagonal Locked Configuration

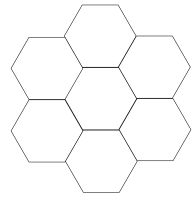

Figure 12: 7 hexagonal configuration

5 Conclusion

We conclude...

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