CALIFORNIA STATE UNIVERSITY, NORTHRIDGE

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

A thesis submitted in partial fulfillment of the requirements for the degree of
Master of Science in Applied Mathematics

by

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August 2014

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Table of Contents

ABSTRACT

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# Chapter 1

# Background

Decidability problems study whether there exists a way to determine whether an element is a member of a set. In this paper we focus on four such decidability problems surrounding graph theory and geometry. The first set of problems involve a special type of graph called a tree and the second set of problems involve something called a polygonal linkage. In each problem, set membership is determined if the tree or polygonal linkage has a particular property when visualized in the plane.

This thesis first presents the preliminary information needed to pose our four problems, then we formally pose each problem and then provide solutions on decidability for each problem.

## 1.1 Graphs

A *graph* is an ordered pair $G = (V,E)$ comprising of a set of vertices $V$ and a multiset of edges $E$. An edge is a 2 element subset of $V$ and denoted as "V choose two", $\binom{V}{2}$. Vertices are said to be *adjacent* if they form an edge in $E$. *Neighbors* of vertex $v$ are the adjecent vertices of $v$. Vertices that are adjacent to themselves are *self-adjacent*, i.e. $u = v$ for $\{u,v\} \in E$. Edges are said to be *incident* if they share a vertex. When an edge is a member of $E$ multiple times, then we say that the graph is a *multigraph*. A *simple graph* has no self-adjacent vertices. If $G' = (V',E')$ such that $V' \subset V$ and $E' \subset E$, then $G'$ is a *subgraph* of $G$. Unless otherwise stated, this thesis will strictly work with simple graphs.

For graph equivalency, we need to define an isomorphism for graphs. Given two graphs $G_1 = (V_1,E_1)$ and $G_2 = (V_2,E_2)$, a *graph isomorphism* a bijective function $f : V_1 \mapsto V_2$ such that for any two vertices $u, v \in V_1$, we have $\{u,v\} \in E_1$, if and only if $(f(u), f(v)) \in E_2$.

| Graph | Vertices | Edges |
|---|---|---|
| $G_1$ | $\{a,b,c,d,e\}$ | $\{(a,b),(b,c),(c,d),(d,e),(e,a)\}$ |
| $G_2$ | $\{1,2,3,4,5\}$ | $\{(1,2),(2,3),(3,4),(4,5),(5,1)\}$ |

Table 1.1: Two graphs that are isomorphic with the alphabetical isomorphism $f(a) = 1$, $f(b) = 2$, $f(c) = 3$, $f(d) = 4$, $f(e) = 5$.

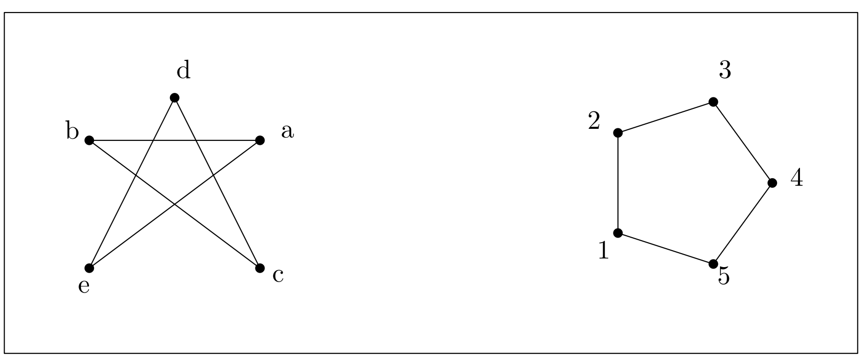


Figure 1.1: This figure depicts the graph isomorphism shown in Table (**??**) between $V_1$ and $V_2$ in the plane.

To visualize a graph, $G$, we create a *drawing* $\Gamma$, of $G$. For a drawing, we use an injective mapping $\Pi : V \mapsto \mathbb{R}^2$ which maps vertices to distinct points in the plane and for each edge $\{u,v\} \in E$, a continuous, injective mapping $c_{u,v} : [0,1] \mapsto \mathbb{R}^2$ such that $c_{u,v}(0) = \Pi(u)$ and $c_{u,v}(1) = \Pi(v)$. The *crossing number* of a graph is the smallest number of edge crossings for a graph, i.e. A drawing is said to be *planar* if no two distinct edges cross [**?**]. For this thesis, we will strictly work with straigt line drawings where all $c_{u,v}$ are straight line segments unless specified otherwise.

A *crossing* is when two edges intersect. Kuratowski's theorem allows one to characterize finite planar graphs, i.e. a finite graph is planar if and only if it does not contain a subgraph that is a subdivision of $K_5$ or $K_{3,3}$ [**?**].

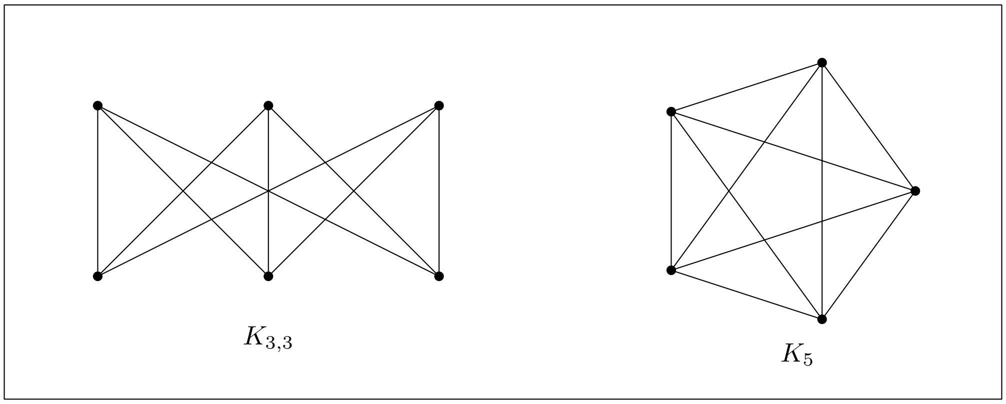


Figure 1.2: The $K_5$ and $K_{3,3}$ drawn in the plane.

A combinatorial *embedding* is a planar drawing with a corresponding circular order of the neighbors of each vertex. Two embeddings of a graph $G$ are equivalent if they determine the same circular orderings of the neighbor sets and the embeddings can be described as a combination of translations and rotations of the other.

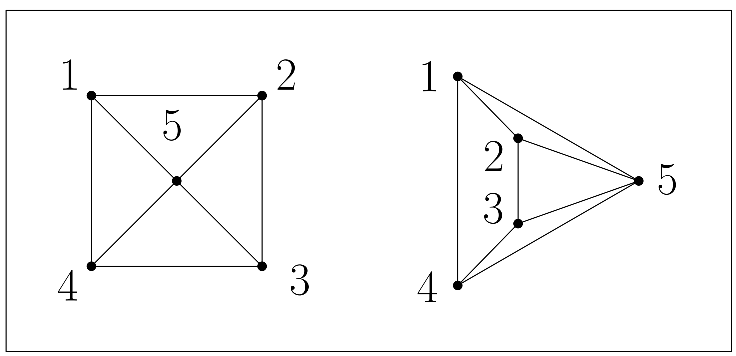


Figure 1.3: Here is a wheel graph, $W_5$, in two separate drawings with the same counterclock

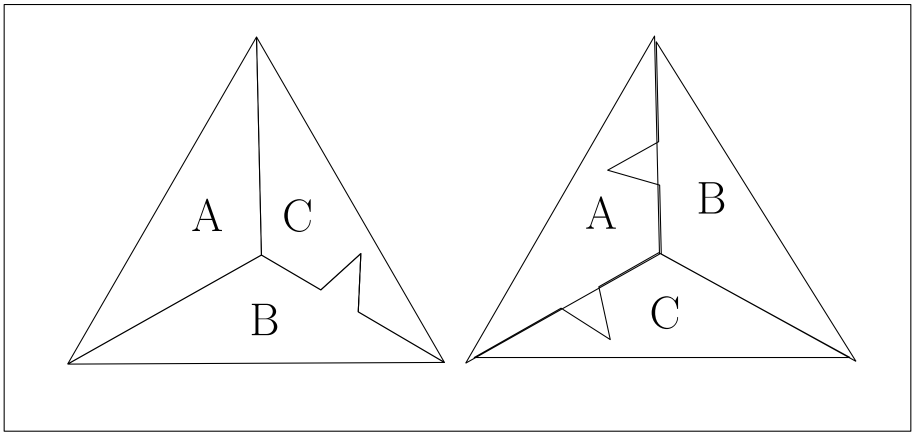


Figure 1.4

### 1.1.1 Trees

Some graphs can be classified by which properties they have. A *path* is a sequence of vertices in which every two consecutive vertices are connected by an edge.

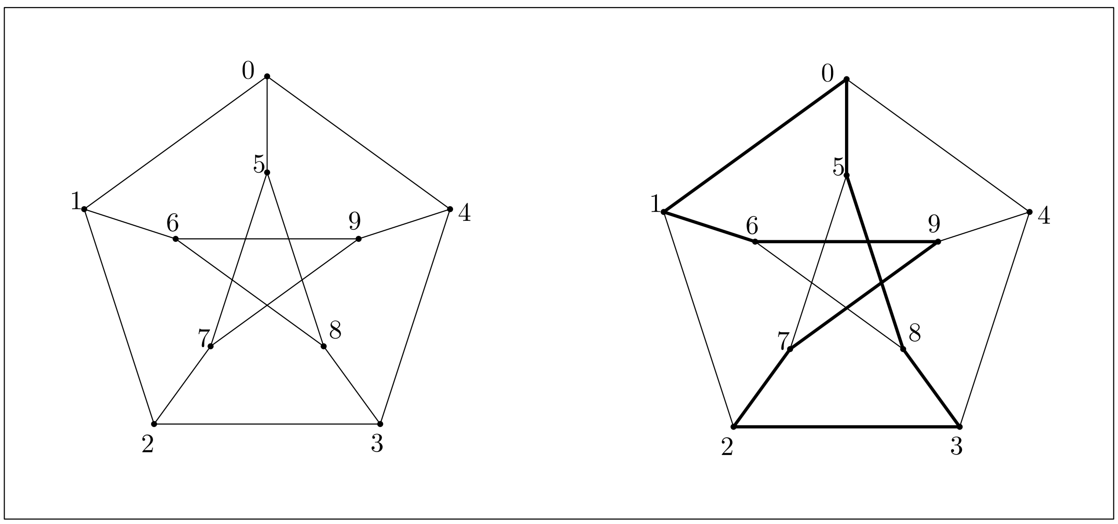


Figure 1.5: An embedding of the Peterson graph with a simple cycle of (2,7,9,6,1,0,5,8,3).

A *simple cycle* of a graph is a sequence, $(v_1, v_2, \ldots, v_{t-1}, v_t)$, of distinct vertices such that every two consecutive vertices are connected by an edge, and the last vertex, $v_t$, connects to $v_1$. A graph is *connected* if for any two vertices, there exists a path between the two points. A *tree* is a graph that has no simple cycles and is connected.

Any two embeddings of trees are equivalent if they can be described as any combination of rotations, translations, and or reflections.

An *ordered tree* is a tree $T$ together with a cyclic order of the neighbors for each vertex, $O$.

Embeddings of ordered trees are equivalent if for each node the counter-clockwise ordering of adjacent nodes are the same and can be described as a combination of translations and rotations of the other. Unlike

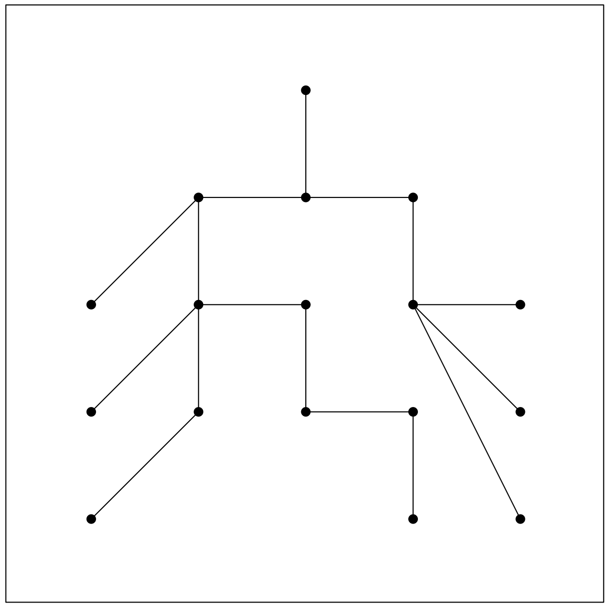

Figure 1.6: An example of a tree.

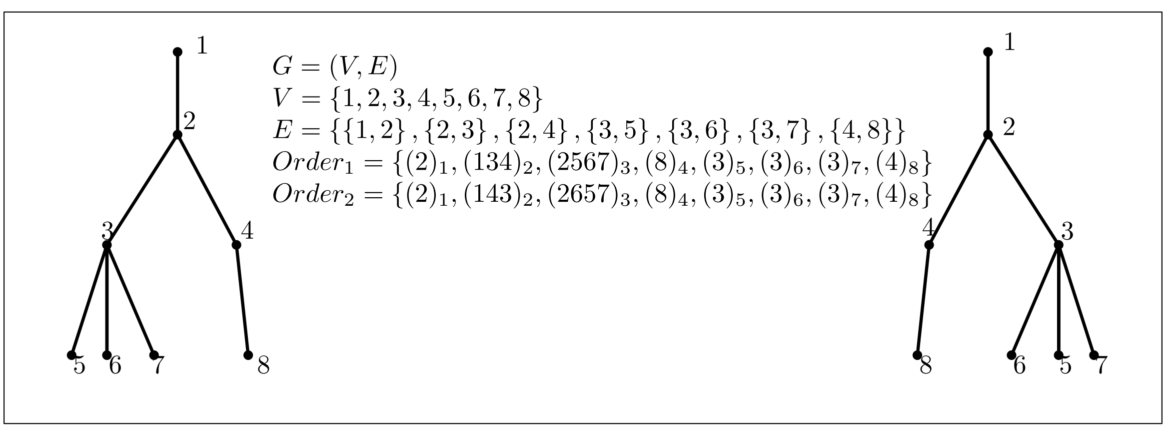


Figure 1.7: A tree with two embeddings with different cyclic orderings around vertices.

embeddings for planar graphs where ordering of adjacent vertices is not a distinguishing condition, we do not consider reflection based transformations for embeddings of ordered trees for equivaliency as that can modify the ordering of adjacent vertices.

### 1.2 Linkages

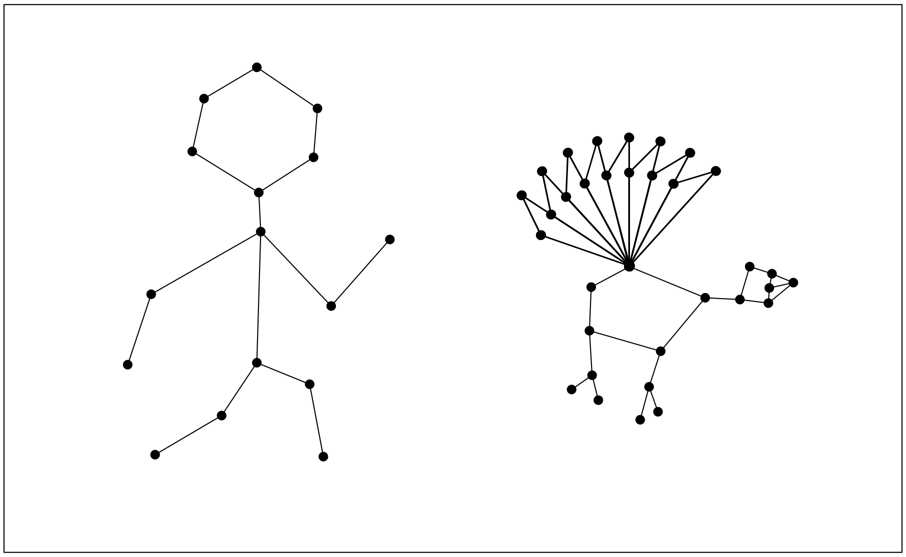

Figure 1.8: Here are skeleton drawings of a human and a turkey. When animating skeletons, one tends to make sure that the lengths of the skeleton segments are kept the same length throught the animation. Otherwise, the animation may depart from what is ideally understood of skeletal motions.

When graph drawings model physical objects, other qualities avout the graph can be contextualized in a geometric sense. Distance, angular relationstips and other geometric qualities of the drawings can be other useful properties of the drawing to perform analysis on. The *length assignment* of a graph $G = (V, E)$ is $\ell : E \mapsto \mathbb{R}^+$. For simple graphs, length assignment must be strictly positive, otherwise it may result in two distinct vertices with the same coordinates. A *linkage* is a graph $G = (V, E)$ with a length assignment $\ell : E \mapsto \mathbb{R}^+$. Length assignments can be thought of as a metric where $\ell(u, v) = \ell(v, u) > 0$.

### 1.3 Polygonal Linkages

Formally, a *polygonal linkage* is an ordered pair $(\mathscr{P}, \mathscr{H})$ where $\mathscr{P}$ is a finite set of polygons and $\mathscr{H}$ is a finite set of hinges; a *hinge* $h \in \mathscr{H}$ corresponds to two points on the boundary of two distinct polygons in $\mathscr{P}$. A *realization of a polygonal linkage* is an interior-disjoint placement of congruent copies of the polygons in $\mathscr{P}$ such that the copies of a hinge are mapped to the same point (e.g., Figure 1.10). A *polygonal linkage realization with fixed orientation* allows for any combination of translations and rotated copies of polygons in $\mathscr{P}$ where every hinge has a cyclic order of of incident polygons. Note that oriented polygonal realizations do not allow for reflection transformations.

These two types of realization types allow one to pose two different types of problems:

*Problem* 1 (Unordered Realizibility Problem for Polygonal Linkages). The realizability problem for a polygonal linkage asks whether a given polygonal linkage has a realization.

Figure 1.9 demonstrates that not all polygonal linkages have a planar realization.

*Problem* 2 (Ordered Realizibility Problem for Polygonal Linkages). The *realizability* problem for a ordered polygonal linkage asks whether a given polygonal linkage has a realization with respect to order.

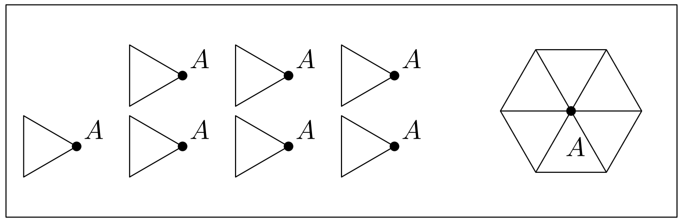


Figure 1.9: Here we have 7 congruent copies of an equilateral triangle with a hinge point of $A$. The polygonal linkage is not realizable. The best we can realize is at most 6 congruent copies of an equilateral triangle with the hinge point of $A$ in the plane.

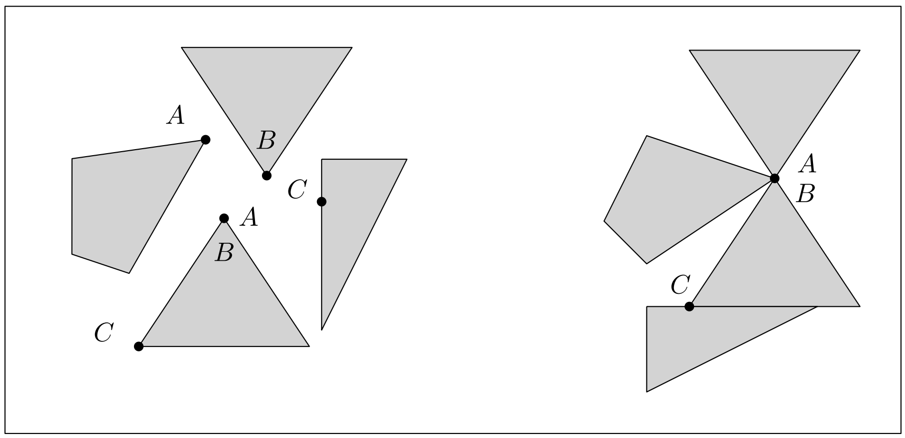


Figure 1.10: (a) A polygonal linkage with a non-convex polygon and two hinge points corresponding to three polygons. Note that hinge points correspond to two distinct polygons.(b) Illustrating that two hinge points can correspond to the same boundary point of a polygon.

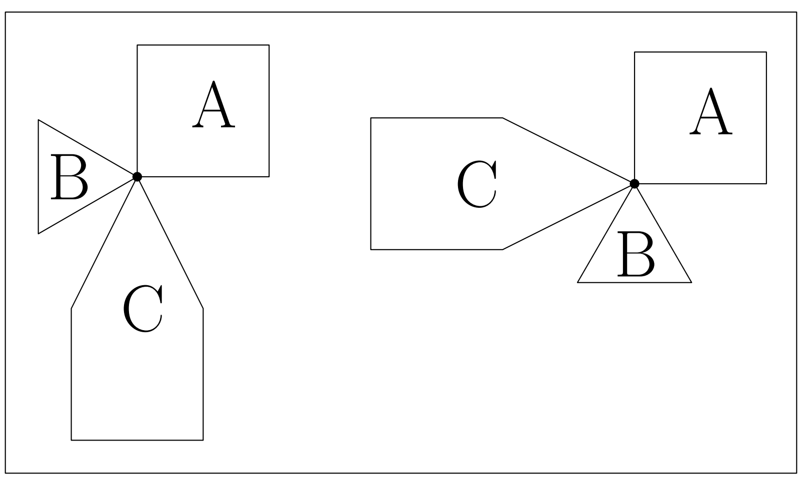


Figure 1.11: The ordering of the polygonal linkages (A,B,C) differs (A,C,B)

**Theorem 1.** *It is strongly NP-hard to decide whether a polygonal linkage whose hinge graph is a **tree** can be realized with fixed orientation.*

Our proof for Theorem 1 is a reduction from PLANAR-3-SAT (P3SAT): decide whether a given Boolean formula in 3-CNF with a planar associated graph is satisfiable. The *graph associated* to a Boolean formula in 3-CNF is a bipartite graph where the two vertex classes correspond to the variables and to the clauses, respectively; there is an edge between a variable $x$ and a clause $C$ iff $x$ or $\neg x$ appears in $C$. See Fig. 1.13(left).

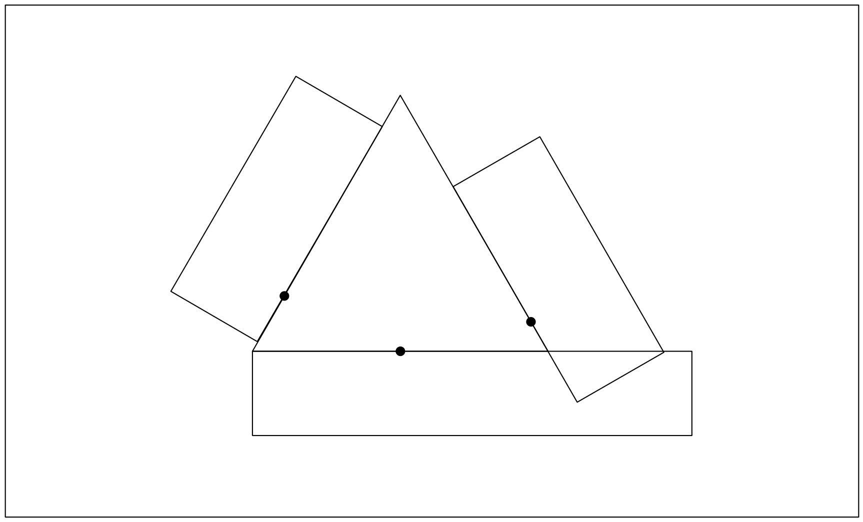

Figure 1.12: This example shows a polygonal linkage with a realization where two polygons intersect another.

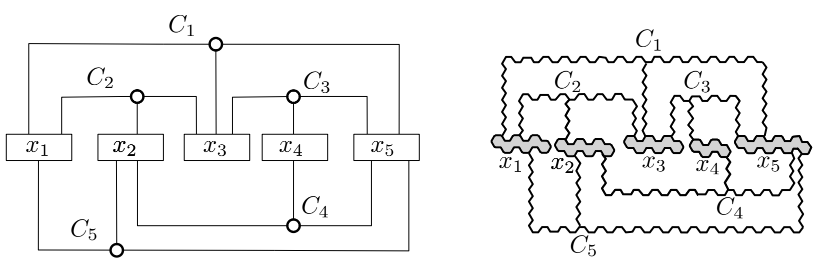


Figure 1.13: Left: the associated graph $A(\Phi)$ for a Boolean formula $\Phi$. Right: the schematic layout of the variable, clause, and transmitter gadgets in our construction.

### 1.3.1 Geometric Dissections

The Wallace-Bolyai-Gerwien Theorem simply states that two polygons are congruent by dissection iff they have the same area. A *dissection* being a collection of smaller polygons that when hinged together form a polygon. Here dissections don't have to be hinged. Hinged dissections preserve adjacent polygon relationships and their points of connection. The question of whether two polygons of equal area have a hinged dissection was an outstanding problem until 2007 [**?**].

The Haberdasher problem was proposed in 1902 by Henry Dudeney which dissects an equilateral triangle into a square.

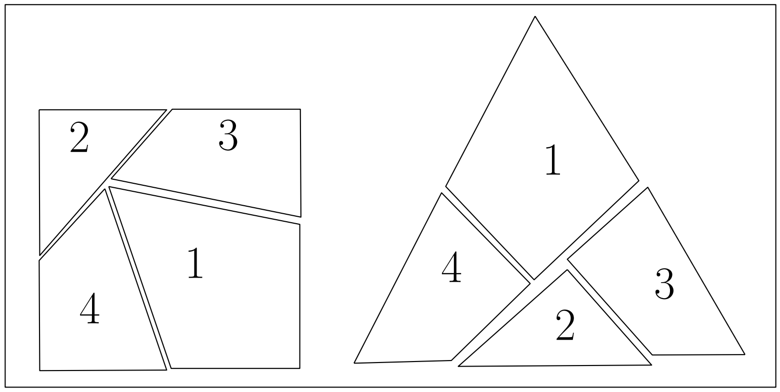


Figure 1.14: The Haberdasher problem was proposed in 1902 and solved in 1903 by Henry Dudeny. The dissection is for polygons that forms a square and equilateral traingle

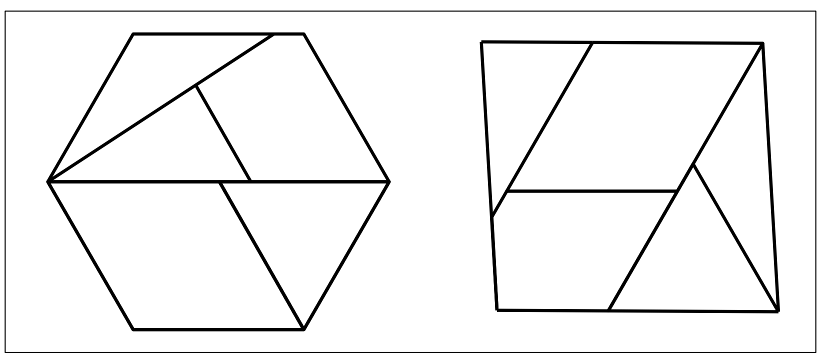

Figure 1.15: Two configurations of polygonal linkage where the polygons touch on boundary segments instead of hinges. These two realizations of the polygonal linkage are invalid to our definitions.